Supporting Information for:

A New Family of High T_c Molecule-based Magnetic Networks:

$V[x\text{-}Cl_nPTCE]_2 \cdot yCH_2Cl_2$

(PTCE = phenyltricyanoethylene)

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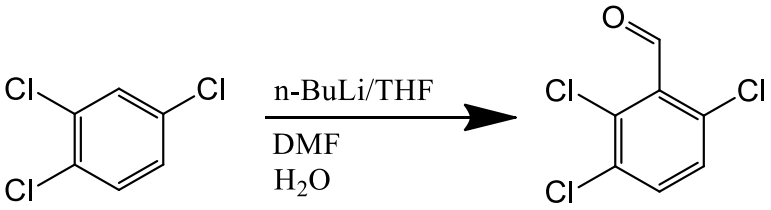
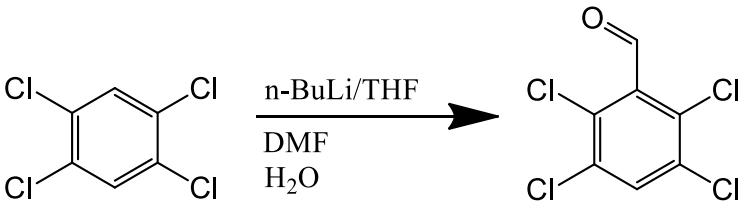
Experimental details.

Synthesis of precursor benzaldehydes from substituted benzenes

The procedure for **1** and **2** was adapted from the literature, where the authors found that quenching the formylation reaction with water while still cold is important for selective preparation of the 2,3,6-trichlorobenzaldehyde over the 2,3,5-trichlorobenzaldehyde.[1] Cold quenching is similarly important for generating any appreciable amount of **2**.

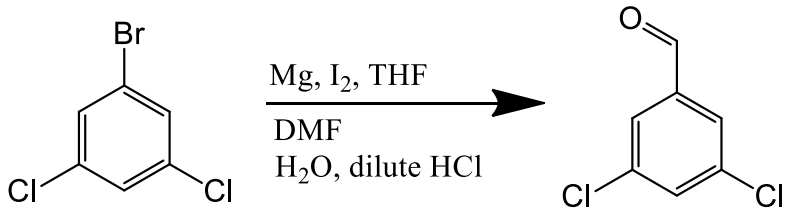


2,3,6-Trichlorobenzaldehyde (1). In a 250 mL Schlenk flask equipped with a stir bar, 1,2,5-trichlorobenzene (3.00 g, 16.5 mmol, 2.06 mL) was dissolved into dry, degassed THF (60 mL) under N_2. The reaction flask was cooled to -78 ºC in a dry ice/acetone cooling bath. Using a disposable syringe, a 2.5 M solution of n-butyllithium in ether (6.6 mL, 26.5 mmol) was added dropwise to the reaction over a period of 20 minutes, and a color change from colorless to yellow was observed. The reaction was stirred for an additional hour at -78 ºC, once all n-BuLi had been added. Next, a 5-fold molar excess of anhydrous/degassed DMF (6.02 g, 82.5 mmol, 6.36 mL) was added to the reaction dropwise over the course of 15 minutes. After all DMF had been added, the reaction was allowed to stir for an additional 30 minutes at -78 ºC. The septum cap was then removed from the reaction flask, and distilled water (20 mL) was rapidly poured into the flask (still at -78 ºC). An immediate precipitate of lithium salts and crystallization of the water was observed. The flask was then removed from the nitrogen line and warmed rapidly to room temperature via water flow along the outside of the flask. During warming, the solution turned dark orange/red. The product was extracted with ether (150 mL), washed with water (3 x 200 mL), and dried over anhydrous sodium sulfate. Evaporation of the solvent yielded light yellow-brown crystals, which were recrystallized from hexanes yielding off-white crystals **1** (2.23 g, 65 %) ^{1}H NMR (400 MHz, $CDCl_3$, vs. TMS): δ 10.41 (s, 1H), 7.55 (d, 1H), 7.34 (d, 1H). *lit. reported (SDBS)* ^{1}H NMR δ 10.426 (s, 1H), 7.564 (d, 1H), 7.353 (d, 1H).



2,3,5,6-Tetrachlorobenzaldehyde (2). The desired product was prepared via similar methods as the synthesis of 2,3,6-trichlorobenzaldehyde (**1**) using 1,2,4,5-tetrachlorobenzene (2.00 g, 9.26 mmol), 2.5 M n-BuLi (3.70 mL, 9.26 mmol), and anhydrous DMF (46.3 mmol, 3.58 mL). Upon removal of the solvent during workup, the crude product crystallized as a light brown solid. ^{1}HNMR analysis revealed ~38 % conversion of the starting material to the desired benzaldehyde

product. The two compounds were separated by dissolving the bulk in hexanes (100 mL) using heat and running a 4-inch silica gel column with hexanes as the mobile phase. 1,2,4,5-tetrachchlorobenzene eluted quickly, and a 1:1 mixture of hexanes:chloroform was used to elute the pure benzaldehyde product. The solvent was removed *in vacuo* to yield pale yellow crystals of **2** (792 mg, 35 %) ^{1}H NMR (400 MHz, $CDCl_3$, vs. TMS): δ 10.36 (s, 1H), 7.77 (s, 1H).



3,5-Dichlorobenzaldehyde (3). In a 250 mL Schlenk flask equipped with a stirbar, 1-bromo-3,5-dichlorobenzene (5.00 g, 22.1 mmol) was dissolved into anhydrous THF (70 mL) under N_2. Magnesium turnings (600 mg, 24.7 mmol) and one crystal of iodine were added and the reaction was heated to reflux under N_2 for 1.5 hours. Upon cooling, the solution was decanted *via* cannula into a dry receiving flask under N_2. Anhydrous DMF (1.75 mL, 22.6 mmol) was added to the reaction via syringe, causing the reaction flask to warm considerably. The solution was stirred for 15 minutes under N_2 at room temperature before quenching with dilute hydrochloric acid (2 mL). The crude product was extracted with dichloromethane (100 mL), washed with water (2 x 200 mL), dried and concentrated to yield a crystalline crude product. Silica gel column chromatography using hexanes:chloroform yielded colorless crystals of **4**. Yield: 2.91 g, (75%). Mp: 63.3-63.7 ºC. IR (KBr): $\nu_{C=O}$ 1693 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$, vs. TMS): δ 9.93 (s, 1H), 7.75 (d, 2H), 7.61 (t, 1H). *lit. reported (SDBS)* ^{1}H NMR δ 9.928 (s, 1H), 7.737 (d, 1H), 7.602 (d, 1H).

Representative synthesis of the organic one-electron acceptors

The synthesis of the 2-(2,3,5,6-tetrachlorophenyl)-1,1,2-tricyanoethylene (2,3,5,6-Cl_4PTCE, **6**) is described in detail here as a representative example of the synthesis used to prepare the family of organic one-electron acceptors.

2-(2,3,5,6-Tetrachlorophenyl)-1,1-dicyanoethylene (4). In a 100 mL round bottom flask, 2,3,5,6-tetrachlorobenzaldehyde (**6**, 2.61 g, 10.7 mmol), and malononitrile (718 mg, 10.9 mmol) were suspended in 100% ethanol (55 mL) at room temperature. While stirring, 2 drops of piperidine were added to initiate the reaction, causing all reactants to dissolve within one minute. The reaction was stirred at room temperature for 30 minutes, during which a white precipitate began to form. The stirbar was then removed and distilled water (5 mL) was added to induce further precipitation of the product. The flask was sealed with a rubber septum and transferred to a freezer overnight. The precipitated off-white crystals were collected by filtration (using a Büchner funnel), rinsed thoroughly with ice-cold 95% ethanol, and dried by suction. The crystals were then dried in open air for several days to yield an off-white, crystalline solid of **7** (2.58 g, 83 %); ^{1}H NMR (400 MHz, $CDCl_3$, vs. TMS): δ 7.87 (s, 1H), 7.77 (s, 1H).

2-(2,3,5,6-Tetrachlorophenyl)-1,1,2-tricyanoethane (5). In a 250 mL round bottom flask, 2-(2,3,5,6-tetrachlorophenyl)-1,1-dicyanoethylene (**7**, 2.44 g, 8.36 mmol) was suspended in 100% ethanol (100 mL), and the reaction was cooled to 0 ºC in an ice/water cooling bath. In a separate

flask, two equivalents of KCN (1.09 mg, 16.8 mmol) were dissolved into distilled water (50 mL) and the flask was cooled to 0 ºC before quickly adding the solution to the reaction flask. Within the first few minutes of the reaction, all reactants entered solution without a significant color change. The reaction was allowed to stir at 0 ºC for 1 hour. Concentrated HCl was then added dropwise until the bulk solution became acidic (pH = 2-3 as measured with pH paper). The reaction was allowed to stir for an additional 15 minutes at 0 ºC after HCl was added. The stirbar was then removed and ice-cold distilled water (50 mL) was added to induce further precipitation of the product. The flask was sealed with a rubber septum and transferred to a freezer overnight. The resulting off-white crystals were collected by filtration (using a Büchner funnel), rinsed thoroughly with ice-cold 95% ethanol, and dried by suction. The crystals were then dried in open air for two days to yield an off-white, crystalline solid of **8** (2.03 g, 76 %); ^{1}H NMR (400 MHz, $CDCl_3$, vs. TMS): δ 7.84 (s, 1H), 5.62 (d, 1H), 4.92 (d, 1H).

2-(2,3,5,6-Tetrachlorophenyl)-1,1,2-tricyanoethylene (6). To a 500 mL round-bottom flask equipped with a stirbar, 2-(2,3,5,6-tetrachlorophenyl)-1,1,2-tricyanoethane (**8**, 1.51 g, 5.97 mmol), water (200 mL) and diethyl ether (200 mL) were added and the mixture was cooled to 0 ºC in an ice/water cooling bath. Upon cooling, *N*-chlorosuccinimide (950 mg, 7.01 mmol) was added to the solution, and the reaction was stirred vigorously for 3 hours at 0 ºC. After the stirring was turned off and the two solvent layers settled completely, the ether layer was separated and washed with water (3 x 300 mL) to remove residual NCS. The ether fraction was dried over anhydrous sodium sulfate, and evaporated *in vacuo*, leaving a crystalline crude product. The final product was then purified by silica gel column chromatography with a dichloromethane mobile phase to yield light yellow crystals of **9** (1.80 g, 81 %). ^{1}H NMR (400 MHz, $CDCl_3$, vs. TMS): δ 7.88 (s, 1H), HRMS-FAB (*m/z*, [M]) Calcd for $C_{11}HN_3Cl_4$: 314.89246, Found: 314.89288.

