Supporting Information

for

Planar Carbenium Ions For Robust Symmetrical All Organic Redox Flow Battery

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I. General Information

All solvents were purified by SPS or distillation over the drying agents indicated. Dried solvents and liquid reagents were transferred by oven-dried syringes or hypodermic syringes. The supporting electrolyte salts tetrabutylammonium hexafluorophosphate ($TBAPF_6$) was recrystallized three times from ethanol, then dried at 80 ˚C for three days prior to use in glovebox.

NMR spectroscopy. ^{1}H-NMR, ^{13}C-NMR, and ^{19}F-NMR spectra were recorded on Bruker Avance III-400 MHz or DRX-500 MHz spectrometers in appropriate solvents using residual solvent signals as standards. The chemical shifts are shown in δ scales. Multiplicities of ^{1}H NMR signals are designated as s (singlet), d (doublet), dd (doublet of doublet), dt (doublet of triplet), t (triplet), quin (quintet), m (multiplet), etc.. (+) and (−) in respect to ^{13}C signals are used to denote uneven and even numbers of attached protons respectively. The data were obtained from ^{13}C 135 DEPT spectra. Compounds were named using ChemDraw and assignments of NMR spectra were done using MestReNova.

Mass spectrometry. HRMS (ESI) were performed via LTQ Orbitrap Velos ETD mass-spectrometer (ThermoFisher Scientific, Bremen, Germany).

UV-visible spectroscopy. Absorption spectra were recorded on a Agilent 8453 UV-Visible spectrophotometer at 25 °C in analytical-grade acetonitrile.

Scanning Electron Microscope

SEM images were taken on an FEI Inspec-S scanning electron microscope containing a tungsten filament with gun voltages of 20 or 30 keV. Carbon felt samples were mounted using sticky carbon tape. Carbon felt samples were not subject to any modification.

Facilities Acknowledgements

All NMR data were collected in the NMR facility of the Department of Chemistry and Biochemistry at the University of Arizona, RRID:SCR_012716. The purchase of the Bruker NEO 500 MHz spectrometer was supported by the National Science Foundation under Grant Number 1920234 and the University of Arizona.

All SEM images and data were collected in the W.M. Keck Center for Nano-Scale Imaging in the Department of Chemistry and Biochemistry at the University of Arizona, RRID:SCR_022884, with funding from the W.M. Keck Foundation Grant.

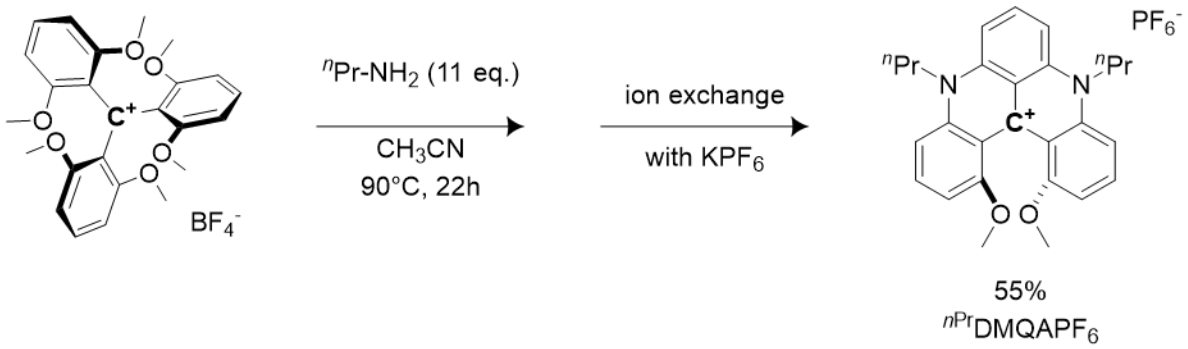
Table S1. D, k^0, Capacity retention and theoretical maximum energy density comparison with relevant reported symmetrical non-aqueous redox flow batteries.

Bipolar Redox Molecules	Theoretical Cell voltage (V)	D (× 10^{-6} cm^2/s)*				k^0 (× 10^{-2} cm/s)*				Capacity retention per cycle†	Theoretical maximum energy density (Wh/L)‡	**Ref**
		Red^2	Red^1	Ox^1	Ox^2	Red^2	Red^1	Ox^1	Ox^2			
DB-134	2.24	1.20	0.48	0.47	1.30	2.80	1.60	1.60	2.00	99.999%	12.0	10
PTIO	1.73		6.20	6.20			-	-		98.60%	11.6	11
PM567	2.32		26.00	27.00			2.40	2.40		99.00%	6.1	12
$PEG(PhPTIO)_2$	1.62		3.45	4.74			-	1.42		98.00%	165.0	13
H_2TPP	2.83	1.01	1.01	12.80	12.80	0.49	0.35	0.52	0.14	99.98%	24.7	14
FcPI	1.94		3.21	3.65			0.03	0.03		98.70%	7.8	15
$C_{60}(Fc)_4$	1.49		-	-			-	39.70		99.40%	80.0	16
p-tolylverdazyl	0.98		4.30	4.00			-	-		98.60%	0.5	17
α-FcEtPI	1.98		1.82	2.35			0.01	0.02		97.80%	21.1	18
Croconate Violet	1.82		7.18	9.76			1.37	1.54		92.00%	24.4	19
Me-TEG-DAAQ	1.80		4.30	2.50			0.49	0.26		99.88%	49.0	20
Oxo-verdazyl	1.42		0.18	0.28			-	0.81		99.20%	45.7	21
FcMeAAQ	1.42		7.82	8.02			0.68	1.86		99.60%	0.3	22
VIODAMB	1.58		4.75	5.14			0.92	0.94		97.00%	2.1	23
Fc4PI-TFSI	2.04		3.10	2.83			0.46	0.36		99.80%	60.4	24
PDI-TEMPO	1.90	1.64	1.10	2.32			0.51	0.18		99.40%	66.2	25
$PhBenzTriazineCF_3+$	1.12		12.00	12.00			1.20	1.30		99.98%	1.5	26
N-MEEE*t*BuPhePhtha-1	2.31		6.70	7.20			2.30	5.00		99.89%	55.7	27
PQ*t*BuTH	1.61		2.79	2.79		0.14	2.70	0.30	0.08	99.88%	16.1	28
BPYPE	1.01		0.37	0.22			-	-		99.65%	67.7	29
$^{nPr}DMQA^+$	2.12		9.40	9.90			2.60	2.00		99.88%	1.8	30
$^{nPr}DMQA^{NO2+}$	2.24	4.30	5.60	9.90		1.20	3.70	0.79		99.68%	9.3	31
$^{PEG}DMQA^+$	2.07		6.10	6.10			24.00	1.10		99.9994%	14.9	*In revision*
$^{nPr}DAOTA^+$	**2.36**		**6.90**	**8.77**			**0.86**	**0.18**		**99.93%**	**6.5**	**This Work**

**If irreversible or not indicated in the reference, left blank.; †Calculated using the data provided in the reference. ‡Calculated using the maximum solubility data provided in the reference*

II. Synthesis

1,13-dimethoxy-5,9-dipropylquinolino[2,3,4-kl]acridinium hexafluorophosphate ($^{n\text{Pr}}$DMQAPF$_6$)[1]



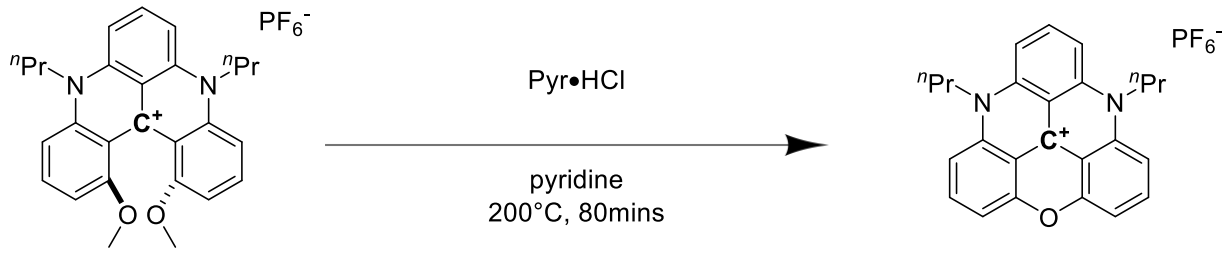
To a solution of tris(2,6 dimethoxyphenyl)carbenium tetrafluoroborate salt[1] (1.001 g, 1.962 mmol) dissolved in MeCN (20 mL) in a bomb flask, *n*Pr-NH_2 (1.61 mL, 20.7mmol) was added. The reaction mixture was heated at 90°C for 22 h, which was associated with a color change from deep purple, to red, then dark green. After 22 h the reaction was cooled to rt, and poured into KPF_6 (0.2 M, 400 mL) under stirring. The suspension was stirred at rt for 2 h, filtered, and the solid was washed with H_2O (3 × 30 mL). The solid was dissolved in CH_2Cl_2:MeCN (4:1 v/v, 12.5 mL) and poured into Et_2O (200 mL) under stirring. The suspension was stirred at rt for 2 h, filtered, and the solid was washed with Et_2O (2 × 50 mL). The dark green solid was collected and dried in vacuo o.n. to yield $^{n\text{Pr}}$DMQAPF$_6$ (0.6079 g, 1.088 mmol, 55%).

^{1}H-NMR (500 MHz, DMSO-*d*$_6$): δ (ppm) = 8.26 (t, *J* = 8.5 Hz, 1H, Ar*H*), 7.96 (t, *J* = 8.0 Hz,nPrDMQAPF6H, Ar*H*), 7.70 (d, *J* = 8.6 Hz,nPrDMQAPF6H, Ar*H*), 7.62 (d, *J* = 8.9 Hz,nPrDMQAPF6H, Ar*H*), 7.02 (d, *J* = 8.0 Hz,nPrDMQAPF6H, Ar*H*), 4.81-4.67 (m,nPrDMQAPF6H, NCH_2), 4.54-4.43 (m,nPrDMQAPF6H, NCH_2), 3.72 (s, 6H, OCH_3),nPrDMQAPF6.10-1.88 (m, 4H, CH_2), 1.16 (t, *J* = 7.3 Hz, 6H, CH_3)

^{13}C-NMR (126 MHz, DMSO-*d*$_6$): δ (ppm) = 159.1 (−), 141.8 (−), 141.6 (−), 138.2(−), 137.1 (+), 136.7 (+), 118.6 (−), 112.2 (−), 107.7 (+), 105.1 (+), 103.0 (+), 55.6 (+), 50.5 (−), 19.3 (−), 10.8 (+).

^{19}F-NMR (471 MHz, DMSO-*d*$_6$): δ (ppm) = −70.50 (d, *J* = 711 Hz, PF_6^-).

8,12-dipropyl-8,12-diaza-4-oxa triangulenium hexaflurophosphate (**$^{n\text{Pr}}$DAOTAPF$_6$**)[2]



$^{n\text{Pr}}$DMQAPF$_6$ **$^{n\text{Pr}}$DAOTAPF$_6$**

Pyr•HCl (10 g) was heated at 200 °C for 1.5 h to drive off excess moisture. $^{n\text{Pr}}$DMQAPF$_6$ (0.2880 g, 0.5157 mmol) was dissolved in pyridine (5 mL) and added to the molten pyr•HCl. The reaction mixture was heated at 200 °C for 1 h 20 min, which was associated with a color change from dark green to deep magenta. After 1 h 20 min the melt was cooled to ambient temperatures and diluted with H_2O (20 mL), before KPF_6 (0.2 M, 100 mL) was added under stirring. The suspension was stirred at rt for 1 h, filtered, and the solid was washed with H_2O (2 × 50 mL) and Et_2O (20 mL). The solid was dissolved in CH_2Cl_2:MeCN (1:1 v/v, 10 mL) and poured into Et_2O (200 mL) under stirring. The suspension was stirred at rt for 20 min, filtered, and the solid was washed with Et_2O (20 mL). The solid was taken up in CH_2Cl_2 (50 mL), and the solution was washed with H_2O (50 mL) and HCl (0.3 M, 2 × 50 mL) to remove excess pyr•HCl. The organic phase was dried ($MgSO_4$), and the solvent was evaporated in vacuo. The resulting magenta solid was dried in vacuo overnight to yield **$^{n\text{Pr}}$DAOTAPF$_6$** (0.2170 g, 0.4234 mmol, 82%).

^{1}H-NMR (500 MHz, DMSO-*d*$_6$): δ (ppm) = 8.28 (t, *J* = 8.6 Hz, 1H, Ar*H*), 8.14 (t, *J* = 8.5 Hz, 2H, Ar*H*), 7.78 (d, *J* = 8.9 Hz, 2H, Ar*H*), 7.65 (d, *J* = 8.6 Hz, 2H, Ar*H*), 7.42 (d, *J* = 8.1 Hz, 2H, Ar*H*), 4.57 (t, *J* = 8.1 Hz, 4H, NC*H*$_2$), 1.87 (h, *J* = 7.4 Hz, 4H, C*H*$_2$), 1.13 (t, *J* = 7.3 Hz, 6H, C*H*$_3$).

^{13}C-NMR (126 MHz, DMSO-*d*$_6$): δ (ppm) = 151.7 (−), 140.2 (−), 139.5 (+), 139.1 (−) 138.9 (−), 138.4 (+), 110.9 (−), 109.4 (+), 108.1 (+), 106.9 (−), 105.6 (+), 48.4 (−), 18.8 (−), 10.6 (+).

^{19}F-NMR (471 MHz, DMSO-*d*$_6$): δ (ppm) = −70.15 (d, *J* = 712 Hz, PF_6^-).

III. Electrochemical Investigations

General methods and materials:

Electrochemical analyses were conducted inside an Argon-filled MBraun Unilab glovebox using a BioLogic SP-200 potentiostat/galvanostat and the EC-Lab® software (v11.33) from BioLogic Science Instruments. For convenience, potentials are expressed versus the internal reference electrode AgNO3/Ag or versus the cell itself in 2 electrode set-up.

Cyclic voltammetry:

Cyclic voltammograms (CV) were measured in a three-electrode electrochemical cell, consisting of a platinum wire counter electrode (Ec), a AgNO3/Ag reference electrode (Eref, 0.01 M AgNO3 in 0.1 M TBAPF6 in CH3CN), and a glassy carbon working electrode (Ew, 0.071 cm², CH Instrument, Inc.). The working electrode was polished prior to each record using aluminium oxide on polishing paper and anhydrous CH_3CN to remove residual particles. CVs were recorded at different scan rates (10, 25, 75, 100, 250, 400, and 500 mV/s) in an CH_3CN electrolyte containing 1 mM $^{n\text{Pr}}$**DAOTAPF$_6$** (**C$^+$**) and 0.1M $TBAPF_6$.

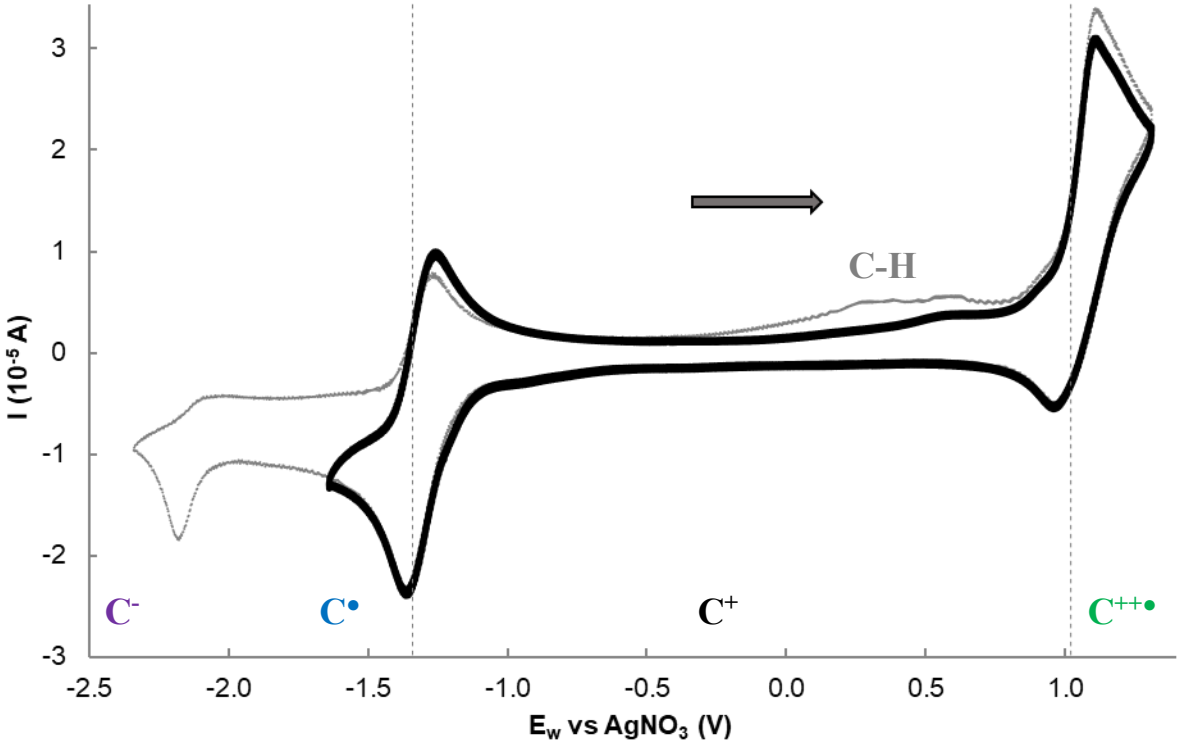


Figure S1. Cyclic voltammogram of **C$^+$** 1 mM in 0.1M $TBAPF_6$ CH_3CN. Recorded at a scan rate of 100 mV/s. Reversible process are indicated by grey dotted lines.

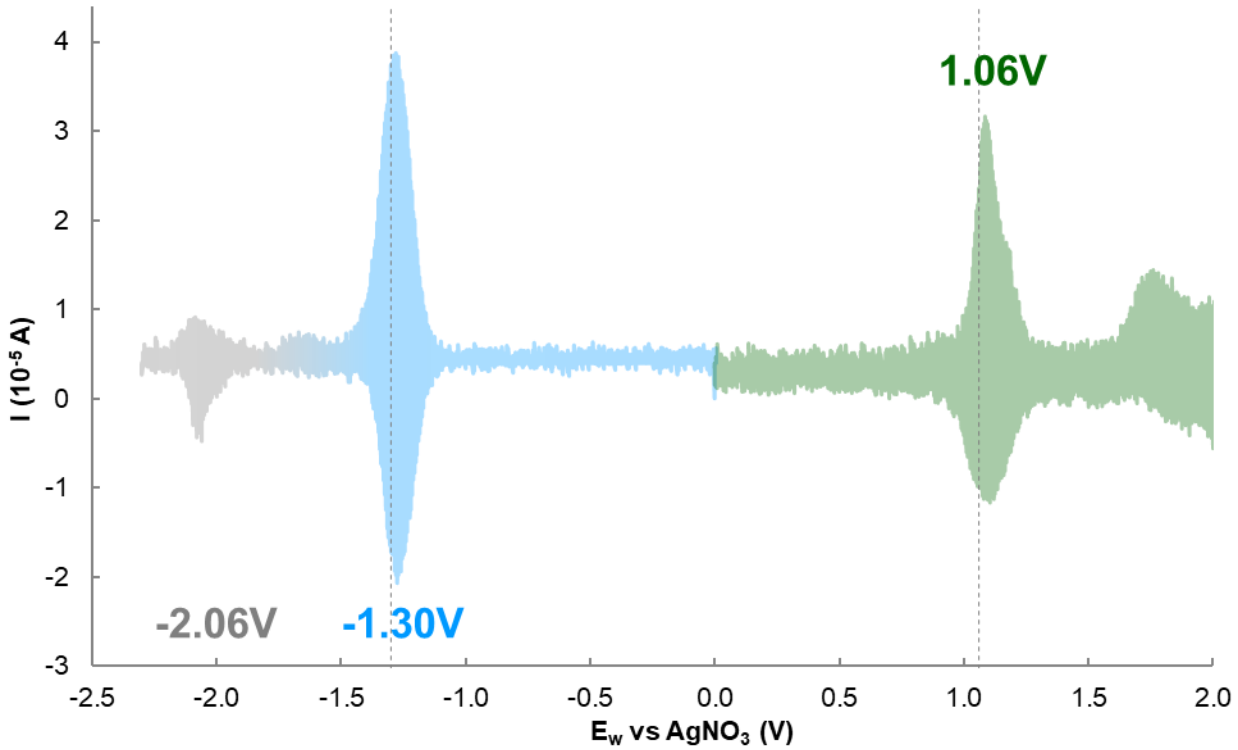


Figure S2. Differential pulse voltammetry (DPV) of $\mathbf{C}^+$ 1 mM in 0.1M $TBAPF_6$ CH_3CN.