^{1}H and ^{13}C NMR Spectra of the Organic One-Electron Acceptors

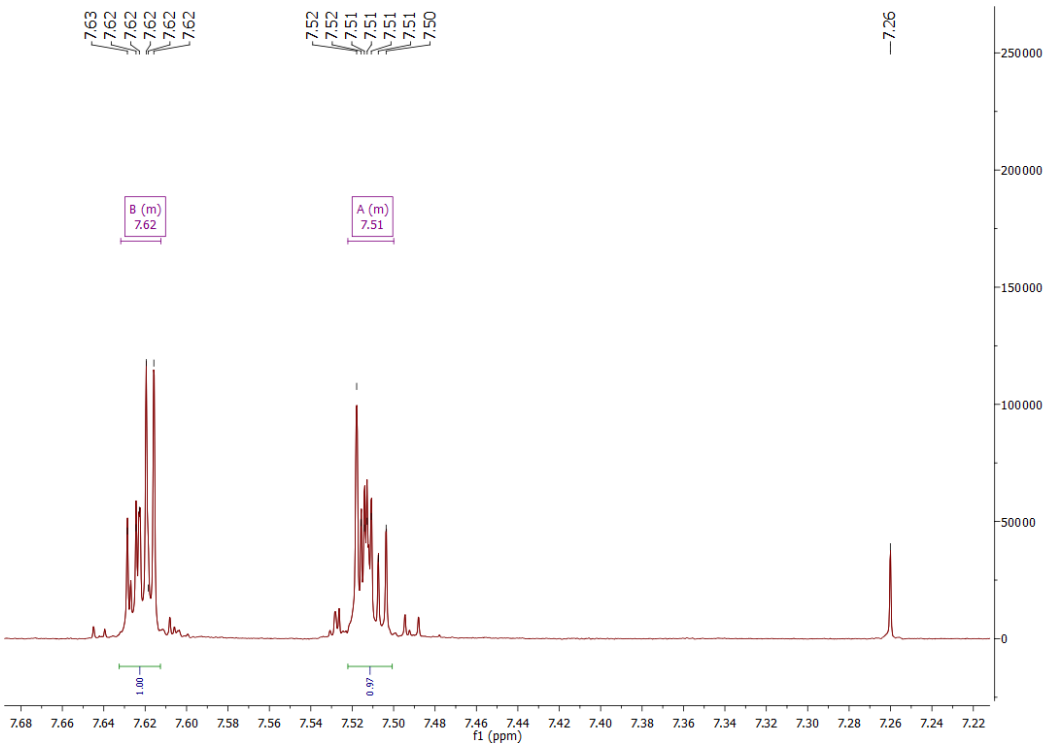


Figure S1. ^{1}H NMR of 2-ClPTCE

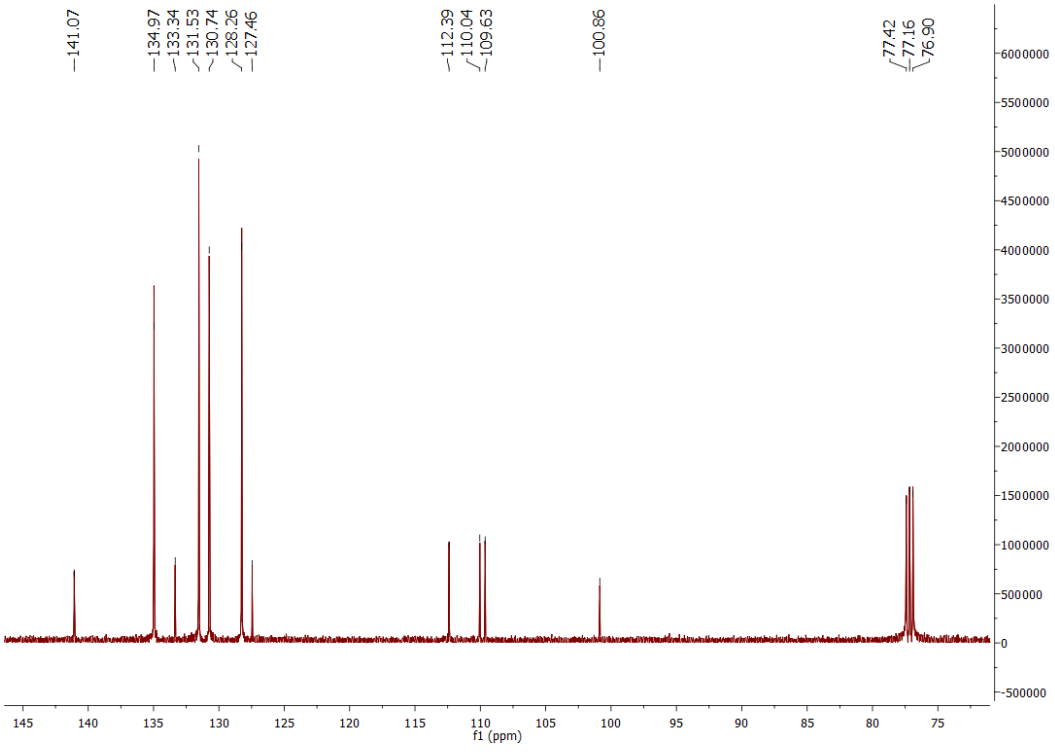


Figure S2. ^{13}C NMR of 2-ClPTCE

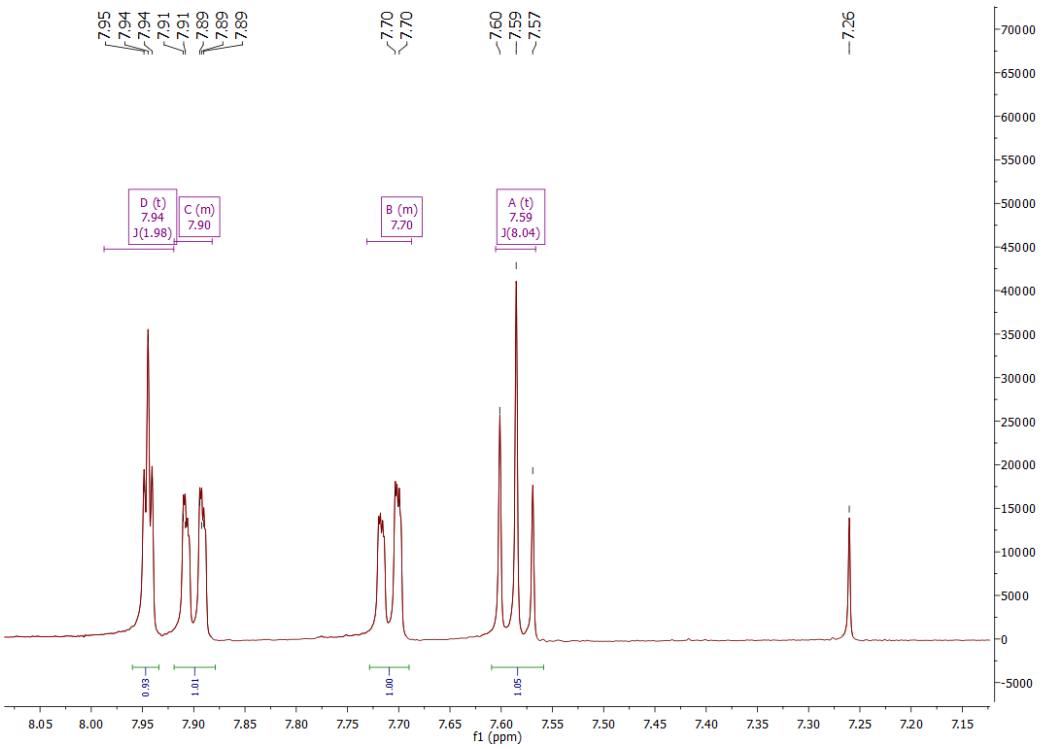


Figure S3. ^{1}H NMR of 3-ClPTCE

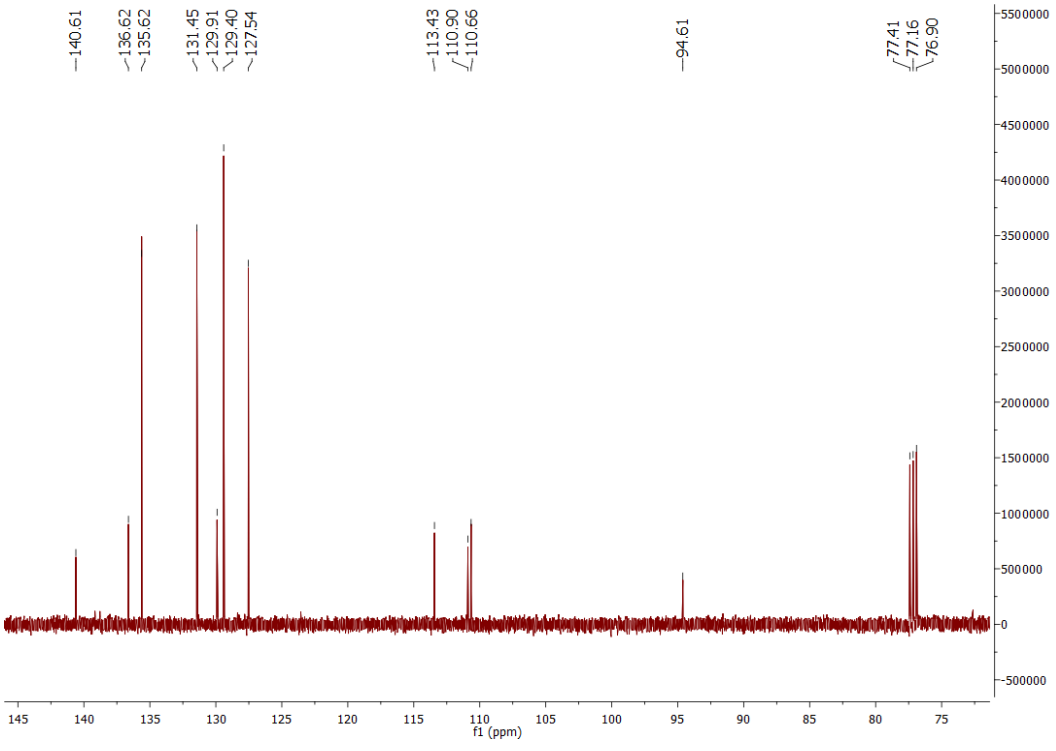
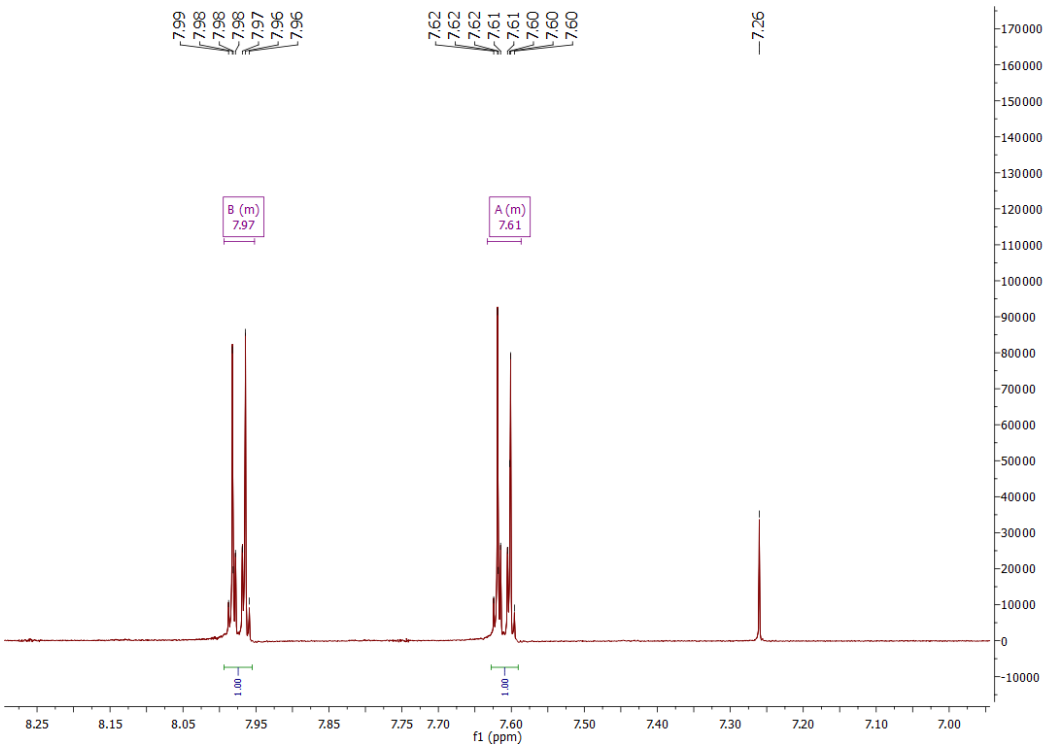


Figure S4. ^{13}C NMR of 3-ClPTCE



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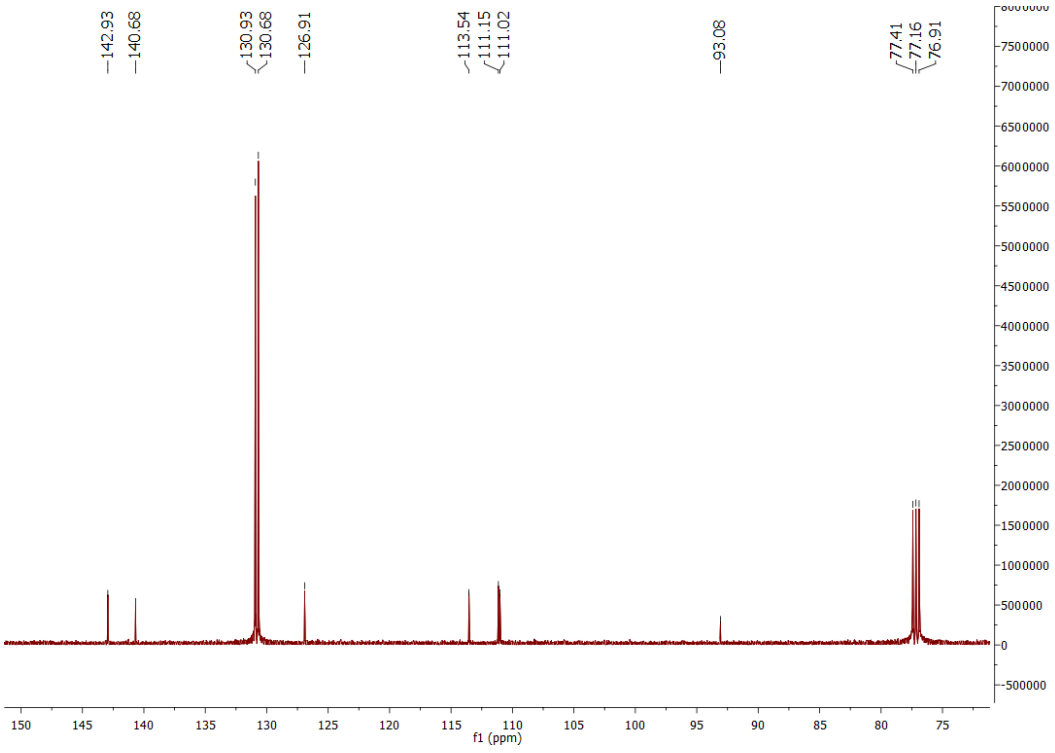