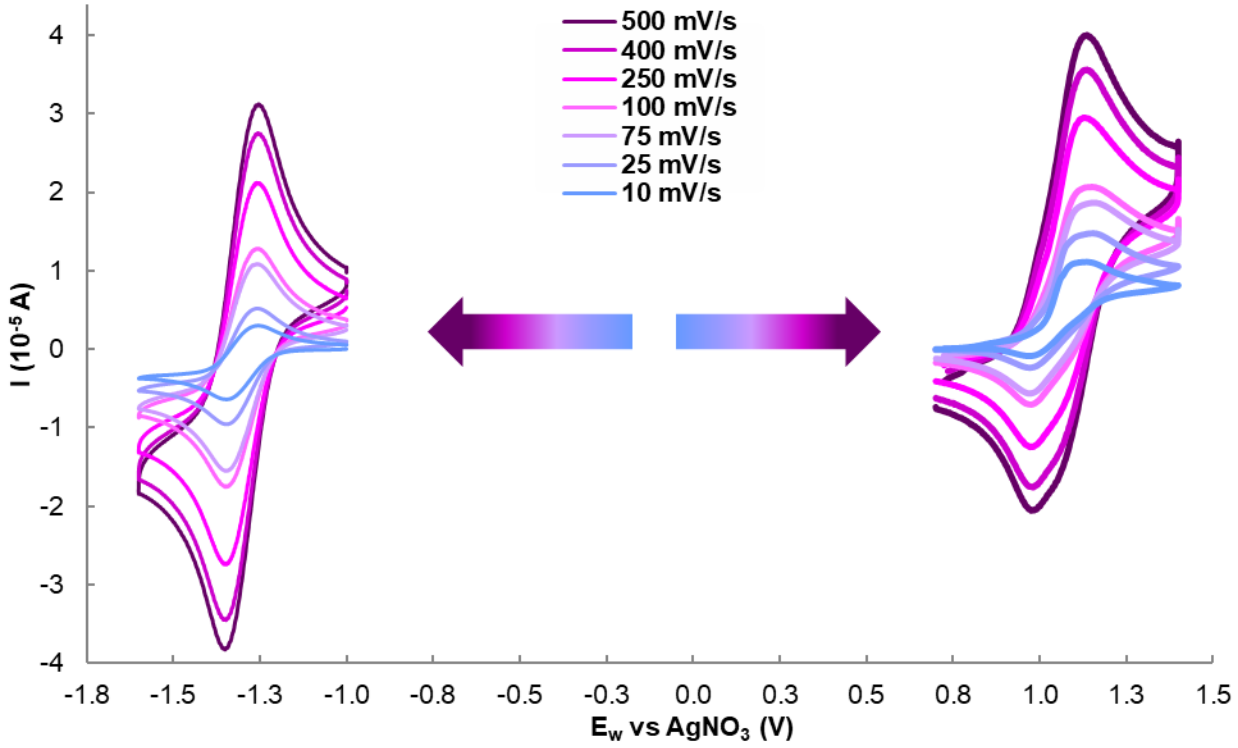


Figure S3. Cyclic voltammogram of reversible electronic process of $\mathbf{C}^+$ 1 mM in 0.1M $TBAPF_6$ CH_3CN at different scan rates.

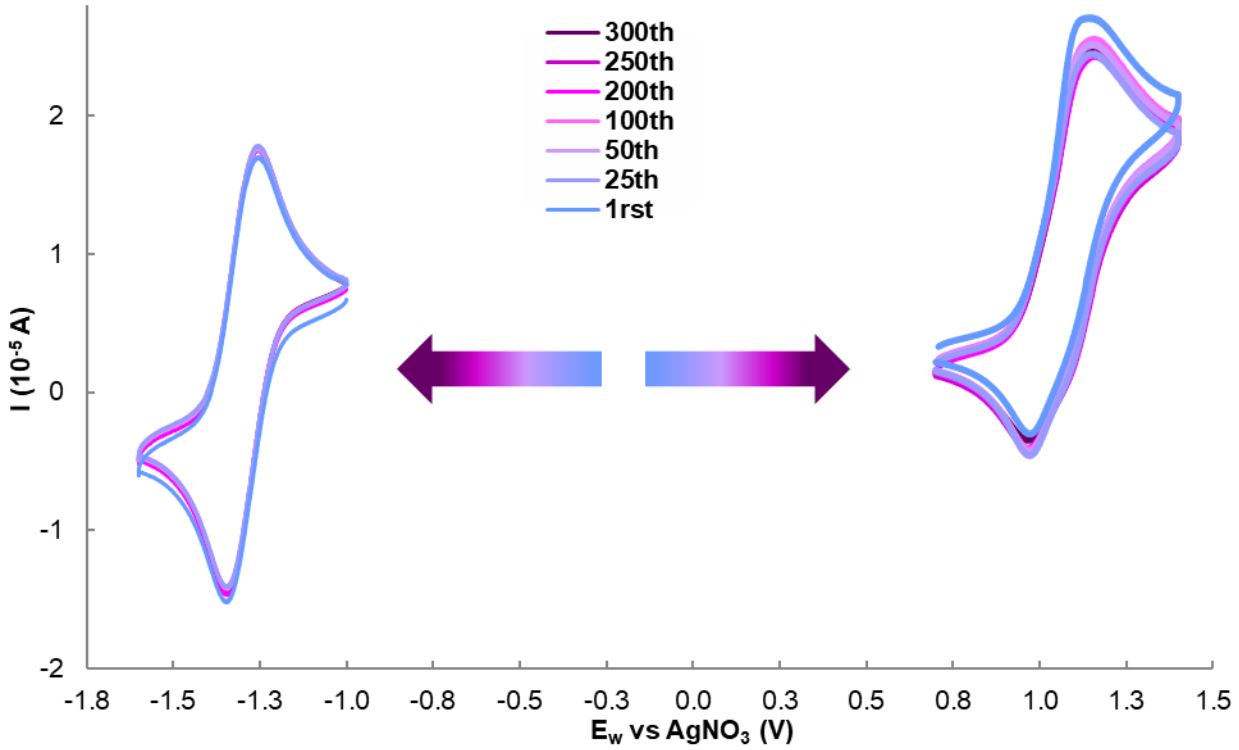


Figure S4. 300 continuous cyclic voltammogram of reversible electronic process of $\mathbf{C}^{+}$ 1 mM in 0.1M $TBAPF_6$ CH_3CN at 100 mV/s.

Table S2. Values used to determine kinetics parameters D and k0.

In 0.1M $TBAPF_6$ $DAOTA^{+}$	**1 mM**
e^- transferred (n)	1
A (cm^2)	0.0707
C (mol/cm^3)	1×10^{-6}
T (K)	298

Table S3. Current values (I) and recorded for processes at -1.30 V and 1.06 V at different scan rates ν for of C^+ 1 mM in 0.1M $TBAPF_6$ CH_3CN.

	-1.30 V		1.06 V	
v (V/s)	**I_{min} (A)**	**I_{max} (A)**	**I_{min} (A)**	**I_{max} (A)**
0.010	-6.38E-06	3.02E-06	-8.50E-07	1.11E-05
0.025	-9.55E-06	5.20E-06	-2.34E-06	1.48E-05
0.075	-1.55E-05	1.09E-05	-5.62E-06	1.87E-05
0.100	-1.75E-05	1.29E-05	-7.04E-06	2.07E-05
0.250	-2.74E-05	2.12E-05	-1.24E-05	2.95E-05
0.400	-3.45E-05	2.76E-05	-1.76E-05	3.57E-05
0.500	-3.83E-05	3.13E-05	-2.06E-05	4.01E-05

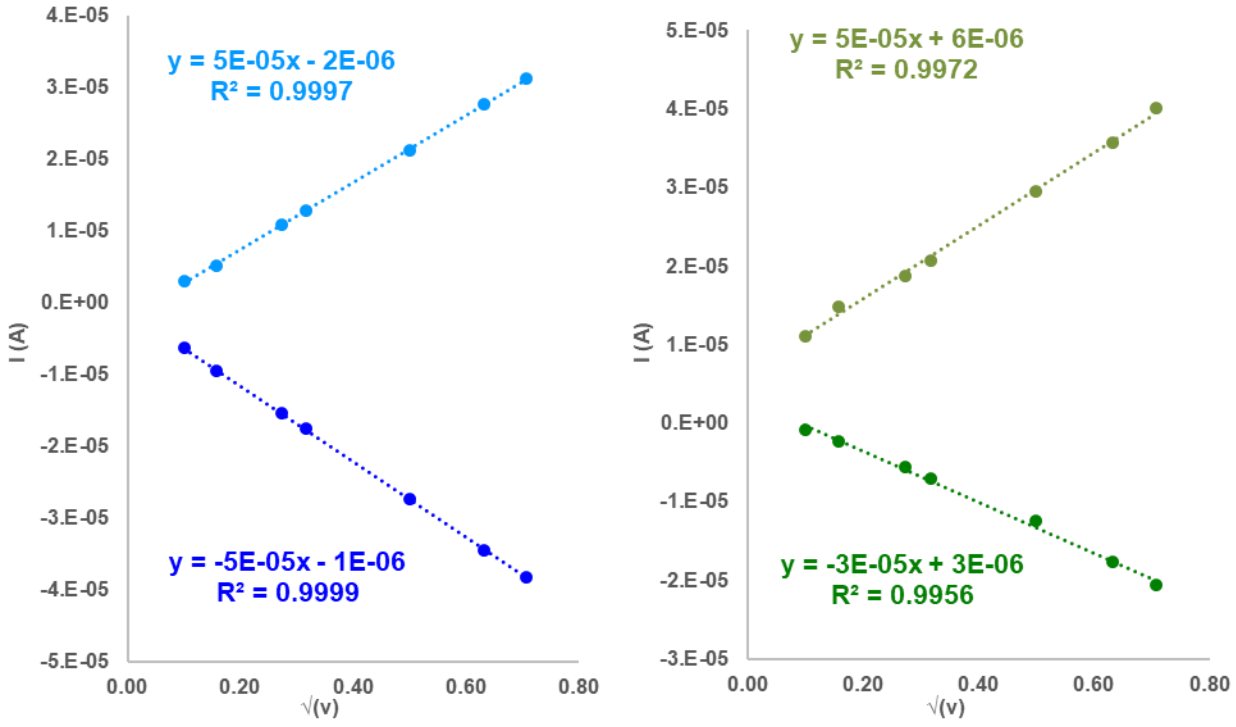


Figure S5. Peak current (I) *vs* square root of scan rate (ν) and linear fits for electronic processes at -1.30 V (blue) and 1.06 V (green) of **C^+** 1 mM in 0.1M $TBAPF_6$ CH_3CN.

$$i_p = 0.4463nFAC\sqrt{\frac{nF\nu D}{RT}} \qquad (1)$$

Equation S1. Randles-Sevcik equation, with i_p the peak current in Amperes, n equals the number of electrons transferred, F equals Faraday's constant, A is the area of the electrode in cm², C the concentration of redox active species in mol cm^{-3}, D the diffusion coefficient in cm² s^{-1}, v the scan rate in V s^{-1}, R the ideal gas constant, and T the temperature in Kelvin.

$$\psi = \frac{(-0.6288+0.0021\Delta E_p)}{(1-0.017\Delta E_p)} \qquad (2)$$

$$\psi = \frac{k^0}{\sqrt{\frac{\pi D n F \nu}{RT}}} \qquad (3)$$

Where: $\Delta E_p = (E_p^{max} - E_p^{min})$

Equation S2-S3. Nicholson's method[3] and the more recent work of reported by Lavagnini et al.[4] were used to determine the electron transfer rate constant (k^0) by relating it with the dimensionless kinetic parameter (Ψ). With n the number of electrons transferred, F equals Faraday's constant, v the scan rate, R the ideal gas constant and T the temperature in Kelvin. D diffusion coefficient at the corresponding scan rate.

Table S4. Diffusion coefficients D and electron transfer rate constant k^0 at $E_{1/2}^{Red}$ and $E_{1/2}^{Ox}$ of $\mathbf{C}^+$ 1 mM in 0.1M $TBAPF_6$ CH_3CN.