Figure S6. ^{13}C NMR of 4-ClPTCE

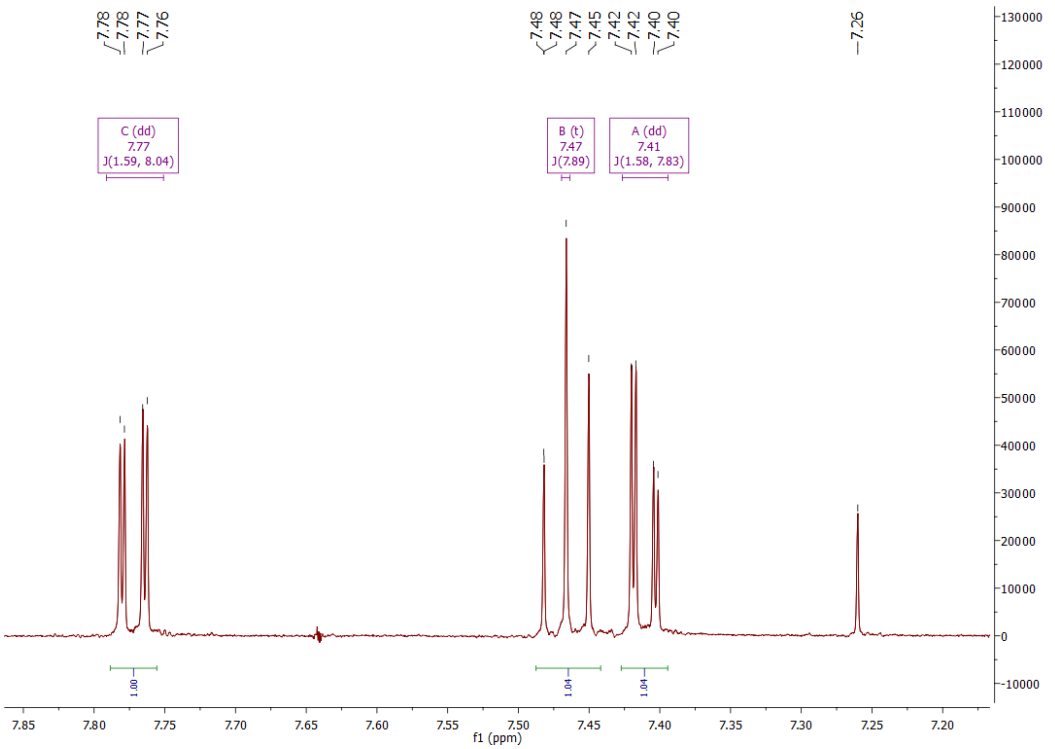

Figure S7. ^{1}H NMR of 2,3-Cl_2PTCE

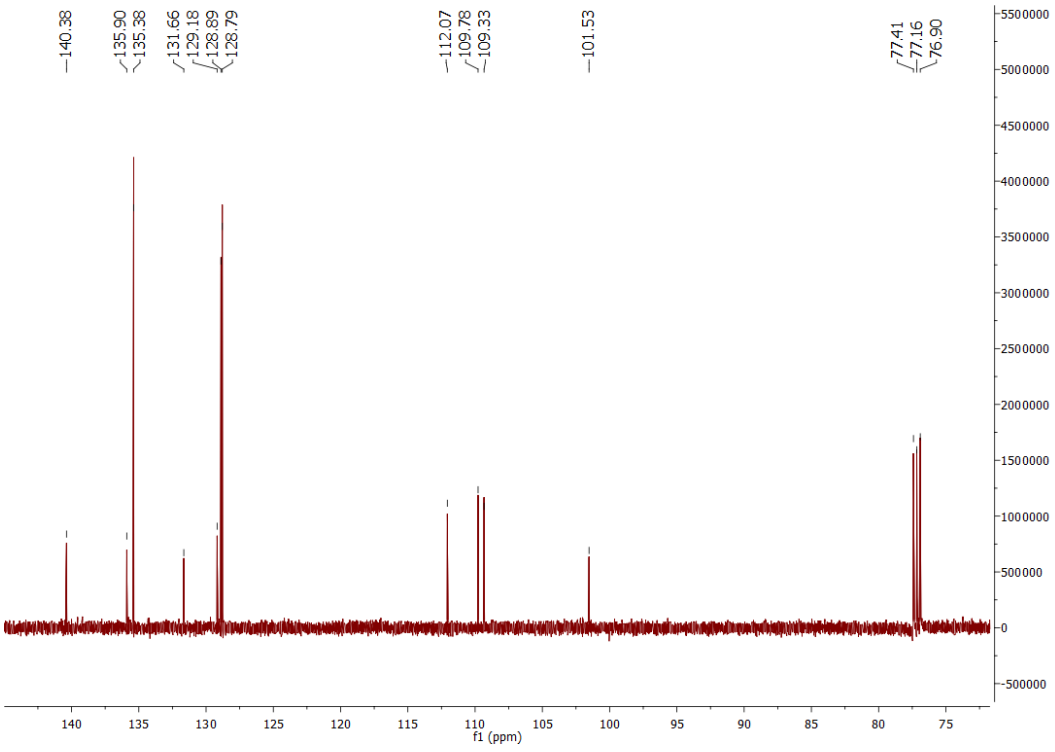

Figure S8. ^{13}C NMR of 2,3-Cl_2PTCE

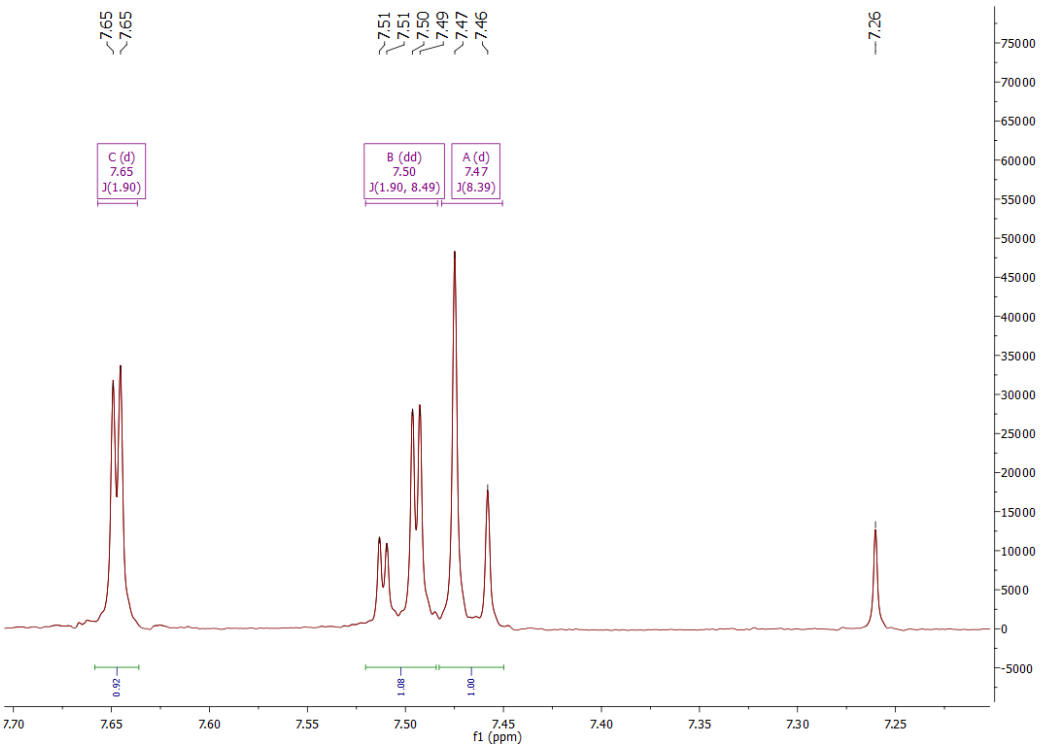

Figure S9. ^{1}H NMR of 2,4-Cl_2PTCE

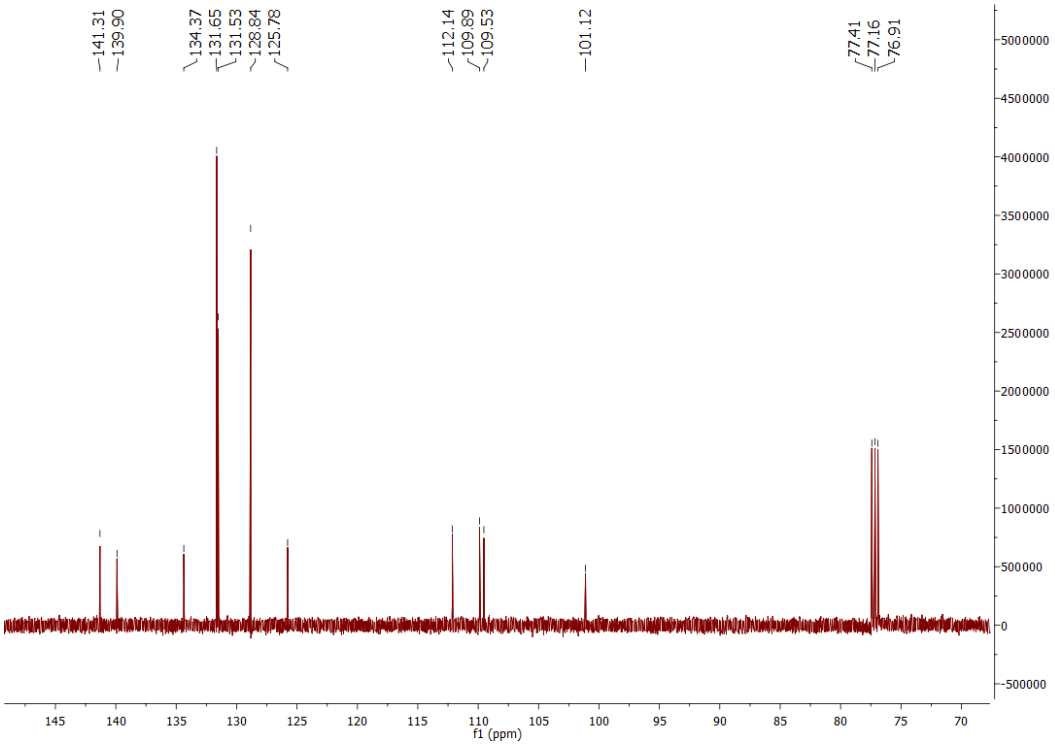

Figure S10. ^{13}C NMR of 2,4-Cl_2PTCE

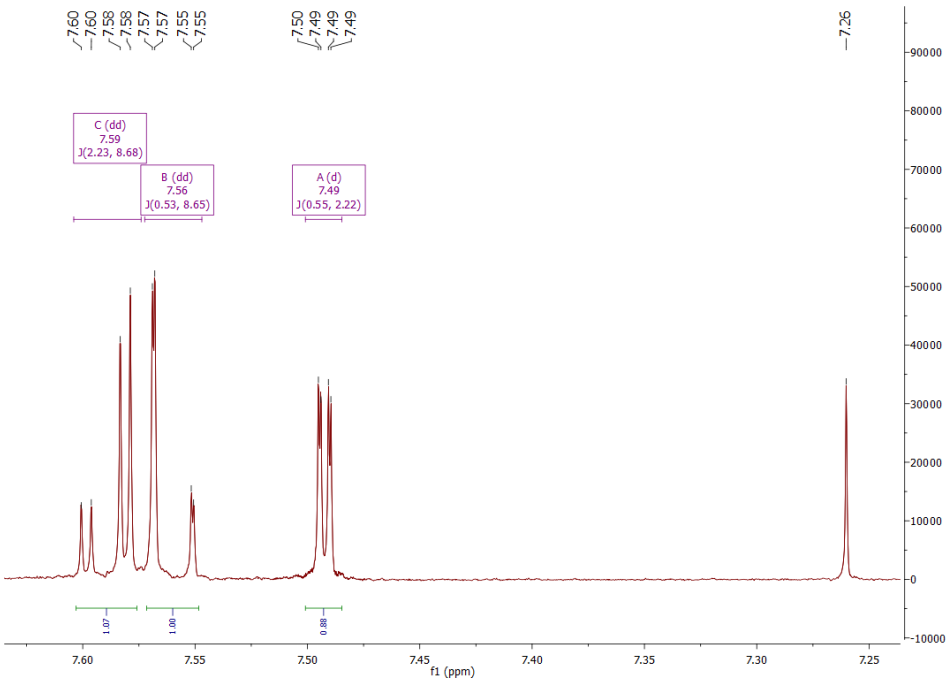

Figure S11. ^{1}H NMR of 2,5-Cl_2PTCE

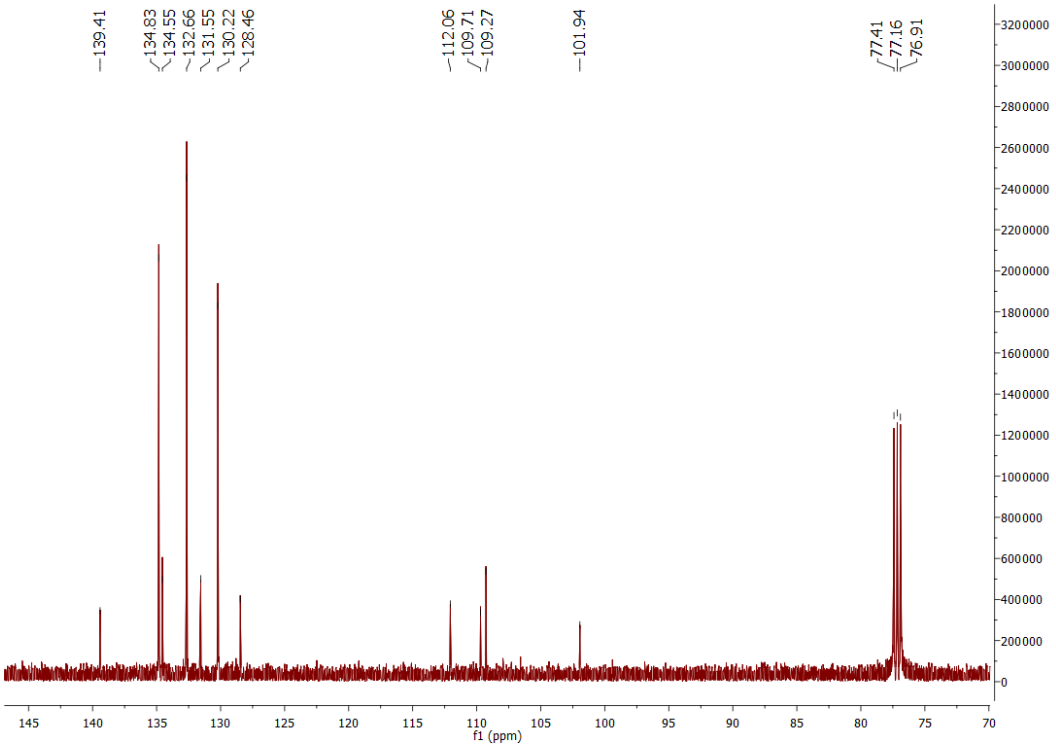

Figure S12. ^{13}C NMR of 2,5-Cl_2PTCE

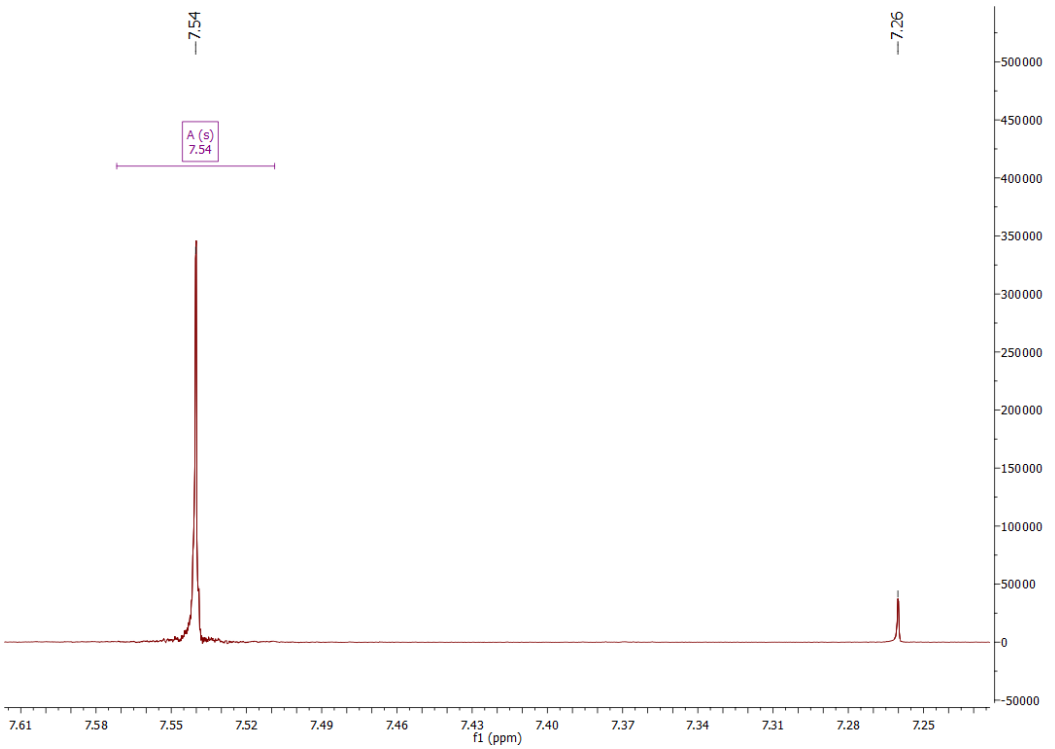

Figure S13. ^{1}H NMR of 2,6-Cl_2PTCE

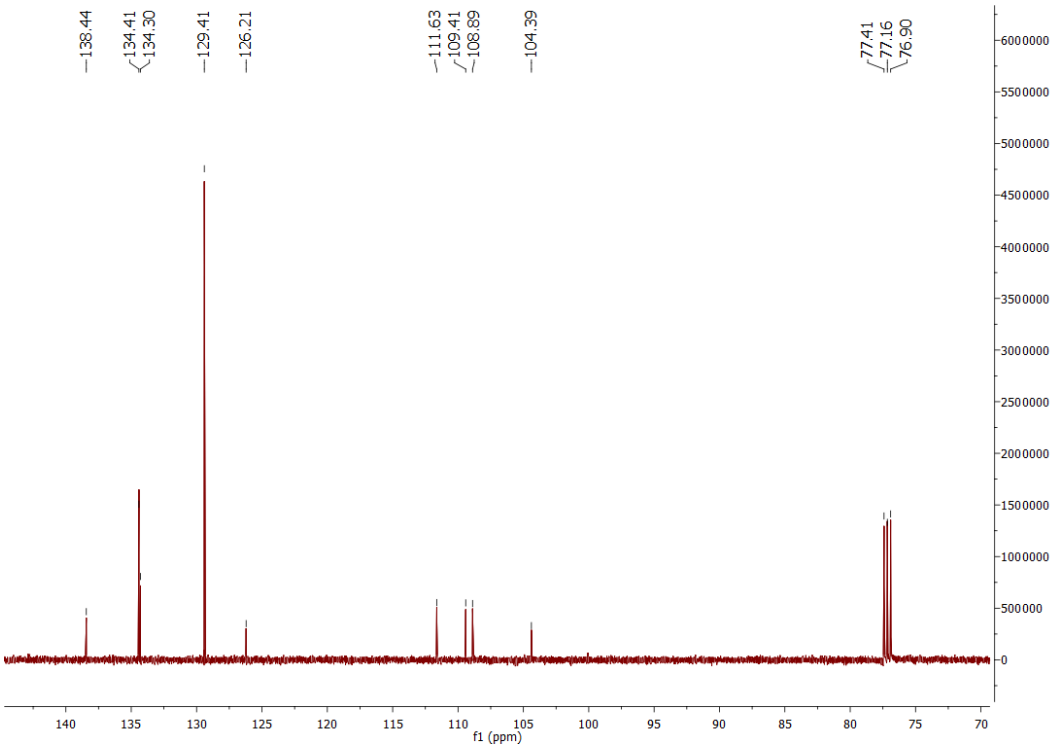

Figure S14. ^{13}C NMR of 2,6-Cl_2PTCE

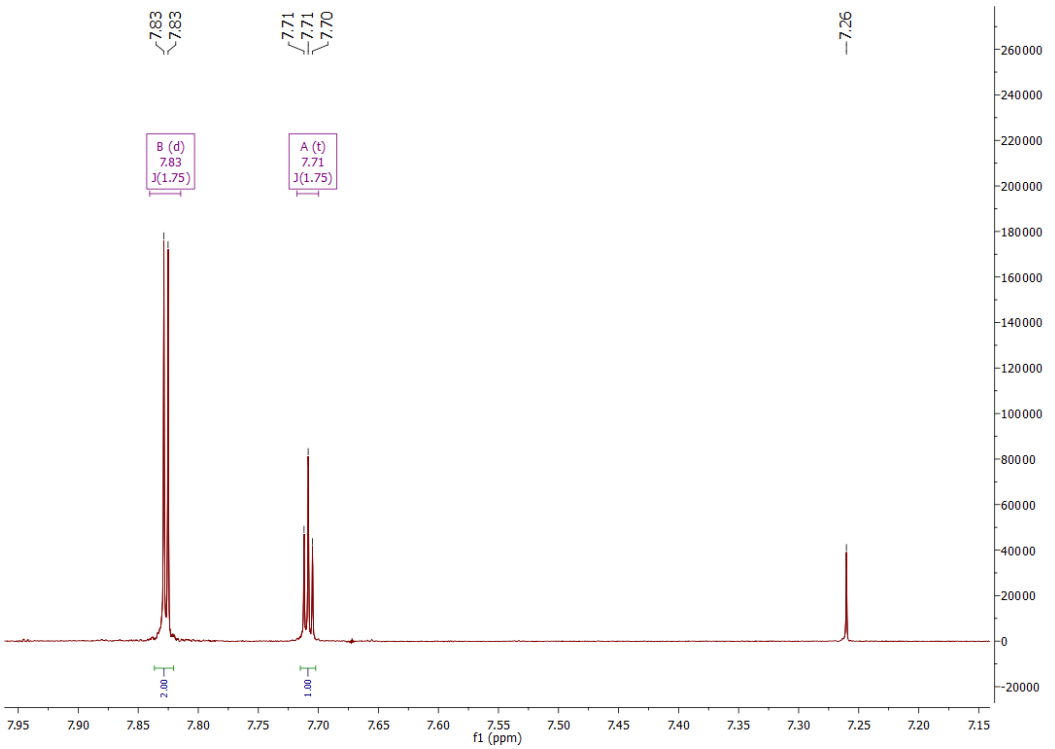

Figure S15. ^{1}H NMR of 3,5-Cl_2PTCE

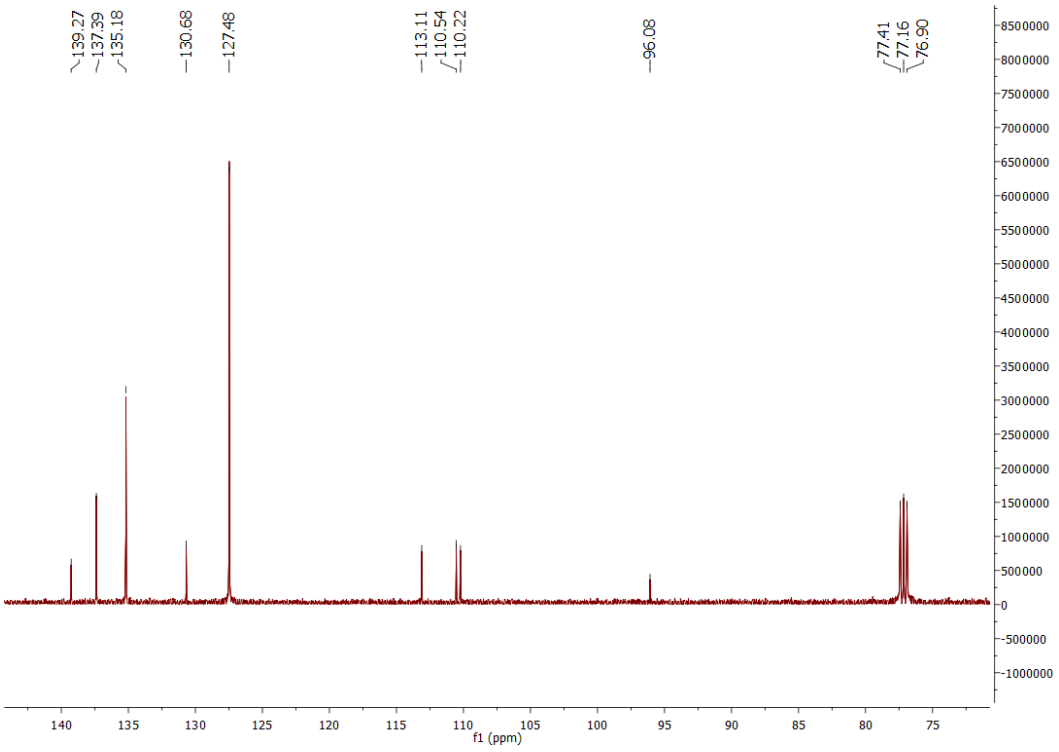

Figure S16. ^{13}C NMR of 3,5-Cl_2PTCE

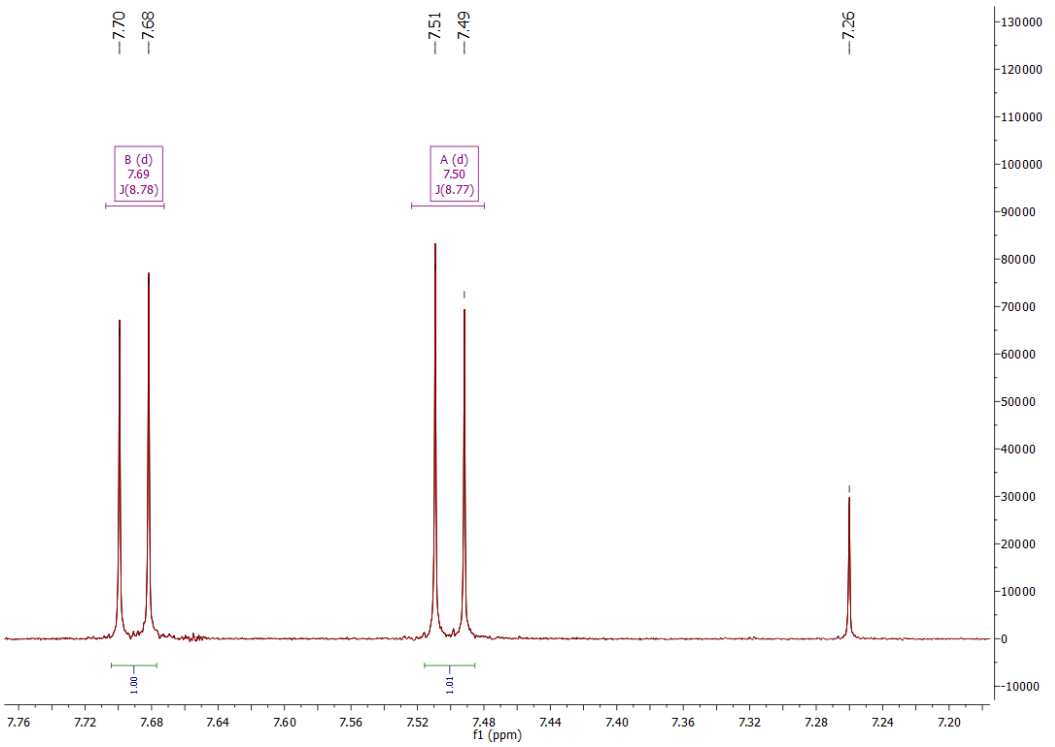

Figure S17. ^{1}H NMR of 2,3,6-Cl_3PTCE

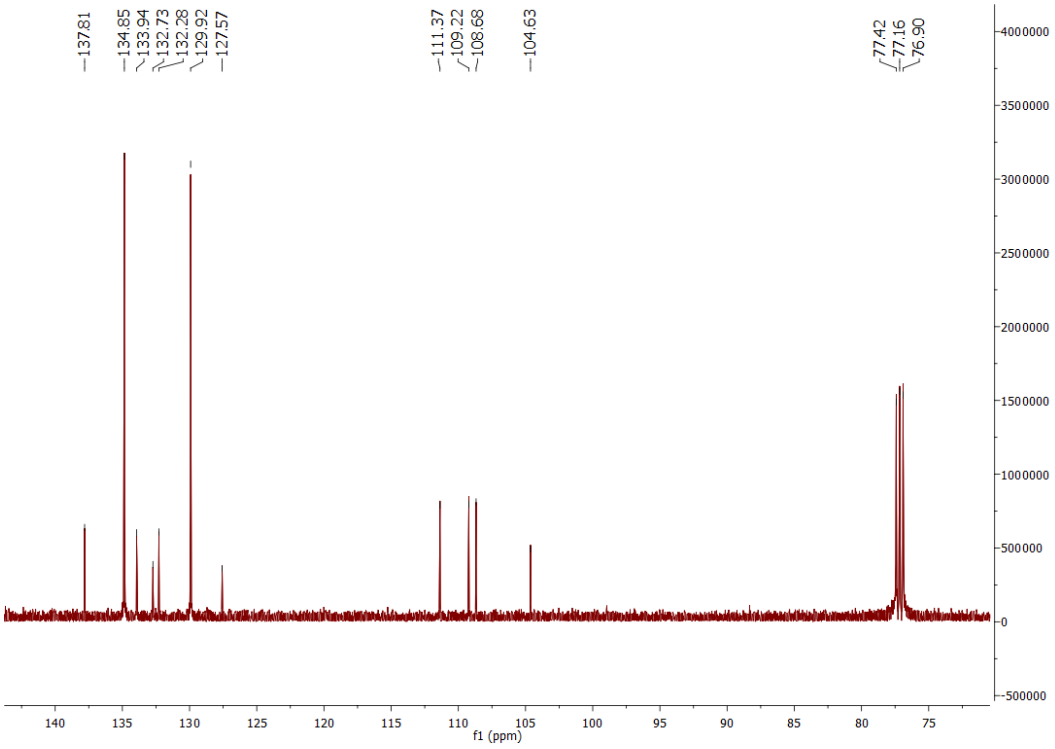

Figure S18. ^{13}C NMR of 2,3,6-Cl_3PTCE

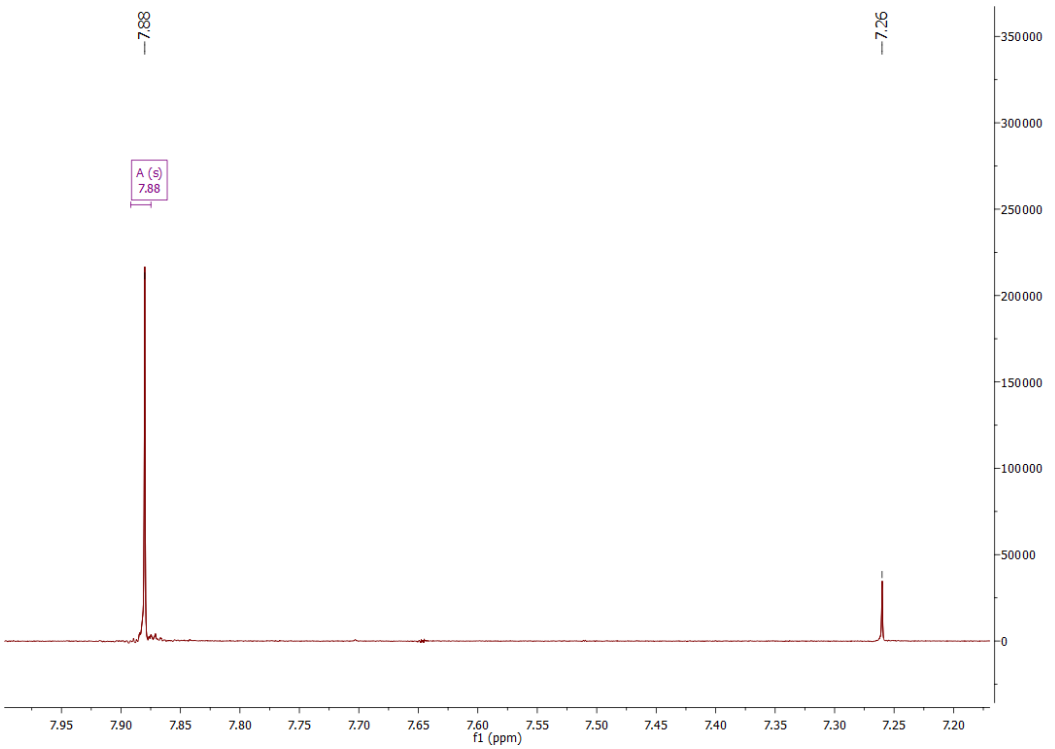

Figure S19. ^{1}H NMR of 2,3,5,6-Cl_4PTCE

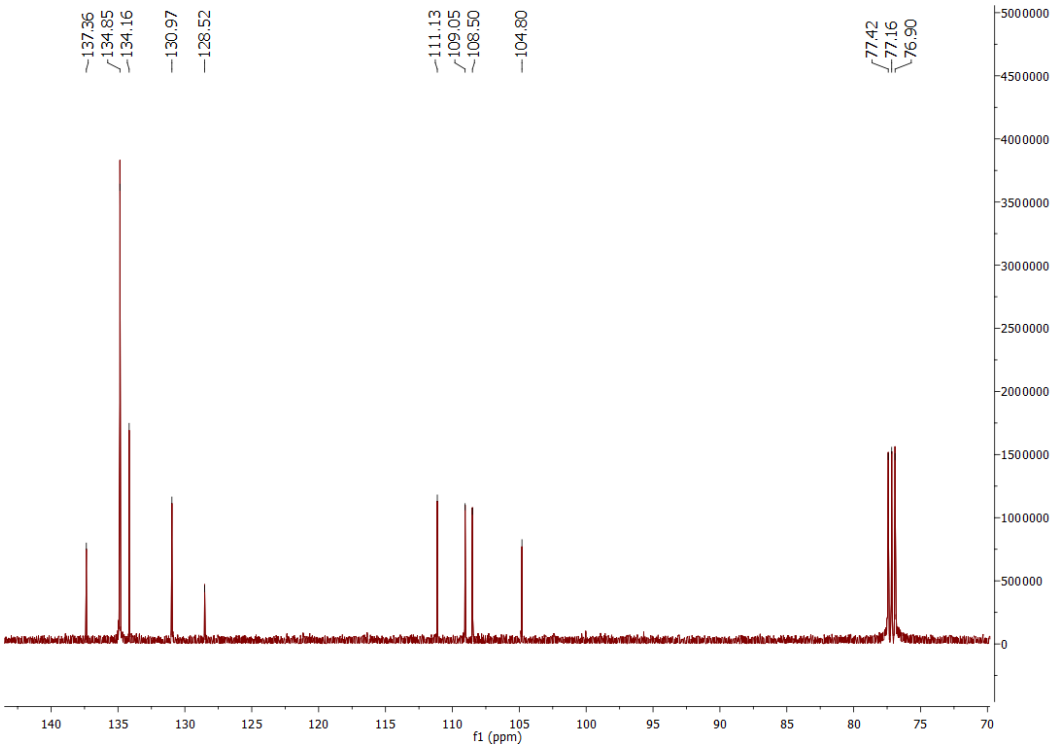

Figure S20. ^{13}C NMR of 2,3,5,6-Cl_4PTCE

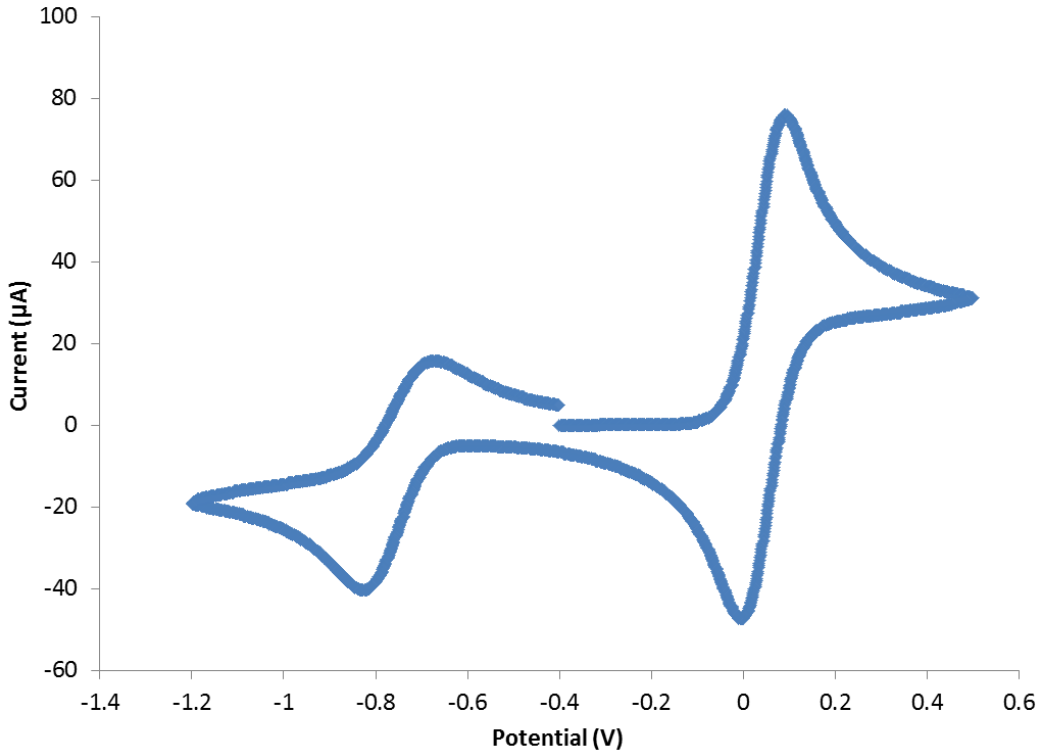