$E_{1/2}^{Red1}$	$E_{1/2}^{Ox1}$
V vs $AgNO_3$/Ag	
-1.30 V	1.06 V
D (cm²/s)	
6.90×10^{-6}	8.77×10^{-6}
k^0 (cm/s)	
8.59×10^{-3}	1.75×10^{-3}

IV. UV-Visible spectrometry and Energy Density

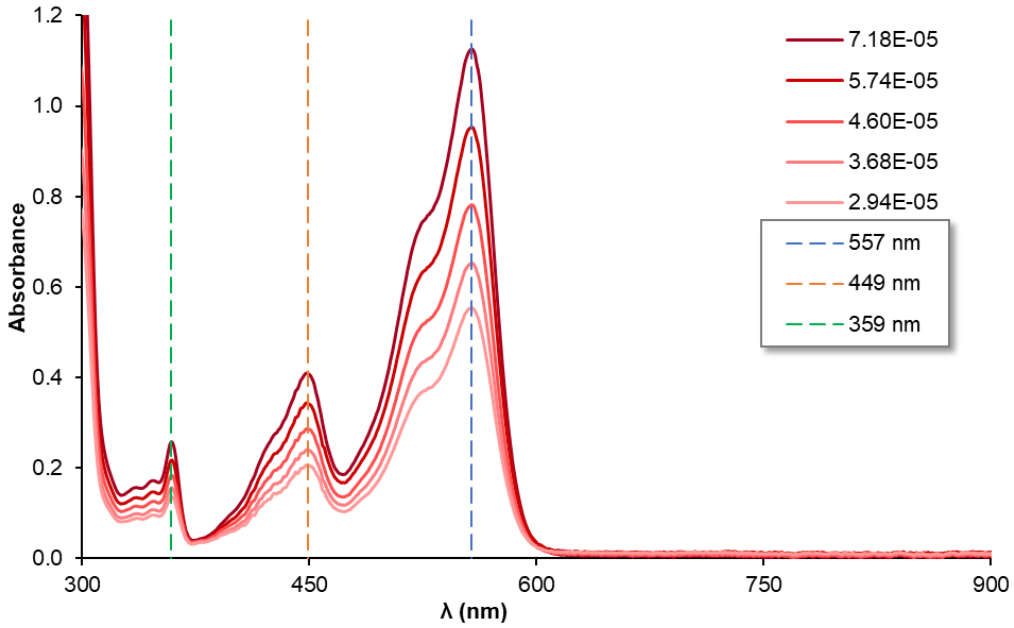


Figure S6. UV-Visible absorption spectrum of $\mathbf{C}^+$ in CH_3CN at 298K at various concentrations (mol/L).

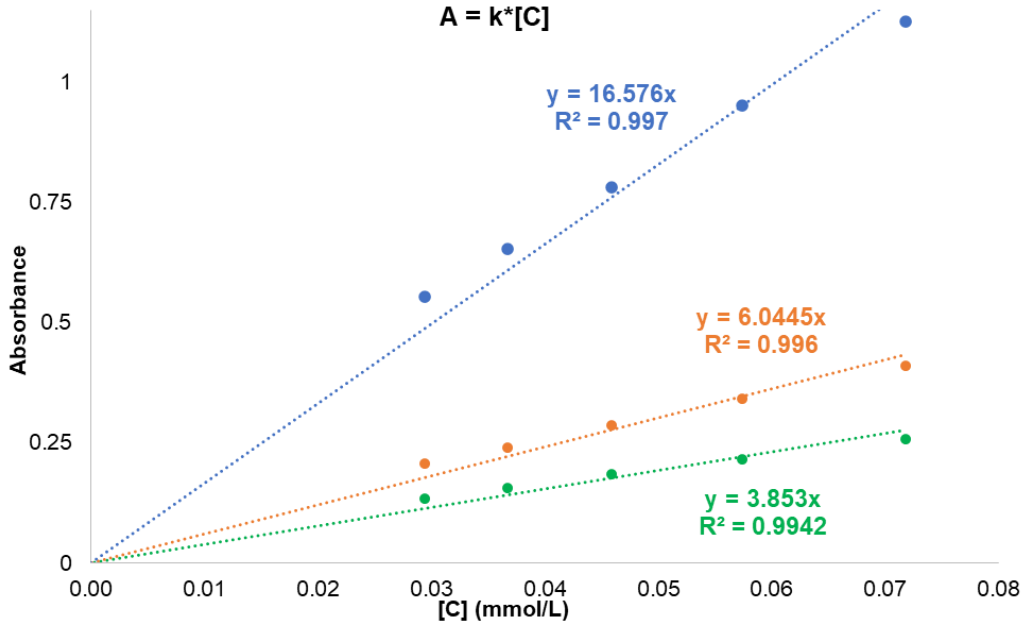


Figure S7. UV-Visible calibration curve of $\mathbf{C}^+$ in CH_3CN at λ_{max} values of 359, 449 and 557 nm.

Table S5. Numerical application to determine $C_{saturation}$ and Energy density for $\mathbf{C}^+$ in CH_3CN.

$C_{saturated}$ diluted 1250x (mM)	$C_{saturated}$ diluted 1563x (mM)	$C_{saturated}$ diluted 1953x (mM)	**C_{max} Average (mM)**	**Energy Density ($Wh.L^{-1}$)**
95	104	109	**103**	**6.51**

V. Computational Details

Density functional theory (DFT)[5] calculations were carried out using a long-range corrected Perdew–Burke–Ernzerhof (LC-wPBE) functional[6] with a 6-311G** basis set applied to all atoms. Initial structures were built using Spartan Student v8.0.3[7] and optimized using Gaussian 16[8]. The optimized structures were determined to be energy minima by lack of imaginary vibrations in the frequency calculations. Solvated models were calculated with the polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM) as the SCRF method. Acetonitrile was used as the solvent and as defined by G16. Free energies of solvation (ΔG_{solv}) (**Table**) were determined as the difference in the sum of electronic and thermal free energies between the solvated and gas phase optimized structures.

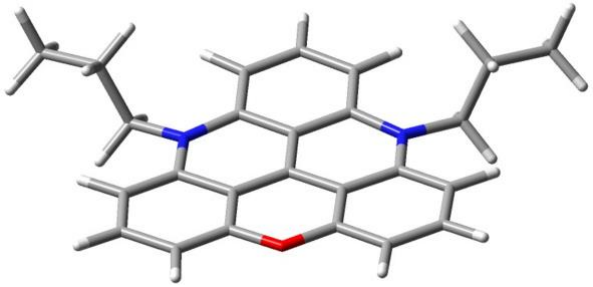
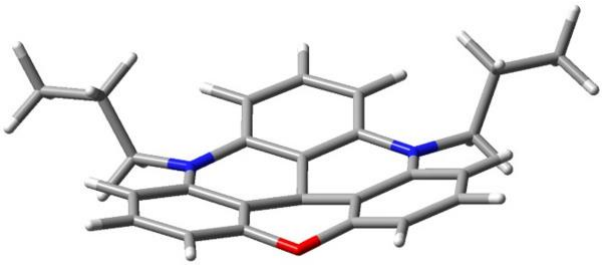
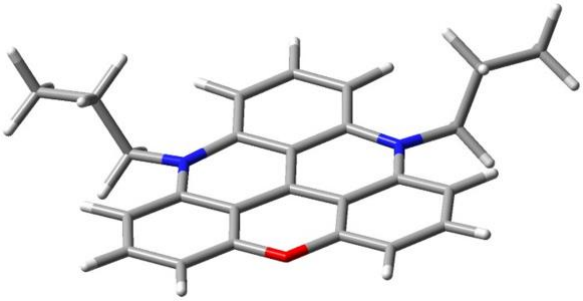
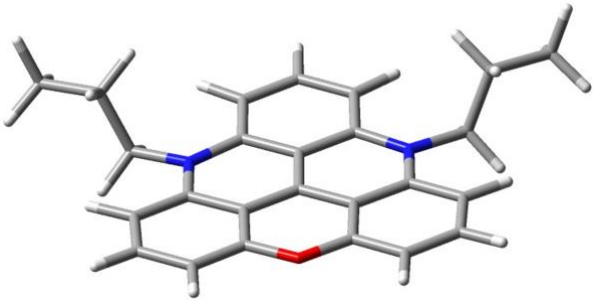
Table S6. Table of ΔG_{solv} in kcal/mol for different oxidation states of **[$^{n\text{Pr}}$DAOTA]**

Oxidation state	ΔG_{solv} (kcal/mol)
$C^{\bullet}$	-6.2
C^{+}	-34.4
$C^{\bullet+++}$	-131.1
$C^{+}(PF_6)$	-26.2
$C^{\bullet+++}(PF_6)_2$	-46.7
C^{-}	-46.6
$C^{-\bullet\bullet}$	-47.3
Side Product	
C-H	-6.2

Table S7. Energies of different redox states and C-H. The energy difference between the triplet and singlet states ($E_{C-\bullet\bullet} - E_{C-}$) is also provided.

Oxidation State	Gas Phase Energies (kcal/mol)	Solvated Phase Energies (kcal/mol)
$C^{\bullet}$	-722073	-722078
C^{+}	-721961	-722013
$C^{\bullet+++}$	-721720	-721851
$C^{+}(PF_6)$	-1312154	-1312178
$C^{\bullet+++}(PF_6)_2$	-1902178	-1902223
C^{-}	-722082	-722129
$C^{-\bullet\bullet}$	-722054	-722101
C-H	-722456	-722462
$E_{C-\bullet\bullet} - E_{C-}$	27.88	28.25

Table S8. Optimized structures for the five potential redox states $\mathbf{C}^{-\bullet\bullet}$, $\mathbf{C}^{-}$,$\mathbf{C}^{\bullet}$, $\mathbf{C}^{+}$, and $\mathbf{C}^{+\bullet\bullet}$. Structures shown are for optimization of solvated phase in CH_3CN but negligible differences were observed in gas phase optimized structures.