Figure S21. Cyclic voltammetry of 2-ClPTCE (peak on left) with added ferrocene (peak on right)

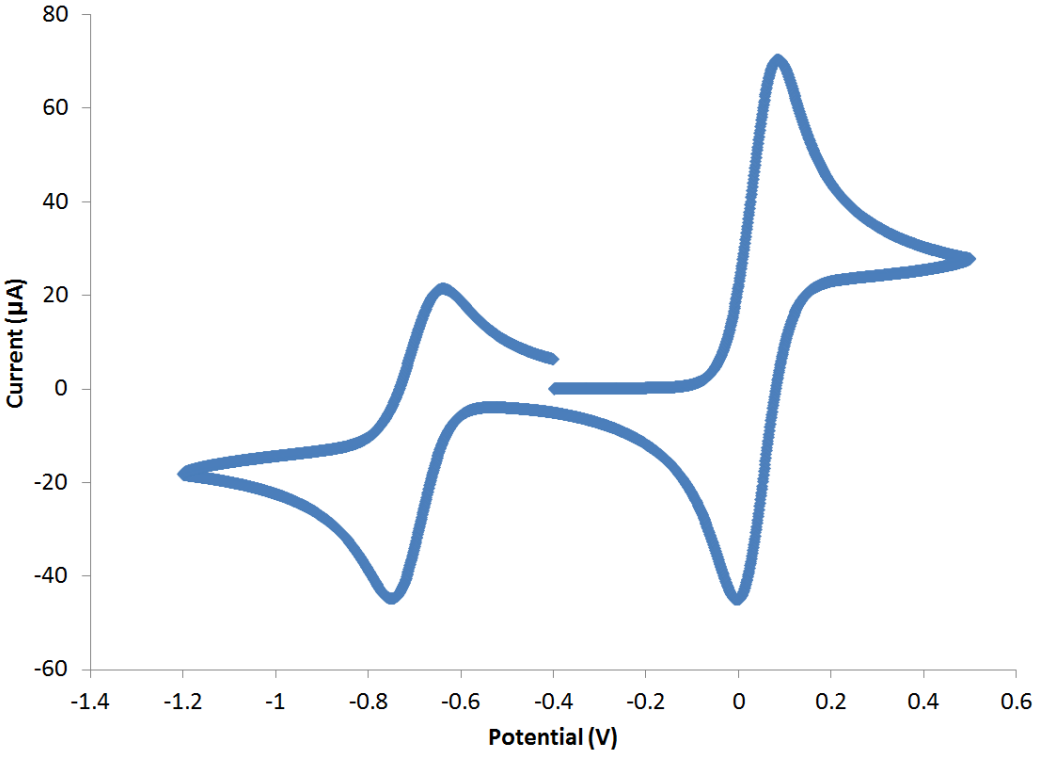

Figure S22. Cyclic voltammetry of 3-ClPTCE (peak on left) with added ferrocene (peak on right)

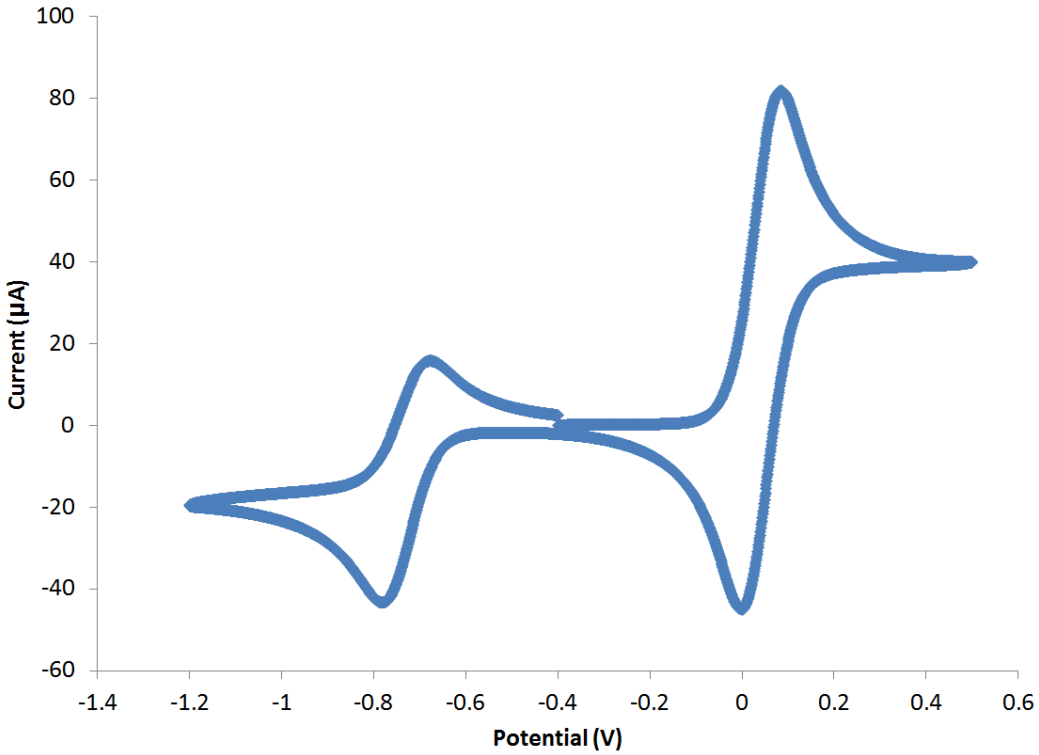

Figure S23. Cyclic voltammetry of 4-ClPTCE (peak on left) with added ferrocene (peak on right)

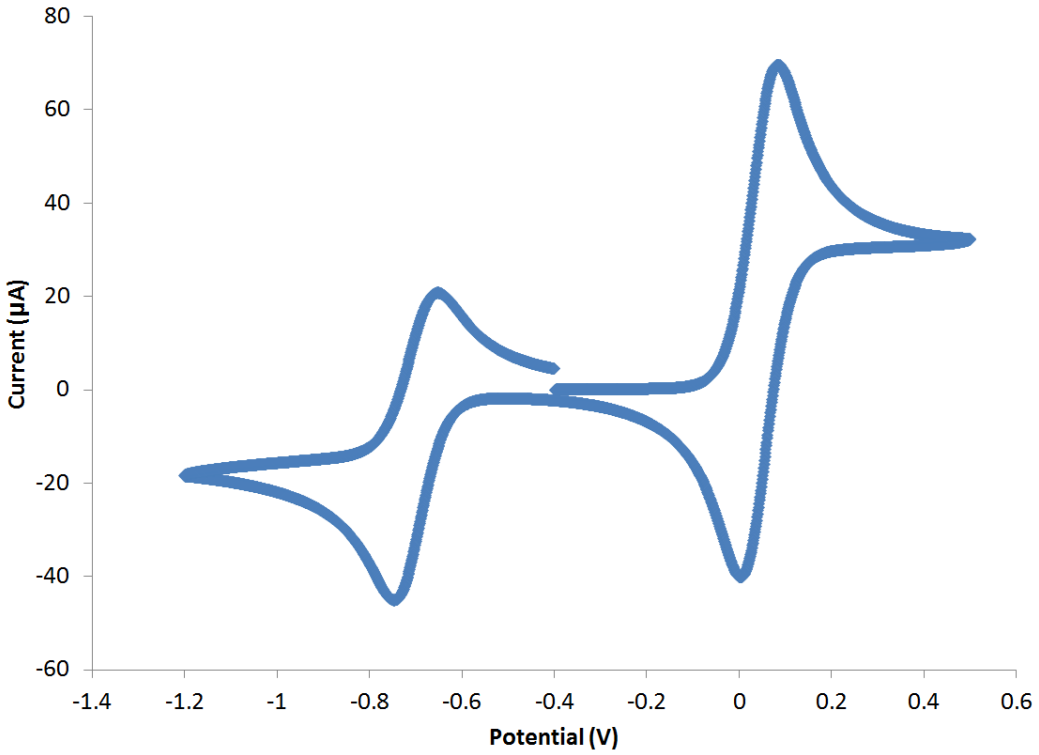

Figure S24. Cyclic voltammetry of 2,3-Cl_2PTCE (peak on left) with added ferrocene (peak on right)

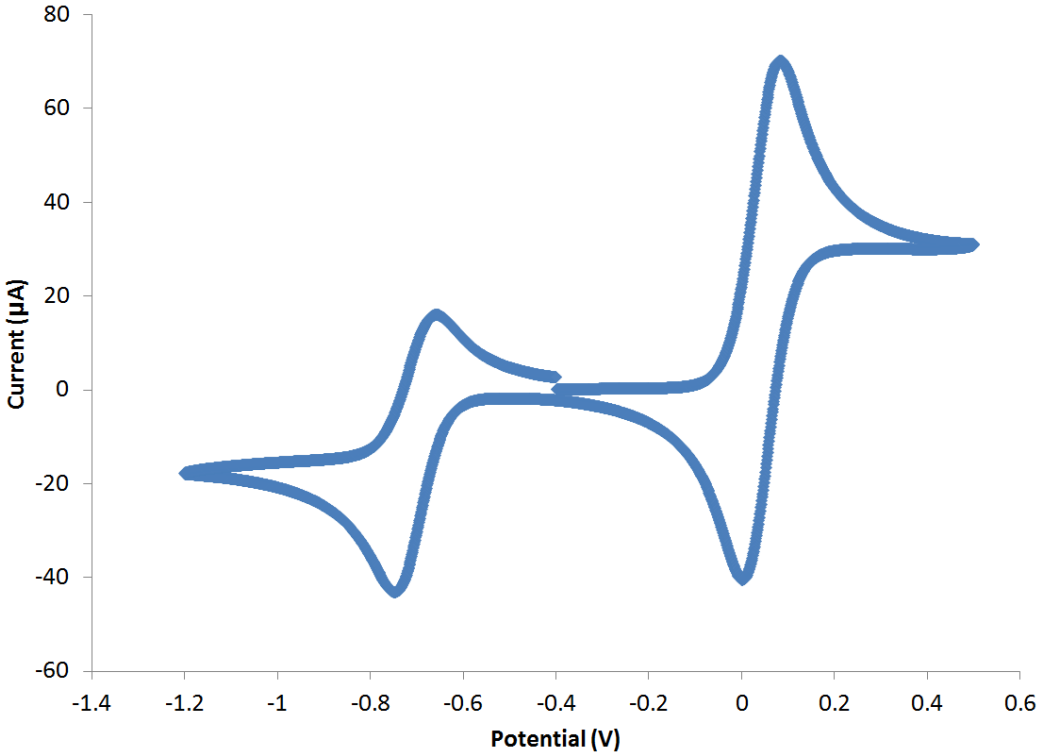

Figure S25. Cyclic voltammetry of 2,4-Cl_2PTCE (peak on left) with added ferrocene (peak on right)

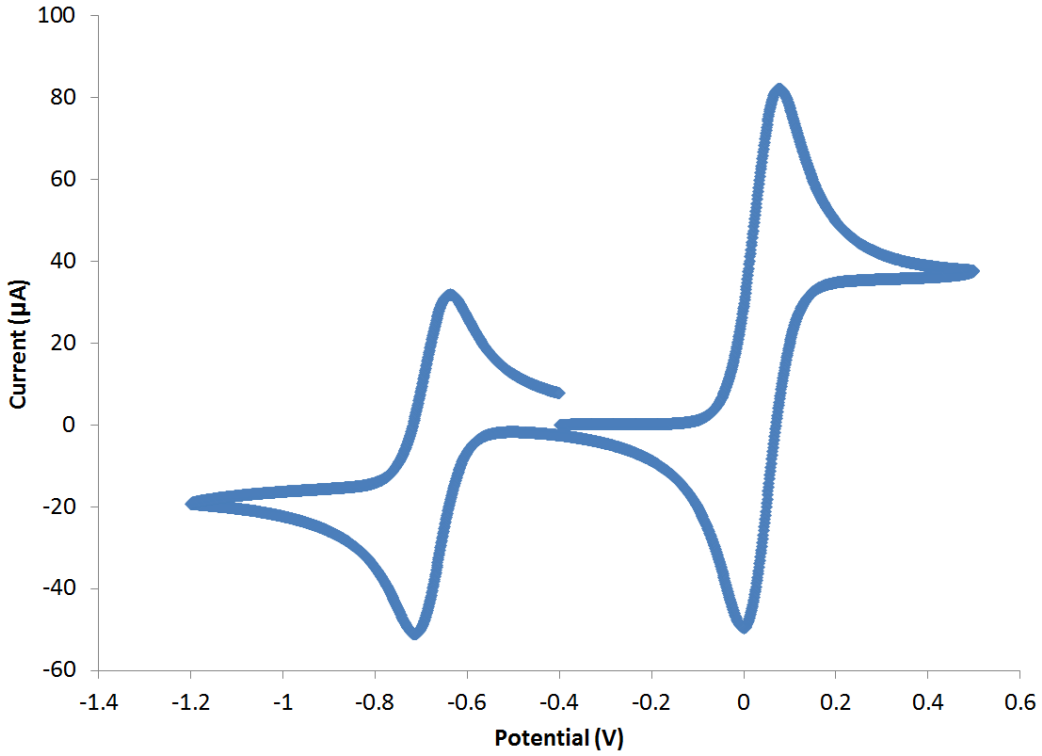

Figure S26. Cyclic voltammetry of 2,5-Cl_2PTCE (peak on left) with added ferrocene (peak on right)

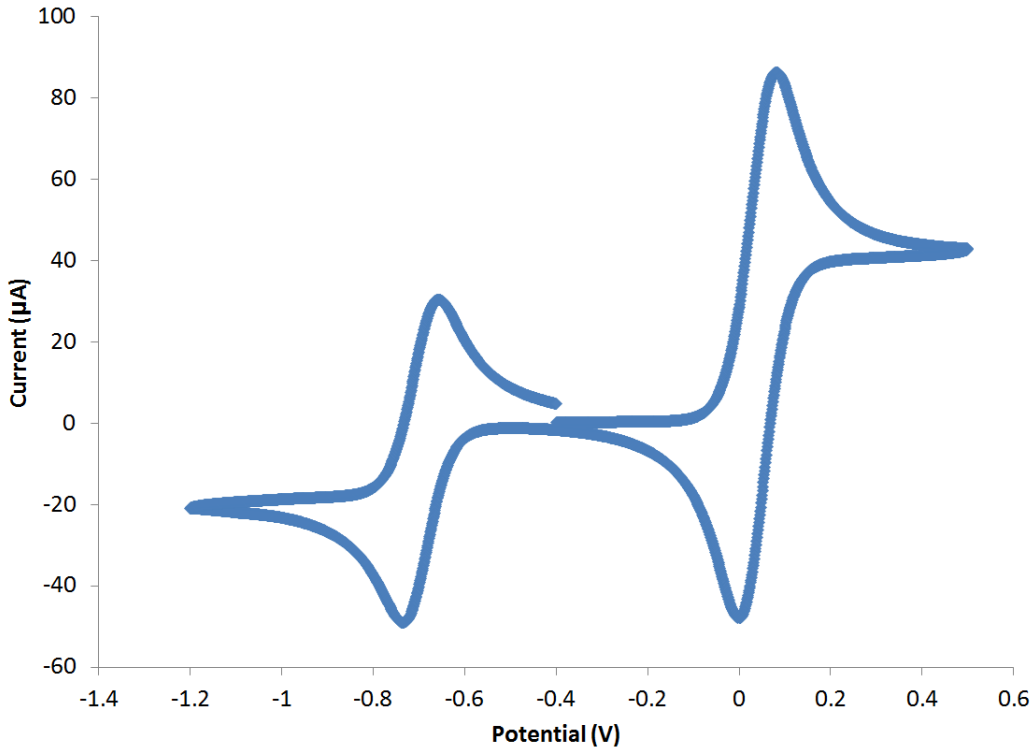

Figure S27. Cyclic voltammetry of 2,6-Cl_2PTCE (peak on left) with added ferrocene (peak on right)

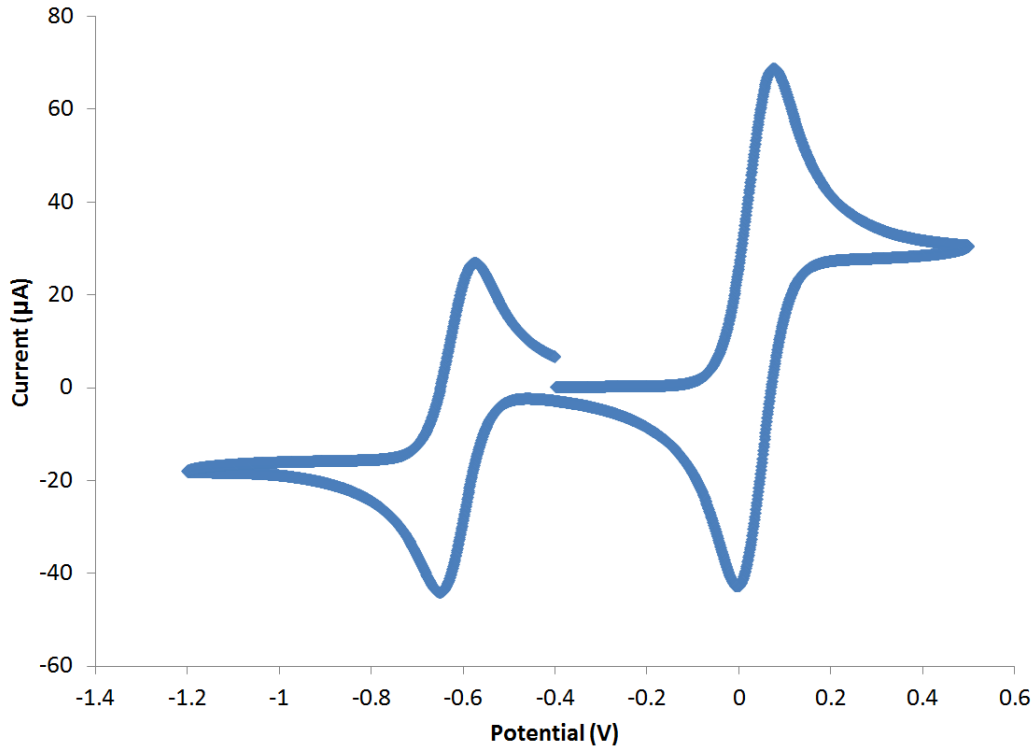

Figure S28. Cyclic voltammetry of 3,5-Cl_2PTCE (peak on left) with added ferrocene (peak on right)

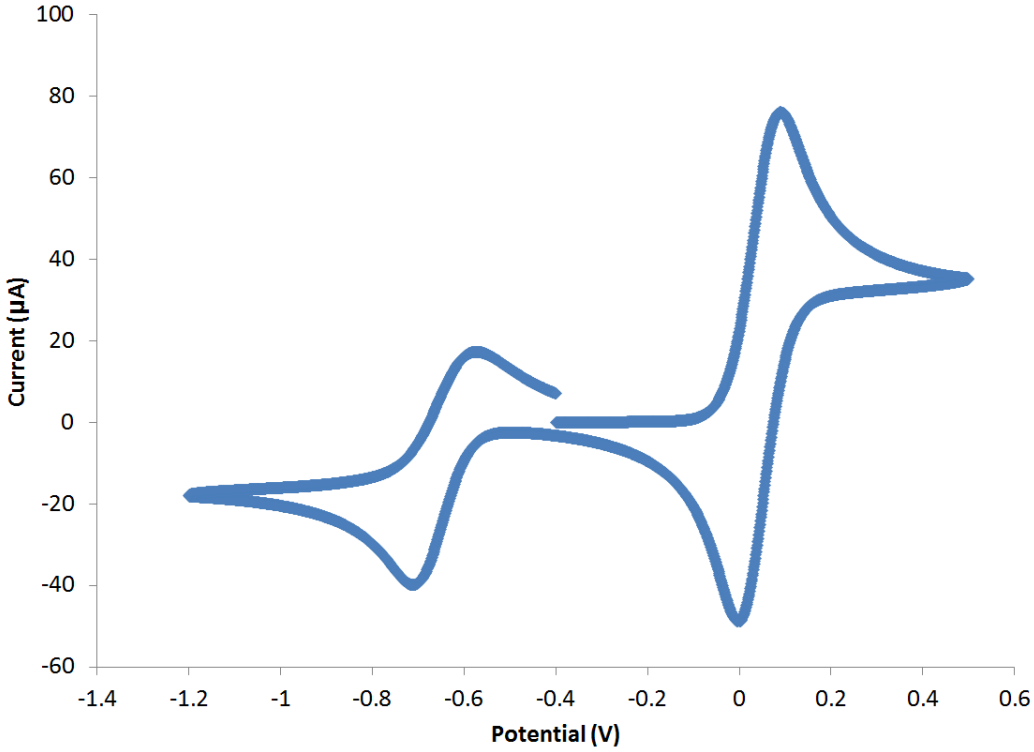

Figure S29. Cyclic voltammetry of 2,3,6-Cl_3PTCE (peak on left) with added ferrocene (peak on right)

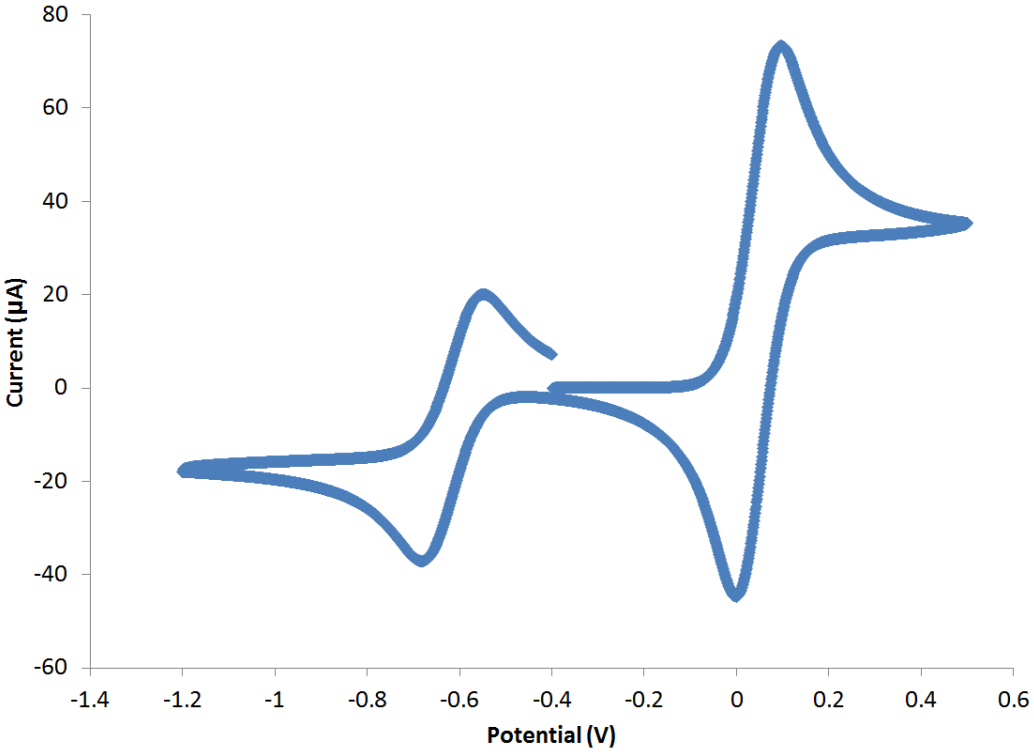

Figure S30. Cyclic voltammetry of 2,3,5,6-Cl_4PTCE (peak on left) with added ferrocene (peak on right)

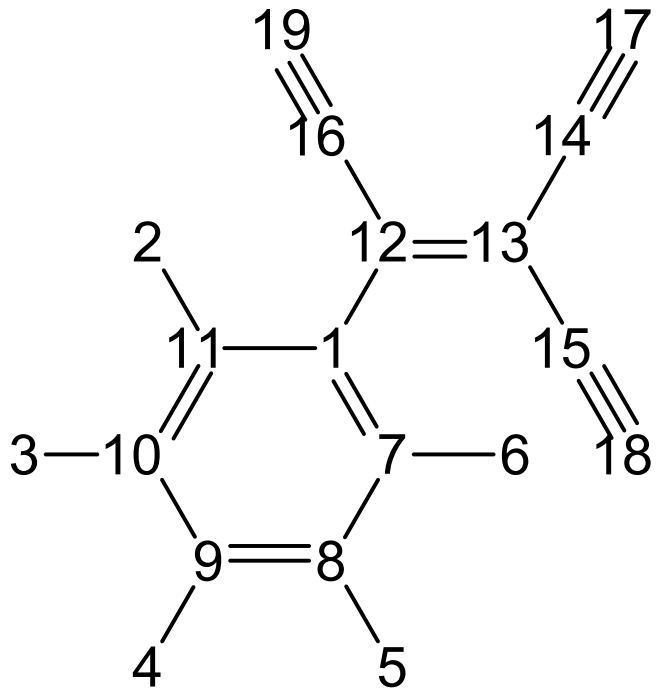

Figure S31. x-Cl_nPTCE numbering scheme for spin density values.