Model	Optimized Structure
$\mathbf{C}^{-\bullet\bullet}$	
$\mathbf{C}^{-}$	
$\mathbf{C}^{\bullet}$	
$\mathbf{C}^{+}$	

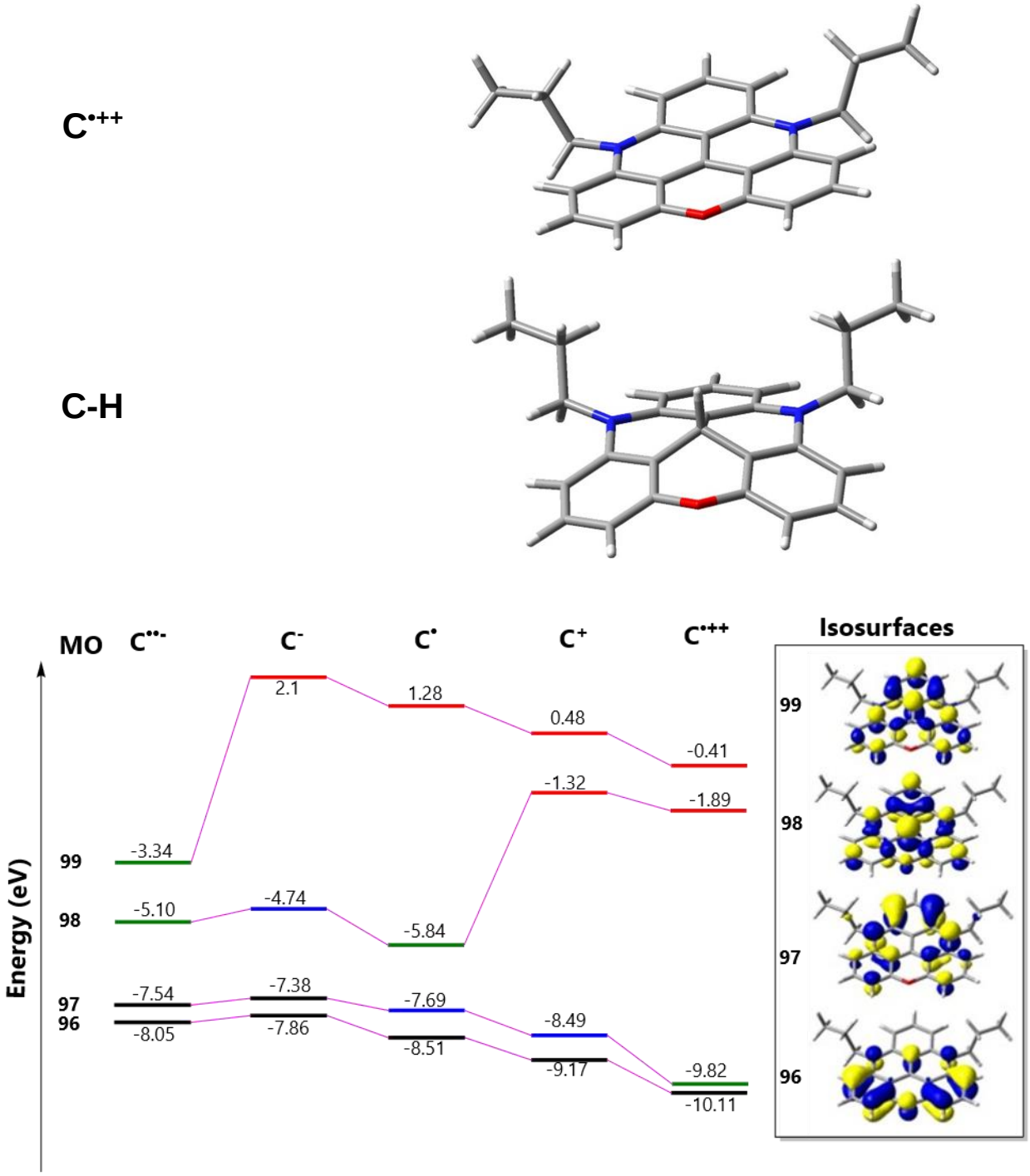


Figure S8. Comparison of frontier molecular orbital (MO) isosurfaces and energies for solvated phase (in CH_3CN) $\mathbf{C}^{-\bullet\bullet}$ $\mathbf{C}^{-}$,$\mathbf{C}^{\bullet}$, $\mathbf{C}^{+}$, and $\mathbf{C}^{+\bullet+}$ models. MOs shown are for $\mathbf{C}^{+}$ though negligible differences were observed for the other redox states. Isosurfaces were plotted at a 0.04 value. MO energy levels correspond to alpha electrons and color representations are as follows: black are core MOs, blue are HOMOs, green are SOMOs, and red are unoccupied orbitals.

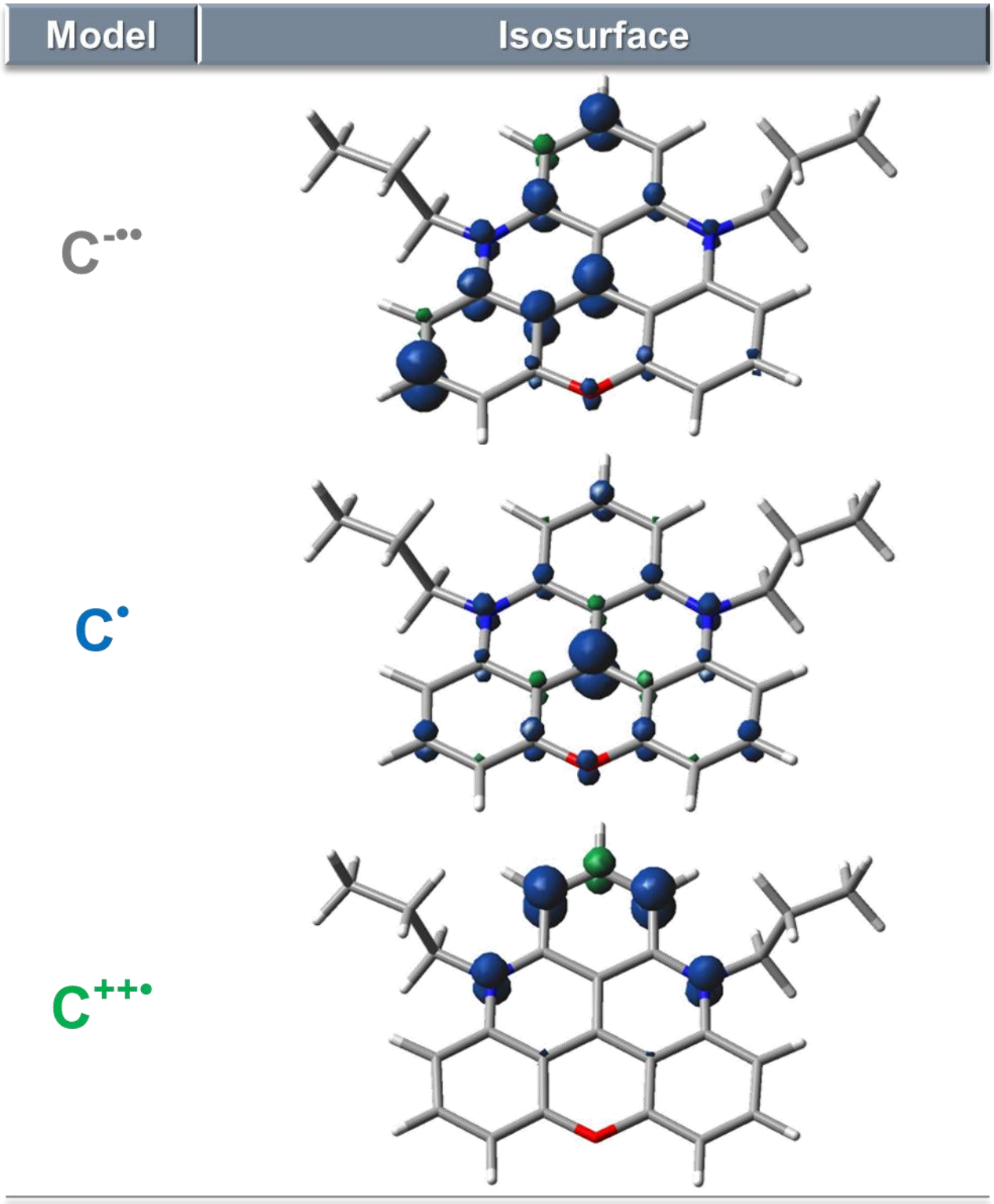


Figure S9. SCRF spin density plots for $\mathbf{C}^{-\bullet}$, $\mathbf{C}^{\bullet}$ and $\mathbf{C}^{+\bullet}$ models. Isosurfaces were plotted at a 0.015 value. Closed-shell state of $\mathbf{C}^{-}$ and $\mathbf{C}^{+}$ arenot shown due to lack of unpaired electrons.

VI. Galvanostatic Cycling

Redox Flow Cell Measurement:

Flow cell measurements were carried out on a BioLogic SP-200 (galvanostatic mode) and the EC-Lab® software (v11.33) (BioLogic Science Instruments) in an Argon-filled MBraun Unilab glovebox. A 5 cm^2 single-cell flow battery (Fuel Cell Technologies Inc., see figure below) was utilized with the acid cell configuration, allowing the tubing to feed directly into the flow plate with no contact with the metallic frame. The cell comes from the supplier with aluminum end plates, electrically insulated from the gold plate current collector (CC), which is in contact with a graphite bipolar plate (BPP) with an engraved serpentine flow path that will guide the liquid electrolyte. A PTFE gasket (TG) with a cutout corresponding to the exchange surface of 5 cm^2 hosts the carbon felt electrodes (2x electrode) which are in direct contact with the exchange membrane (EM). this succession of 5 elements is repeated in reverse order on the other side of the EM to complete the assembly of the cell. Daramic-175 porous separators were purchased from Daramic LLC (Owensboro, KY). and used as exchange membrane betweem the anolyte and catholyte. ePTFE gaskets (Compressible ePTFE Plastic Sheet - 1/64" Thick, USA Sealing Inc.) were used in the flow cell to avoid leakage of liquid. Commercial carbon felt electrodes (Sigracet® 29AA, from SGL Carbon) and commercial separator were ultra-sonically cleaned with isopropanol and dried under vacuum prior to use. All components of the flow cell were dried in an oven overnight, assembled outside of the glovebox, and immediately brought into the glovebox through an antechamber via a 5-hour evacuation/argon backfill process. The assembled flow cell was allowed to equilibrate in the glovebox for 12 hours prior to use. If require, even more detailed assembly is available in the Supporting Information of the work of Marshak and coworkers.[9]

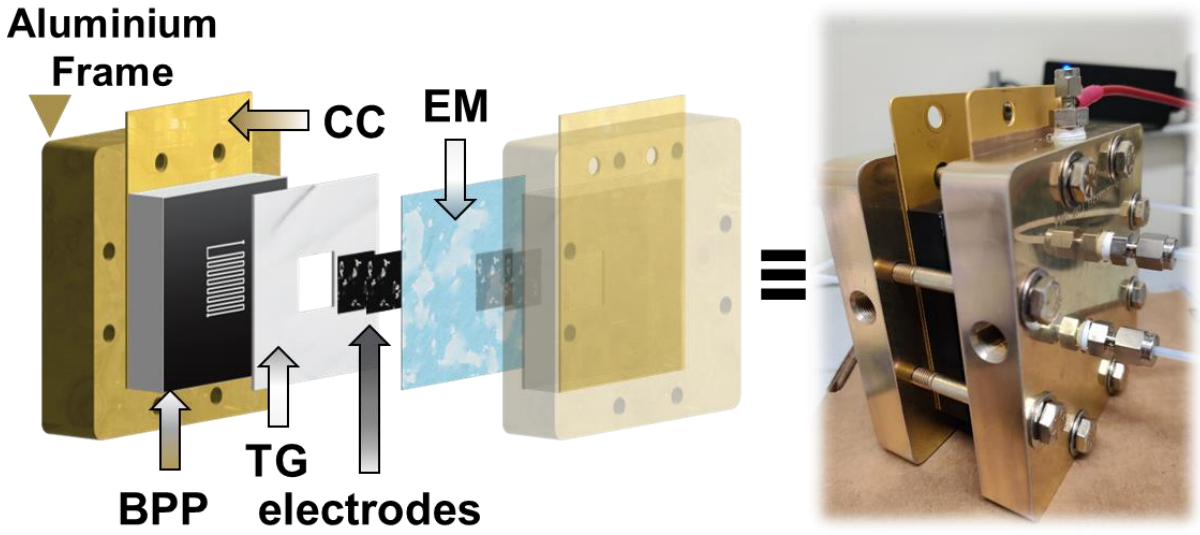


Figure S10. Left: scheme of the open RFB cell used with the gold plate current collector (CC), graphite bipolar plate (BPP), teflon gasket (TG), the carbon felt electrodes (electrodes) and the exchange membrane (EM). Right: picture of the actual cell assembled.