Table S1. Atomic Mulliken Spin Densities by Atom

Atom #	H_5PTCE	2-ClPTCE	3-ClPTCE	4-ClPTCE	2,3-ClPTCE	2,4-ClPTCE	2,5-ClPTCE	2,6-ClPTCE	3,5-ClPTCE	2,3,6-ClPTCE	2,3,5,6-ClPTCE
1	-0.079902	-0.046062	-0.070759	-0.07021	-0.038939	-0.060418	-0.026057	-0.040488	-0.060112	-0.042228	-0.029123
2	-0.006997	0.009649	-0.006906	-0.007	0.009506	0.009157	0.009196	0.004902	-0.006592	0.007115	0.006661
3	0.002969	0.002796	-0.000941	0.002912	-0.000669	0.002871	0.002728	0.001554	-0.00077	-0.001545	-0.001678
4	-0.009773	-0.006909	-0.010157	0.007831	-0.007109	0.005677	-0.007335	-0.003806	-0.010439	-0.004568	-0.004772
5	0.003529	0.002975	0.003438	0.003443	0.002759	0.003017	-0.001577	0.00196	-0.001153	0.001746	0.000617
6	-0.007511	-0.005117	-0.007644	-0.007706	-0.005291	-0.005755	-0.004134	-0.001585	-0.007468	-0.001196	-0.006576
7	0.12329	0.060727	0.125959	0.13043	0.067437	0.079825	0.04574	0.03695	0.125138	0.046036	0.043559
8	-0.055978	-0.039507	-0.052532	-0.059777	-0.034238	-0.040504	-0.031387	-0.017789	-0.053314	-0.021431	-0.024977
9	0.139367	0.097827	0.14775	0.130845	0.101093	0.095719	0.108385	0.052065	0.157582	0.057688	0.070836
10	-0.052367	-0.042958	-0.052979	-0.054813	-0.052162	-0.050706	-0.041734	-0.024906	-0.050393	-0.027095	-0.016125
11	0.105209	0.097066	0.103041	0.107826	0.085377	0.08732	0.106955	0.042885	0.105254	0.05086	0.037795
12	0.401934	0.390055	0.373313	0.380558	0.397837	0.408238	0.348742	0.450808	0.341832	0.431794	0.402685
13	0.278641	0.317252	0.30532	0.287973	0.321039	0.309206	0.338892	0.318185	0.326861	0.327964	0.338554
14	-0.066895	-0.073387	-0.073556	-0.0698	-0.081092	-0.074657	-0.079198	-0.068206	-0.07998	-0.07187	-0.076864
15	-0.097914	-0.11256	-0.106957	-0.107563	-0.106905	-0.110774	-0.117076	-0.124493	-0.115842	-0.127008	-0.128549
16	-0.106555	-0.099169	-0.103967	-0.101718	-0.101753	-0.102349	-0.095231	-0.114069	-0.096582	-0.105459	-0.084859
17	0.121659	0.130858	0.126106	0.123467	0.133201	0.132008	0.13479	0.137825	0.13098	0.139254	0.140682
18	0.141677	0.136718	0.146309	0.14516	0.138263	0.13831	0.13877	0.150817	0.150769	0.152077	0.152894
19	0.165618	0.179744	0.155161	0.158144	0.171645	0.173814	0.169532	0.197392	0.144228	0.187865	0.17924

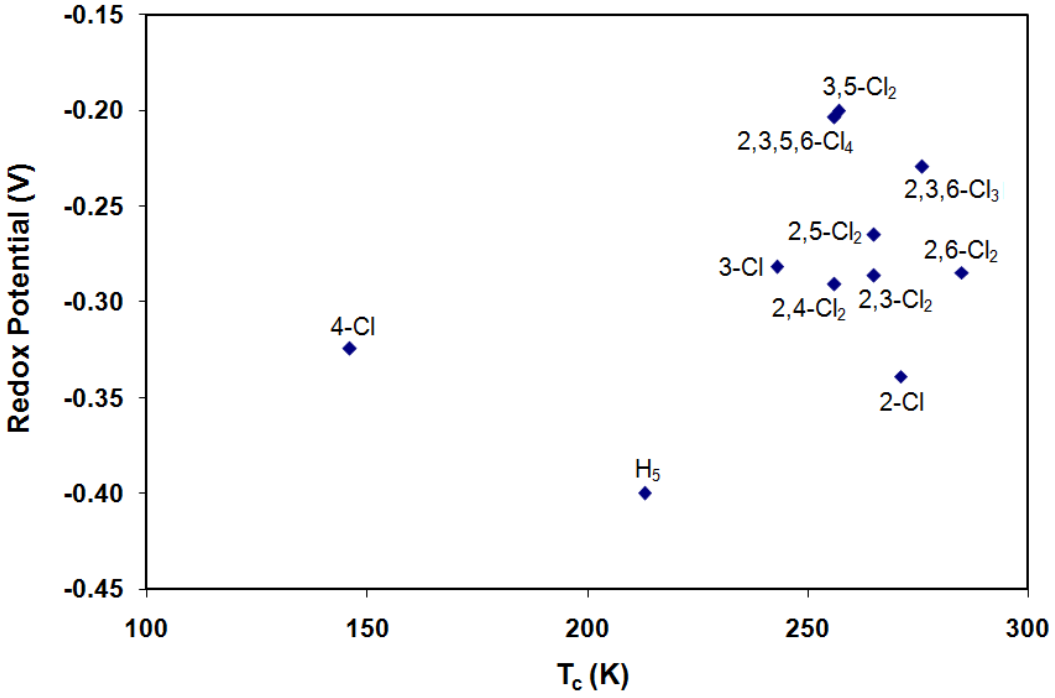

Figure S32. Redox Potential (E_{red}) vs. Ordering Temperature for Chloro-substituted PTCE Magnets

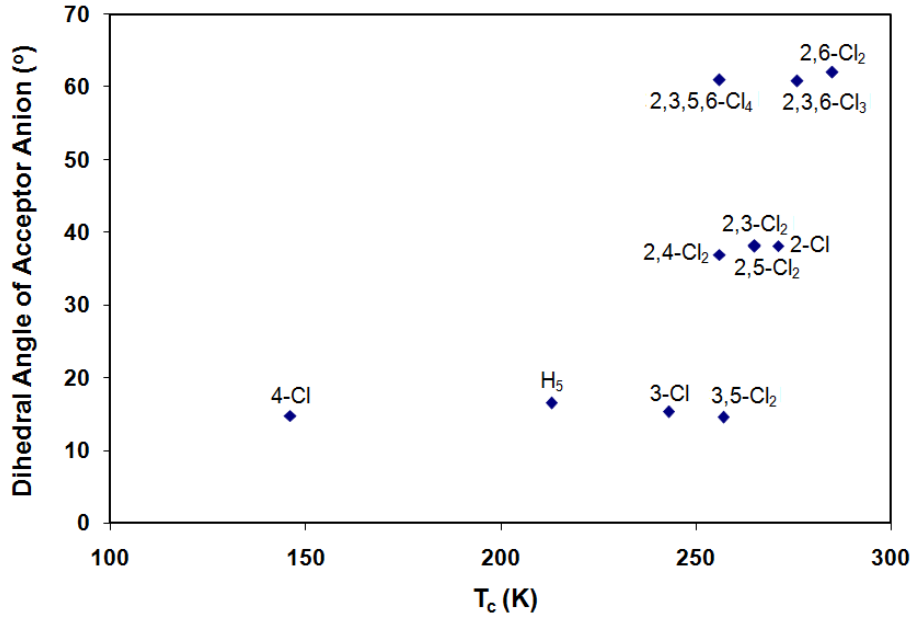

Figure S33. Radical Anion Dihedral Angle vs. Ordering Temperature for Chloro-substituted PTCE Magnets

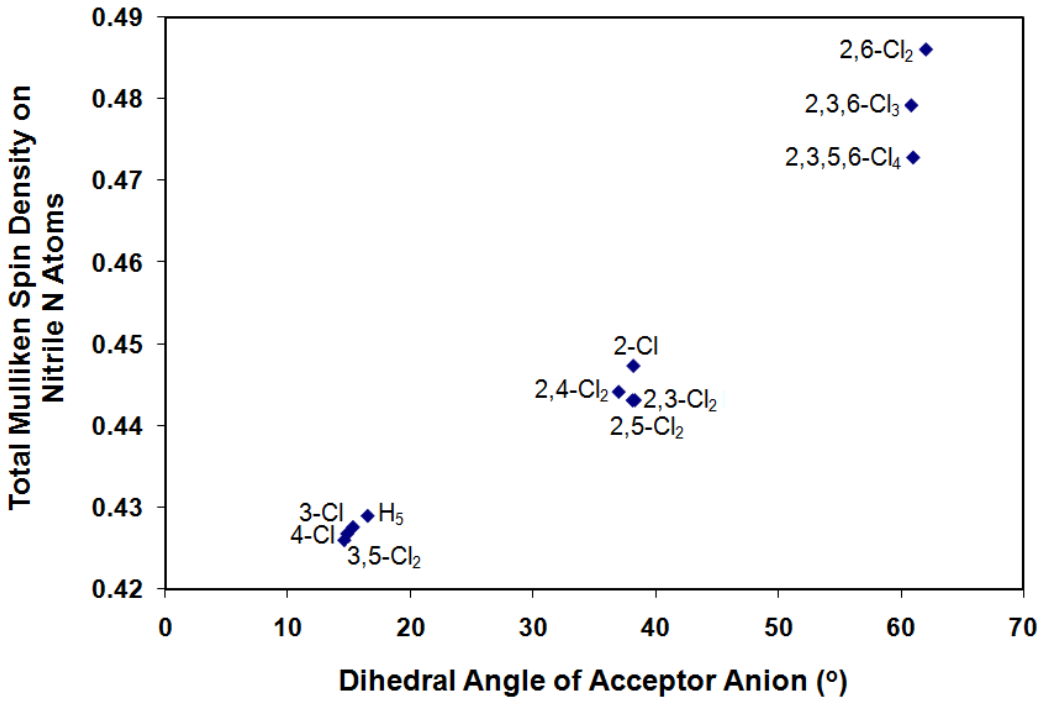

Figure S34. Mulliken Spin Density on Nitrile Nitrogen Atoms vs. Radical Anion Dihedral Angle for Chloro-substituted PTCE Magnets

Table S2. Atomic Coordinates of DFT minimized 2-ClPTCE

C	-2.217000	-1.220000	0.027000
C	-1.360000	-0.928000	-1.032000
C	-0.680000	0.283000	-1.055000
C	-0.840000	1.217000	-0.021000
C	-1.709000	0.904000	1.036000
C	-2.397000	-0.304000	1.059000
H	-2.753000	-2.162000	0.051000
H	-1.219000	-1.639000	-1.836000
H	-0.001000	0.507000	-1.869000
H	-3.072000	-0.515000	1.878000
C	-0.061000	2.481000	-0.056000
C	-0.148000	3.381000	-1.078000
C	0.672000	4.550000	-1.139000
C	-1.083000	3.219000	-2.149000
C	0.872000	2.713000	1.001000
N	-1.826000	3.125000	-3.028000
N	1.647000	2.857000	1.845000
N	1.323000	5.501000	-1.210000
Cl	-1.992000	2.058000	2.320000

Table S3. Atomic Coordinates of DFT minimized 2-ClPTCE radical anion

C	-2.193000	-1.261000	0.013000
C	-1.462000	-0.825000	-1.094000
C	-0.825000	0.406000	-1.068000
C	-0.882000	1.271000	0.050000
C	-1.654000	0.805000	1.140000
C	-2.284000	-0.435000	1.130000
H	-2.693000	-2.223000	0.008000
H	-1.378000	-1.451000	-1.976000
H	-0.240000	0.719000	-1.923000
H	-2.864000	-0.735000	1.994000
C	-0.153000	2.542000	0.022000
C	-0.062000	3.344000	-1.171000
C	0.893000	4.374000	-1.311000
C	-0.969000	3.211000	-2.244000
C	0.605000	2.920000	1.146000
N	-1.702000	3.109000	-3.143000
N	1.269000	3.212000	2.058000
N	1.672000	5.227000	-1.450000
Cl	-1.922000	1.815000	2.562000

Table S4. Atomic Coordinates of DFT minimized 3-ClPTCE

C	-2.308000	-1.202000	0.078000
C	-1.668000	-0.831000	-1.102000
C	-0.956000	0.360000	-1.182000
C	-0.871000	1.201000	-0.061000
C	-1.491000	0.816000	1.141000
C	-2.210000	-0.370000	1.191000
H	-2.866000	-2.127000	0.141000
C	-0.126000	2.474000	-0.096000
C	0.006000	3.310000	-1.175000
C	0.791000	4.502000	-1.105000
C	-0.646000	3.094000	-2.427000
C	0.503000	2.873000	1.128000
N	-1.160000	2.971000	-3.454000
N	0.992000	3.162000	2.133000
N	1.420000	5.471000	-1.078000
H	-0.451000	0.613000	-2.102000
H	-1.723000	-1.481000	-1.967000
H	-1.422000	1.439000	2.023000
Cl	-2.999000	-0.830000	2.685000

Table S5. Atomic Coordinates of DFT minimized 3-ClPTCE radical anion

C	-2.273000	-1.261000	0.096000
C	-1.768000	-0.775000	-1.112000
C	-1.106000	0.443000	-1.187000
C	-0.922000	1.249000	-0.036000
C	-1.432000	0.746000	1.190000
C	-2.082000	-0.472000	1.229000
H	-2.788000	-2.210000	0.159000
C	-0.224000	2.525000	-0.065000
C	0.095000	3.292000	-1.241000
C	1.006000	4.373000	-1.180000
C	-0.509000	3.110000	-2.501000
C	0.183000	3.054000	1.181000
N	-0.988000	2.987000	-3.556000
N	0.503000	3.459000	2.224000
N	1.755000	5.262000	-1.158000
H	-0.724000	0.768000	-2.143000
H	-1.889000	-1.366000	-2.013000
H	-1.313000	1.320000	2.099000
Cl	-2.708000	-1.058000	2.785000

Table S6. Atomic Coordinates of DFT minimized 4-ClPTCE

C	-2.320000	-1.179000	0.084000
C	-1.717000	-0.812000	-1.118000
C	-1.007000	0.377000	-1.191000
C	-0.885000	1.212000	-0.066000
C	-1.479000	0.802000	1.143000
C	-2.203000	-0.378000	1.219000
C	-0.140000	2.480000	-0.103000
C	0.040000	3.302000	-1.188000
C	0.826000	4.492000	-1.100000
C	-0.558000	3.076000	-2.464000
C	0.443000	2.903000	1.137000
N	-1.028000	2.939000	-3.511000
N	0.895000	3.212000	2.153000
N	1.456000	5.460000	-1.059000
H	-0.528000	0.634000	-2.125000
H	-1.384000	1.418000	2.029000
H	-2.669000	-0.678000	2.148000
H	-1.797000	-1.455000	-1.985000
Cl	-3.221000	-2.672000	0.174000

Table S7. Atomic Coordinates of DFT minimized 4-ClPTCE radical anion

C	-2.175000	-1.291000	-0.013000
C	-1.662000	-0.784000	-1.203000
C	-1.049000	0.462000	-1.216000
C	-0.932000	1.247000	-0.042000
C	-1.464000	0.686000	1.148000
C	-2.074000	-0.558000	1.168000
C	-0.282000	2.548000	-0.016000
C	0.057000	3.355000	-1.160000
C	0.918000	4.470000	-1.036000
C	-0.483000	3.176000	-2.449000
C	0.051000	3.061000	1.258000
N	-0.910000	3.054000	-3.527000
N	0.309000	3.449000	2.324000
N	1.628000	5.388000	-0.960000
H	-0.651000	0.822000	-2.153000
H	-1.392000	1.246000	2.073000
H	-2.472000	-0.957000	2.093000
H	-1.735000	-1.361000	-2.116000
Cl	-2.958000	-2.880000	0.004000

Table S8. Atomic Coordinates of DFT minimized 2,3-Cl_2PTCE

C	-2.182000	-1.234000	0.034000
C	-1.322000	-0.941000	-1.017000
C	-0.647000	0.273000	-1.047000
C	-0.822000	1.204000	-0.019000
C	-1.693000	0.911000	1.044000
C	-2.372000	-0.312000	1.062000
H	-2.716000	-2.174000	0.069000
C	-0.049000	2.474000	-0.057000
C	-0.180000	3.390000	-1.058000
C	0.630000	4.567000	-1.129000
C	-1.151000	3.236000	-2.097000
C	0.922000	2.687000	0.969000
N	-1.924000	3.145000	-2.949000
N	1.725000	2.814000	1.790000
N	1.272000	5.523000	-1.206000
H	0.034000	0.498000	-1.859000
H	-1.180000	-1.661000	-1.813000
Cl	-1.955000	2.094000	2.294000
Cl	-3.471000	-0.712000	2.353000

Table S9. Atomic Coordinates of DFT minimized 2,3-Cl_2PTCE radical anion

C	-2.168000	-1.266000	0.022000
C	-1.452000	-0.819000	-1.086000
C	-0.821000	0.413000	-1.065000
C	-0.877000	1.268000	0.058000
C	-1.642000	0.815000	1.167000
C	-2.256000	-0.441000	1.138000
H	-2.658000	-2.231000	0.030000
C	-0.152000	2.540000	0.027000
C	-0.076000	3.343000	-1.164000
C	0.877000	4.376000	-1.313000
C	-0.995000	3.211000	-2.227000
C	0.625000	2.916000	1.140000
N	-1.738000	3.107000	-3.117000
N	1.303000	3.206000	2.041000
N	1.652000	5.230000	-1.459000
H	-0.243000	0.732000	-1.921000
H	-1.375000	-1.448000	-1.966000
Cl	-1.888000	1.857000	2.550000
Cl	-3.198000	-1.026000	2.508000

Table S10. Atomic Coordinates of DFT minimized 2,4-Cl_2PTCE

C	-2.214000	-1.209000	0.026000
C	-1.372000	-0.919000	-1.045000
C	-0.698000	0.294000	-1.058000
C	-0.843000	1.222000	-0.017000
C	-1.702000	0.898000	1.045000
C	-2.391000	-0.308000	1.071000
C	-0.065000	2.485000	-0.052000
C	-0.140000	3.379000	-1.081000
C	0.685000	4.545000	-1.141000
C	-1.064000	3.213000	-2.161000
C	0.857000	2.725000	1.012000
N	-1.799000	3.112000	-3.045000
N	1.624000	2.876000	1.863000
N	1.339000	5.494000	-1.211000
H	-0.030000	0.518000	-1.880000
Cl	-1.979000	2.036000	2.342000
H	-3.059000	-0.535000	1.890000
H	-1.245000	-1.630000	-1.850000
Cl	-3.073000	-2.729000	0.062000

Table S11. Atomic Coordinates of DFT minimized 2,4-Cl_2PTCE radical anion

C	-2.191000	-1.237000	0.016000
C	-1.478000	-0.816000	-1.103000
C	-0.843000	0.415000	-1.069000
C	-0.885000	1.277000	0.053000
C	-1.648000	0.807000	1.148000
C	-2.283000	-0.432000	1.143000
C	-0.155000	2.545000	0.023000
C	-0.053000	3.340000	-1.171000
C	0.907000	4.368000	-1.308000
C	-0.952000	3.205000	-2.250000
C	0.595000	2.929000	1.151000
N	-1.680000	3.097000	-3.153000
N	1.252000	3.227000	2.065000
N	1.689000	5.218000	-1.444000
H	-0.267000	0.725000	-1.931000
Cl	-1.907000	1.805000	2.575000
H	-2.859000	-0.746000	2.002000
H	-1.409000	-1.446000	-1.980000
Cl	-3.003000	-2.807000	0.005000

Table S12. Atomic Coordinates of DFT minimized 2,5-Cl_2PTCE

C	-2.252000	-1.204000	0.013000
C	-1.390000	-0.911000	-1.039000
C	-0.687000	0.286000	-1.070000
C	-0.838000	1.214000	-0.031000
C	-1.708000	0.914000	1.027000
C	-2.412000	-0.285000	1.044000
H	-2.796000	-2.140000	0.027000
C	-0.043000	2.471000	-0.067000
C	-0.160000	3.394000	-1.063000
C	0.665000	4.560000	-1.123000
C	-1.131000	3.260000	-2.104000
C	0.924000	2.666000	0.966000
N	-1.908000	3.186000	-2.956000
N	1.721000	2.779000	1.794000
N	1.319000	5.509000	-1.192000
H	-0.010000	0.494000	-1.888000
Cl	-1.967000	2.066000	2.316000
H	-3.090000	-0.494000	1.862000
Cl	-1.181000	-2.063000	-2.338000

Table S13. Atomic Coordinates of DFT minimized 2,5-Cl_2PTCE radical anion

C	-2.222000	-1.252000	0.010000
C	-1.497000	-0.798000	-1.089000
C	-0.846000	0.420000	-1.084000
C	-0.888000	1.274000	0.045000
C	-1.645000	0.806000	1.146000
C	-2.285000	-0.428000	1.130000
H	-2.728000	-2.208000	-0.010000
C	-0.149000	2.537000	0.016000
C	-0.062000	3.345000	-1.171000
C	0.904000	4.365000	-1.313000
C	-0.991000	3.236000	-2.227000
C	0.622000	2.901000	1.137000
N	-1.747000	3.155000	-3.109000
N	1.295000	3.183000	2.044000
N	1.691000	5.210000	-1.453000
H	-0.269000	0.722000	-1.946000
Cl	-1.887000	1.805000	2.576000
H	-2.858000	-0.735000	1.996000
Cl	-1.381000	-1.833000	-2.520000

Table S14. Atomic Coordinates of DFT minimized 2,6-Cl_2PTCE

C	-2.244000	-1.196000	-0.028000
C	-1.206000	-1.069000	-0.946000
C	-0.467000	0.108000	-0.977000
C	-0.750000	1.171000	-0.108000
C	-1.795000	1.006000	0.811000
C	-2.544000	-0.164000	0.855000
H	-2.824000	-2.111000	0.000000
H	-0.966000	-1.870000	-1.633000
H	-3.347000	-0.259000	1.573000
C	0.053000	2.430000	-0.143000
C	-0.286000	3.487000	-0.926000
C	0.480000	4.694000	-0.963000
C	-1.445000	3.442000	-1.763000
C	1.210000	2.481000	0.689000
N	-2.377000	3.424000	-2.445000
N	2.137000	2.476000	1.379000
N	1.085000	5.676000	-1.007000
Cl	-2.170000	2.295000	1.934000
Cl	0.845000	0.256000	-2.125000

Table S15. Atomic Coordinates of DFT minimized 2,6-Cl_2PTCE radical anion

C	-2.398000	-1.131000	-0.013000
C	-1.488000	-0.913000	-1.043000
C	-0.698000	0.230000	-1.034000
C	-0.786000	1.219000	-0.027000
C	-1.723000	0.944000	0.994000
C	-2.510000	-0.202000	1.016000
H	-3.015000	-2.022000	-0.012000
H	-1.371000	-1.632000	-1.844000
H	-3.215000	-0.348000	1.824000
C	0.044000	2.440000	-0.036000
C	-0.050000	3.398000	-1.100000
C	0.881000	4.447000	-1.255000
C	-1.111000	3.362000	-2.027000
C	0.942000	2.620000	1.025000
N	-1.990000	3.335000	-2.790000
N	1.699000	2.730000	1.907000
N	1.637000	5.320000	-1.393000
Cl	-1.968000	2.106000	2.293000
Cl	0.505000	0.372000	-2.308000

Table S16. Atomic Coordinates of DFT minimized 3,5-Cl_2PTCE

C	-2.324000	-1.193000	0.067000
C	-1.669000	-0.818000	-1.103000
C	-0.946000	0.365000	-1.187000
C	-0.870000	1.200000	-0.063000
C	-1.500000	0.824000	1.134000
C	-2.228000	-0.357000	1.177000
H	-2.885000	-2.116000	0.116000
C	-0.112000	2.468000	-0.097000
C	-0.003000	3.316000	-1.168000
C	0.790000	4.504000	-1.103000
C	-0.689000	3.117000	-2.405000
C	0.547000	2.842000	1.118000
N	-1.231000	3.006000	-3.419000
N	1.060000	3.110000	2.117000
N	1.424000	5.469000	-1.078000
H	-0.435000	0.608000	-2.107000
H	-1.434000	1.448000	2.015000
Cl	-3.035000	-0.814000	2.658000
Cl	-1.750000	-1.871000	-2.495000

Table S17. Atomic Coordinates of DFT minimized 3,5-Cl_2PTCE radical anion

C	-2.284000	-1.260000	0.096000
C	-1.785000	-0.755000	-1.103000
C	-1.124000	0.456000	-1.201000
C	-0.927000	1.251000	-0.043000
C	-1.424000	0.743000	1.187000
C	-2.076000	-0.472000	1.227000
H	-2.798000	-2.208000	0.146000
C	-0.225000	2.522000	-0.071000
C	0.101000	3.293000	-1.240000
C	1.009000	4.375000	-1.167000
C	-0.493000	3.116000	-2.506000
C	0.181000	3.046000	1.178000
N	-0.965000	2.999000	-3.564000
N	0.500000	3.447000	2.223000
N	1.755000	5.267000	-1.134000
H	-0.755000	0.774000	-2.163000
H	-1.293000	1.312000	2.097000
Cl	-2.687000	-1.067000	2.780000
Cl	-1.998000	-1.731000	-2.564000

Table S18. Atomic Coordinates of DFT minimized 2,3,6-Cl_3PTCE

C	-2.196000	-1.219000	-0.020000
C	-1.201000	-1.053000	-0.972000
C	-0.475000	0.132000	-1.007000
C	-0.738000	1.163000	-0.099000
C	-1.740000	0.979000	0.868000
C	-2.471000	-0.212000	0.904000
H	-2.768000	-2.137000	0.015000
H	-0.986000	-1.838000	-1.684000
C	0.049000	2.434000	-0.135000
C	-0.304000	3.484000	-0.922000
C	0.451000	4.697000	-0.968000
C	-1.466000	3.423000	-1.753000
C	1.207000	2.498000	0.693000
N	-2.401000	3.390000	-2.429000
N	2.138000	2.504000	1.378000
N	1.047000	5.684000	-1.019000
Cl	-2.052000	2.252000	2.013000
Cl	0.788000	0.318000	-2.201000
Cl	-3.725000	-0.470000	2.082000

Table S19. Atomic Coordinates of DFT minimized 2,3,6-Cl_3PTCE radical anion

C	-2.360000	-1.149000	-0.004000
C	-1.475000	-0.906000	-1.046000
C	-0.695000	0.242000	-1.041000
C	-0.777000	1.213000	-0.020000
C	-1.694000	0.937000	1.028000
C	-2.460000	-0.230000	1.035000
H	-2.965000	-2.046000	0.011000
H	-1.370000	-1.620000	-1.852000
C	0.042000	2.441000	-0.033000
C	-0.064000	3.395000	-1.097000
C	0.864000	4.444000	-1.264000
C	-1.137000	3.357000	-2.012000
C	0.950000	2.628000	1.019000
N	-2.025000	3.325000	-2.764000
N	1.716000	2.746000	1.891000
N	1.618000	5.318000	-1.412000
Cl	-1.903000	2.108000	2.306000
Cl	0.488000	0.402000	-2.329000
Cl	-3.597000	-0.579000	2.330000

Table S20. Atomic Coordinates of DFT minimized 2,3,5,6-Cl_4PTCE

C	-2.252000	-1.183000	-0.039000
C	-1.254000	-1.040000	-0.996000
C	-0.491000	0.131000	-1.039000
C	-0.745000	1.158000	-0.120000
C	-1.744000	1.002000	0.851000
C	-2.500000	-0.174000	0.884000
H	-2.841000	-2.090000	-0.011000
C	0.070000	2.413000	-0.158000
C	-0.296000	3.492000	-0.898000
C	0.478000	4.693000	-0.938000
C	-1.492000	3.474000	-1.682000
C	1.261000	2.430000	0.624000
N	-2.455000	3.474000	-2.319000
N	2.218000	2.398000	1.272000
N	1.089000	5.671000	-0.984000
Cl	-2.022000	2.275000	2.003000
Cl	0.774000	0.330000	-2.214000
Cl	-3.756000	-0.411000	2.062000
Cl	-0.984000	-2.339000	-2.119000

Table S21. Atomic Coordinates of DFT minimized 2,3,5,6-Cl_4PTCE radical anion

C	-2.404000	-1.108000	0.043000
C	-1.263000	-1.175000	-0.745000
C	-0.416000	-0.073000	-0.869000
C	-0.682000	1.134000	-0.178000
C	-1.836000	1.168000	0.645000
C	-2.685000	0.065000	0.732000
H	-3.064000	-1.959000	0.121000
C	0.209000	2.303000	-0.304000
C	-0.265000	3.551000	-0.822000
C	0.488000	4.741000	-0.727000
C	-1.501000	3.642000	-1.496000
C	1.536000	2.156000	0.127000
N	-2.519000	3.711000	-2.056000
N	2.625000	2.016000	0.518000
N	1.100000	5.728000	-0.661000
Cl	-2.151000	2.565000	1.638000
Cl	0.960000	-0.165000	-1.937000
Cl	-4.119000	0.079000	1.745000
Cl	-0.956000	-2.677000	-1.599000

References

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