Both anolyte and catholyte tank were loaded with 4 mL of electrolyte/ROM in 0.1 M $TBAPF_6$ in CH_3CN at the desired **DAOTA**$^+$ concentration. The electrolytes solutions were pumped into and out from the flow cell using Masterflex® L/S® Digital Miniflex® Dual Channel peristaltic pump (Masterflex®) at a rate of 16 $mL.min^{-1}$. An equilibration period of 4 h was used before active charging and discharging, during which

the working solutions were flowed through the cell. The experiment involved conducting Potentiostatic Electrochemical Impedance Spectroscopy (PEIS) measurements at 0% state of charge (SOC) both before and after cycling, ranging from 1 GHz to 100 mHz, using a 10 mV sine perturbation. Energy efficiencies (EE) were calculated by dividing the time-integrated output power density by the input power density during both the discharging and charging phases over each cycle. The Voltage Efficiency (VE) was then obtained by dividing EE by CE.

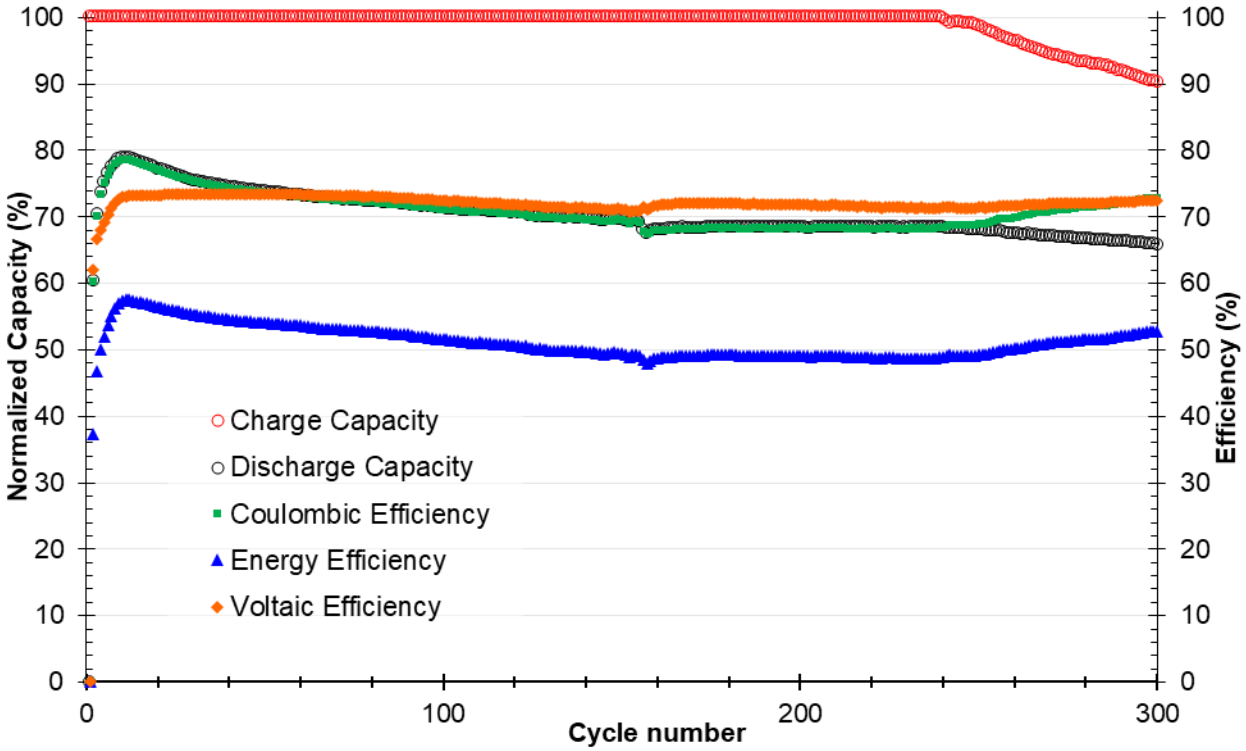


Figure S11. Flow cycling data showing Charge and Discharge capacities and Coulombic, Energy and Voltaic Efficiencies, each data point represents 1 cycle. Both cell reservoirs were charged with 4 mL of 1 mM $\mathbf{C}^{+}$ in 0.1 M $TBAPF_6/CH_3CN$. Charging and discharging were performed at a C-rate of 2 with voltage cutoff of ± 200 mV from the E_{cell} of 2.36 V. The 300 cycles cover a time of approximately 9.5 days.

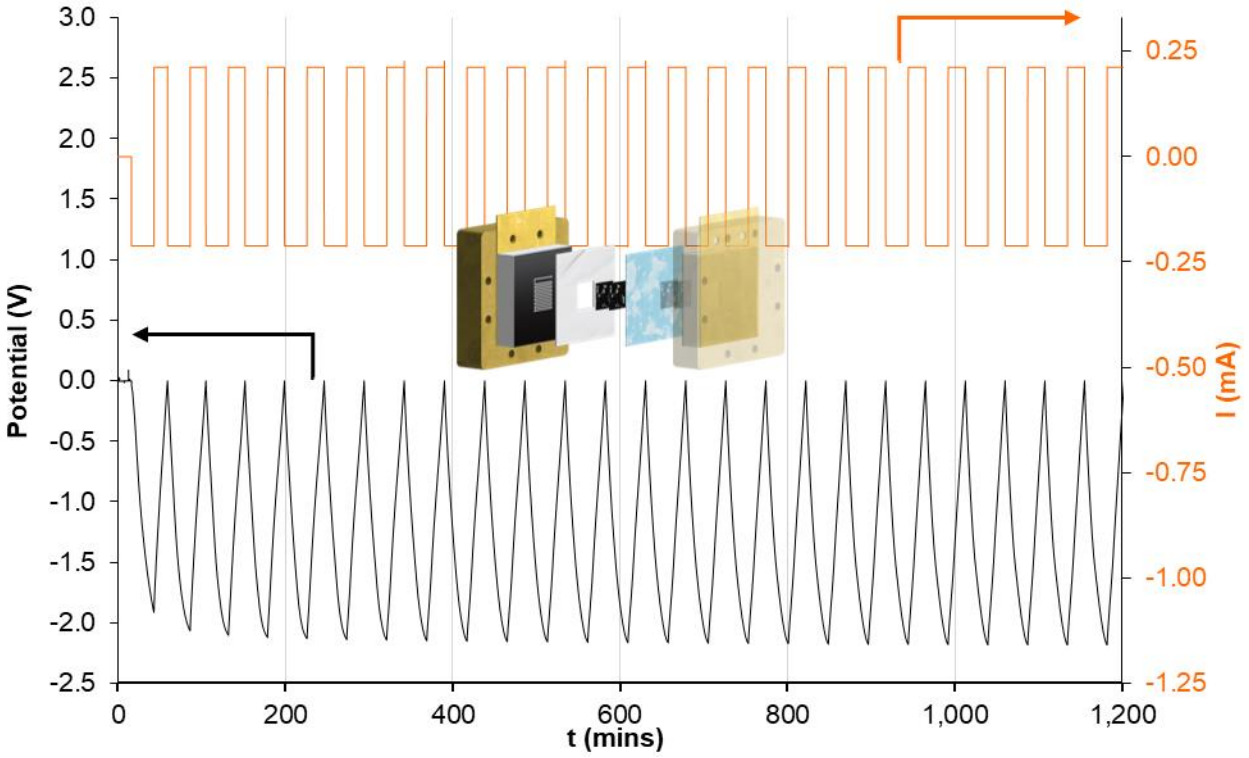


Figure S12. Plot of E_{we} potential and current (I) at over 25 cycles for the 1 mM $\mathbf{C}^{+}$ in 0.1 M $TBAPF_6/CH_3CN$ solution during the first 25 cycles.

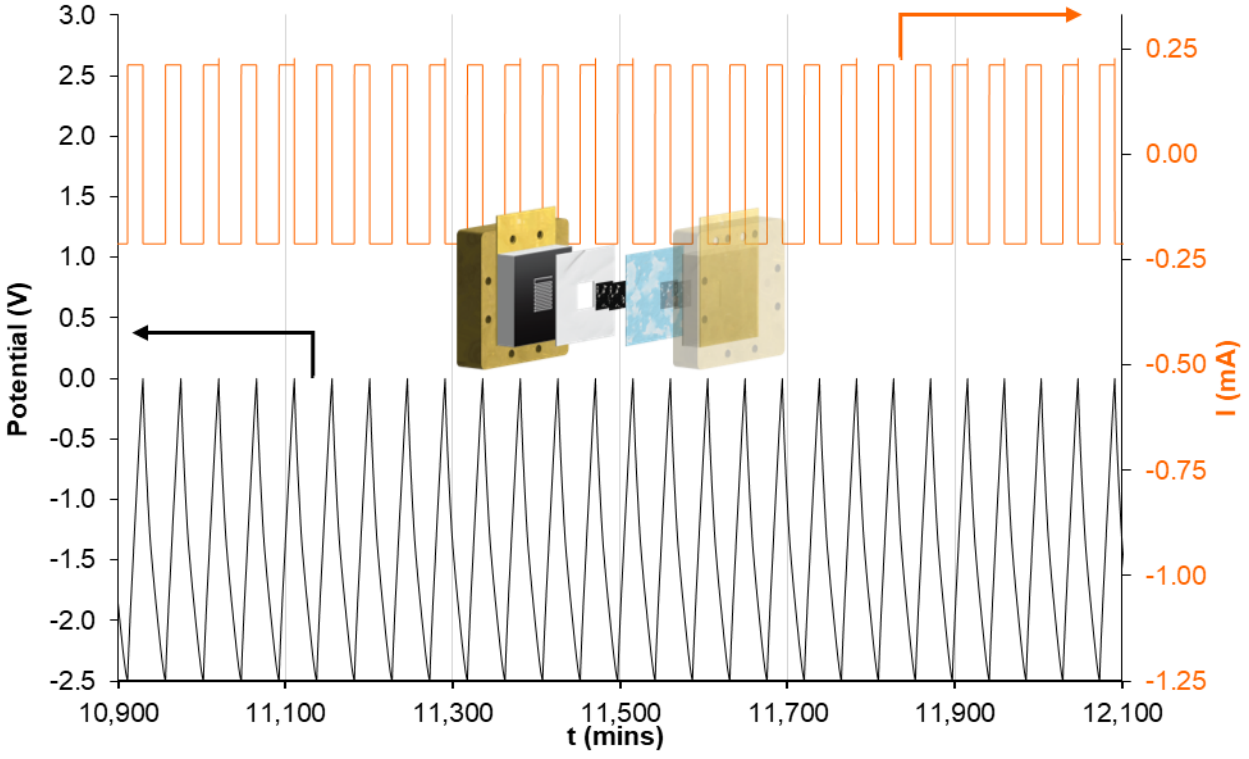


Figure S13. Plot of E_{we} potential and current (I) at over 25 cycles for the 1 mM $\mathbf{C}^{+}$ in 0.1 M $TBAPF_6/CH_3CN$ solution from the 235th to 260th cycle.

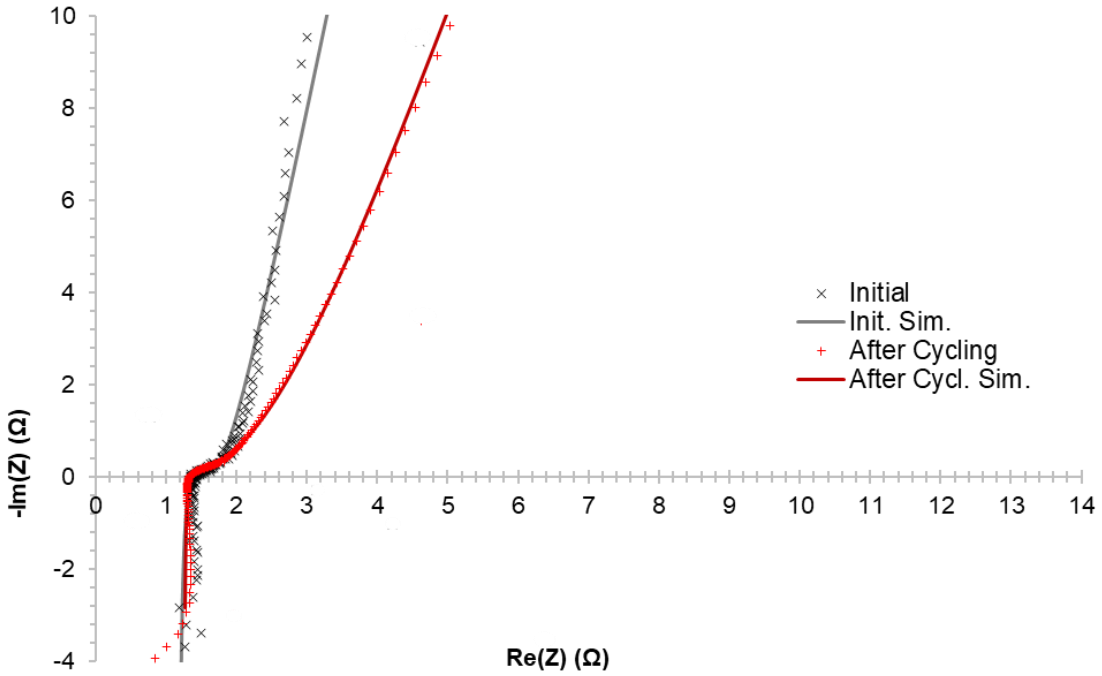


Figure S14. Potential electrochemical impedance spectroscopy (PEIS) from 1Ghz to 0.1Hz with an amplitude of 10mV before and after cycling (at 0% SOC) as Nyquist plot and fit of the flow cell 1 mM $\mathbf{C}^+$ in 0.1 M $TBAPF_6/CH_3CN$. The first intercept with the Z'-axis represents the ohmic resistance originating from cables, membrane, and solution (initial 1.40 Ω; after cycling 1.34 Ω).

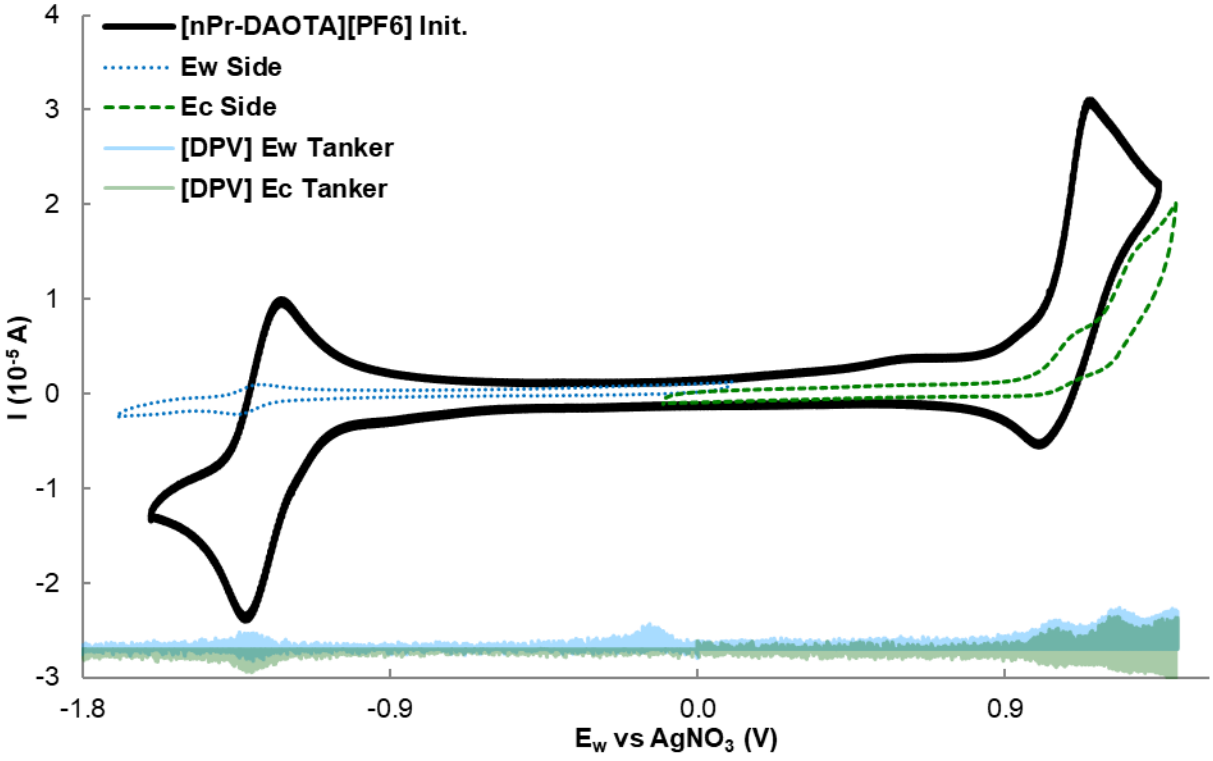


Figure S15. Cyclic voltammograms and DPV (in pastel) of the tank's solution at E_{we} and E_c after 300 cycles and comparison with initial $\mathbf{C}^+$ Cyclic voltammogram.

VII. Scanning Electron Microscope

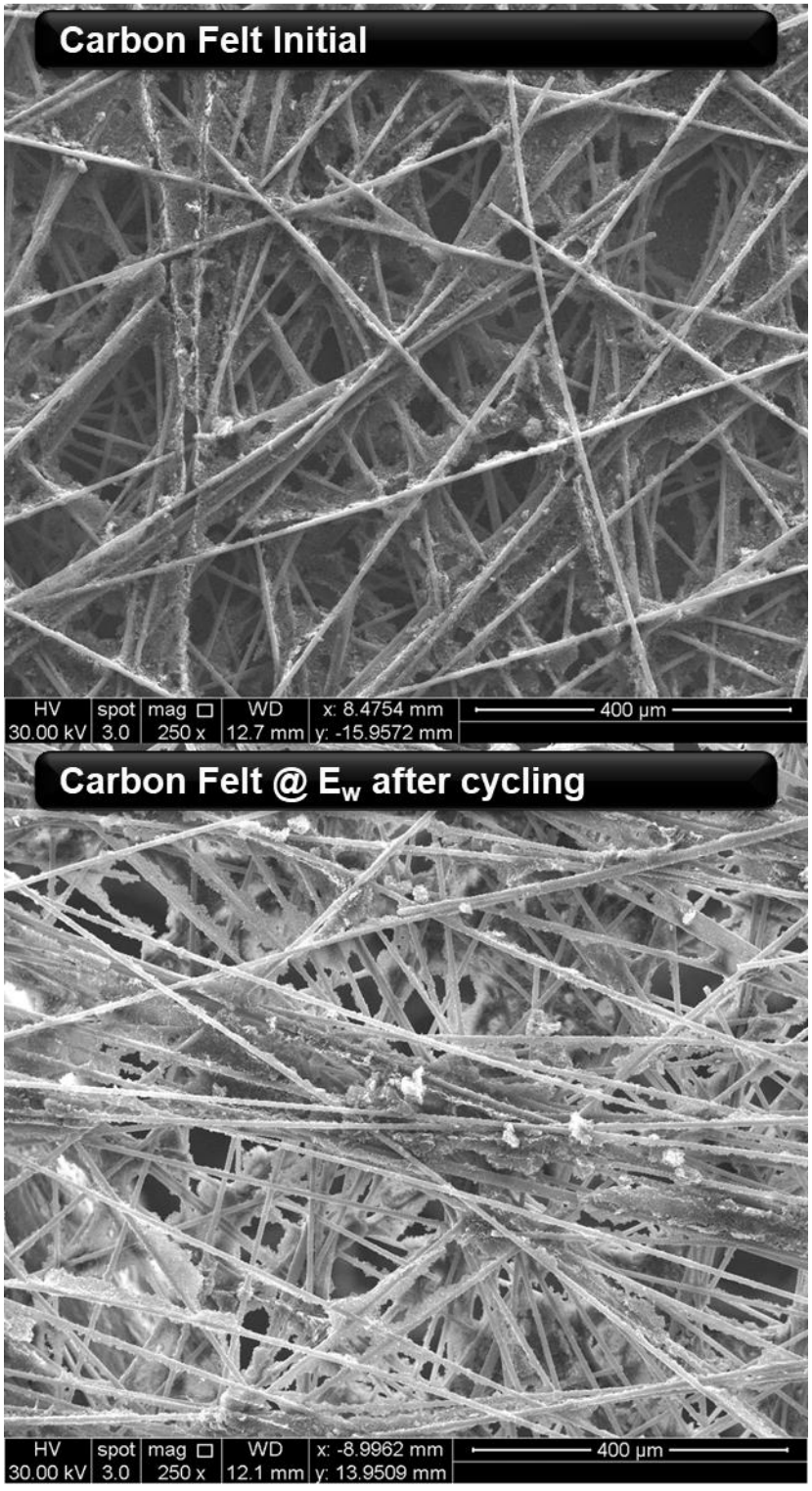


Figure S16. SEM pictures of the E_w carbon felt electrodes before and after cycling, magnification x250.

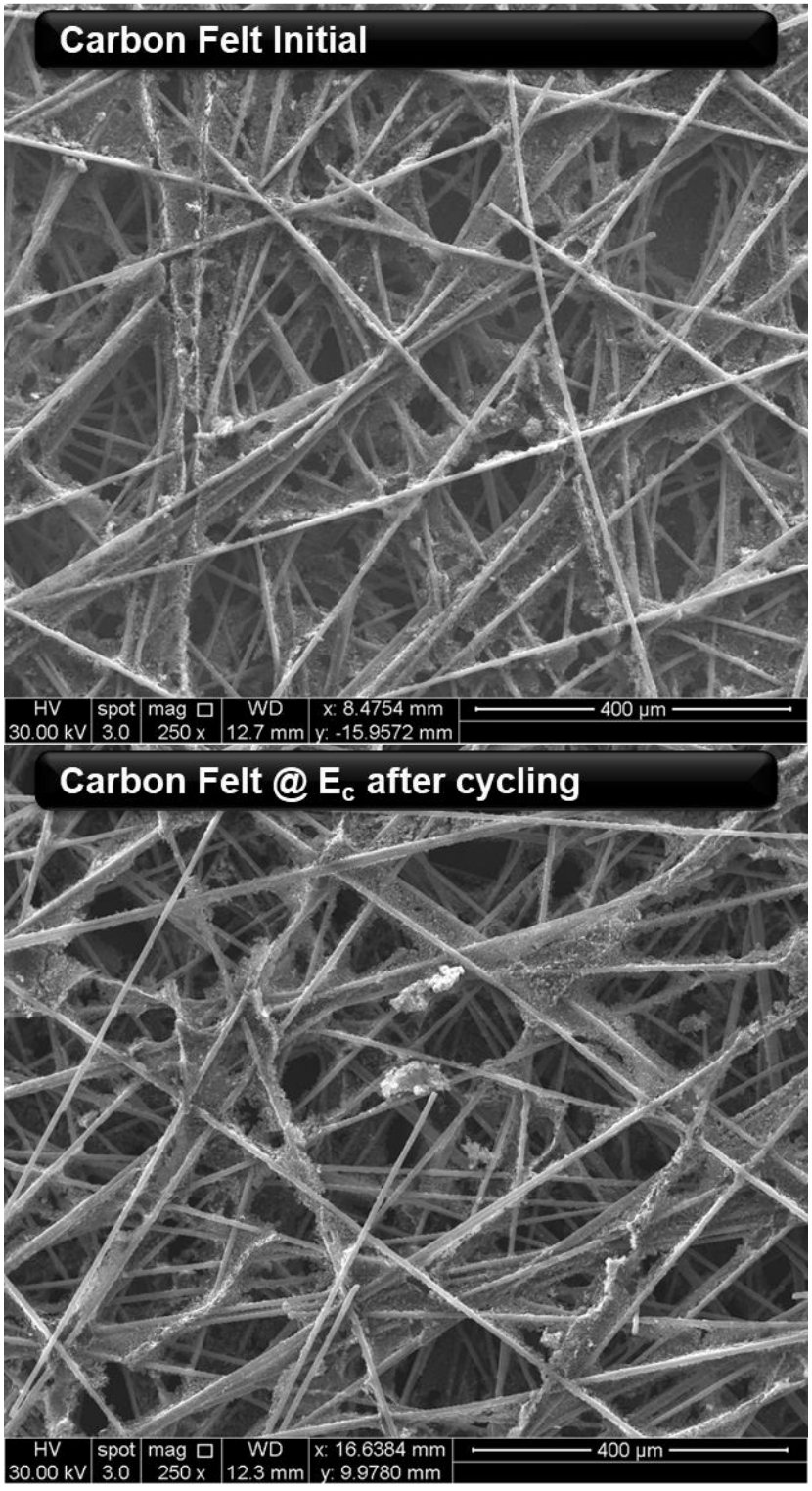


Figure S17. SEM pictures of the E_c carbon felt electrodes before and after cycling, magnification x250.

VIII. References

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IX. Copies of Spectrum

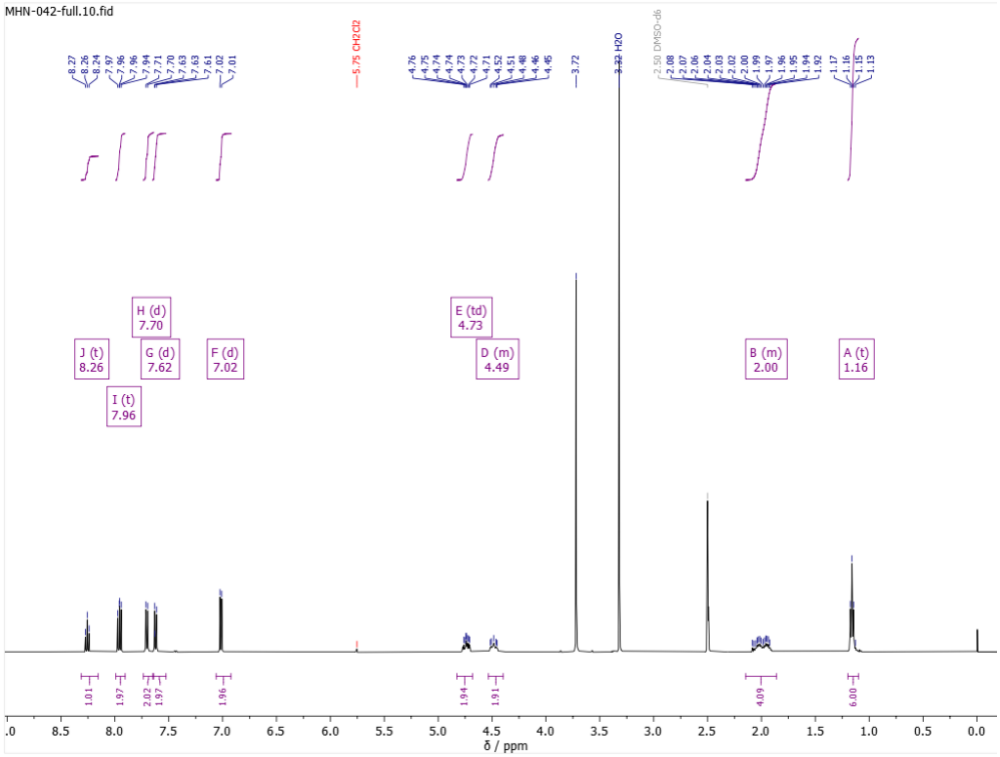

Figure S18. 1H-NMR spectrum (500 MHz, DMSO-d6) of $^{n\text{Pr}}$DMQAPF$_6$.

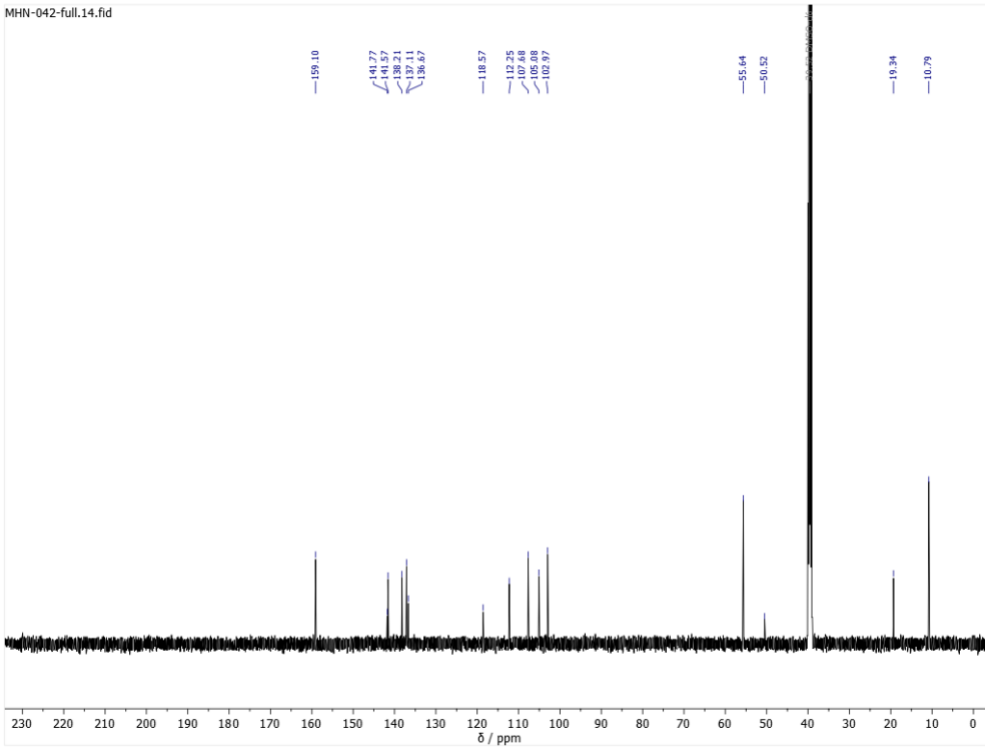

Figure S19. ^{13}C-NMR spectrum (126 MHz, DMSO-d_6) of $^{n\text{Pr}}$DMQAPF$_6$.

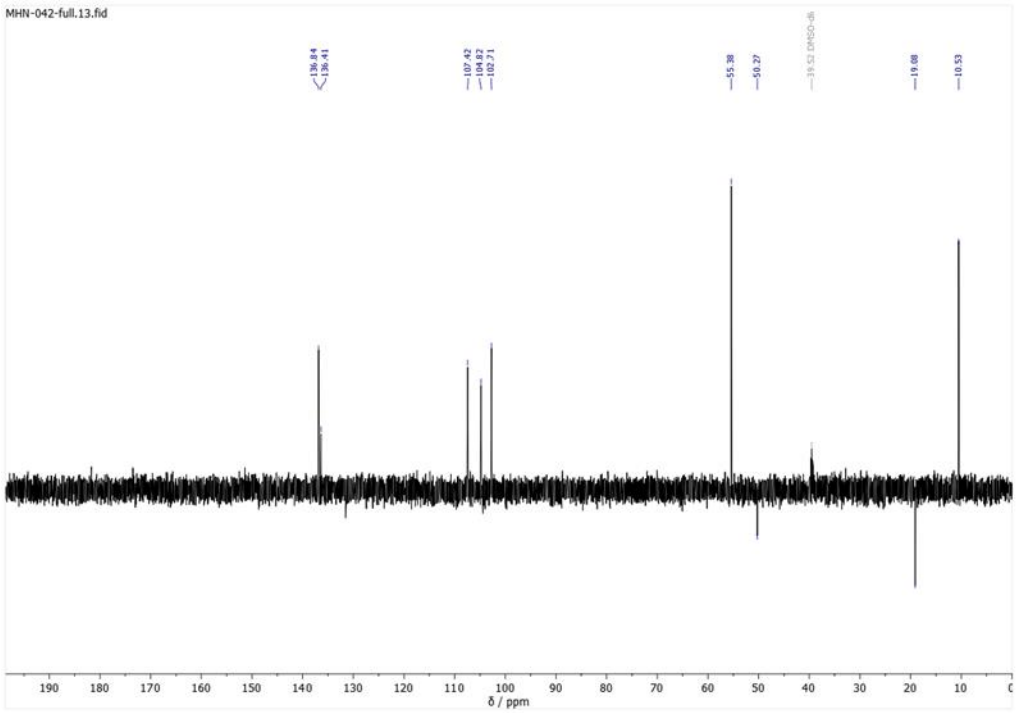

Figure S20. 135 DEPT ^{13}C-NMR spectrum (126 MHz, DMSO-d_6) of $^{n\text{Pr}}$DMQAPF$_6$.

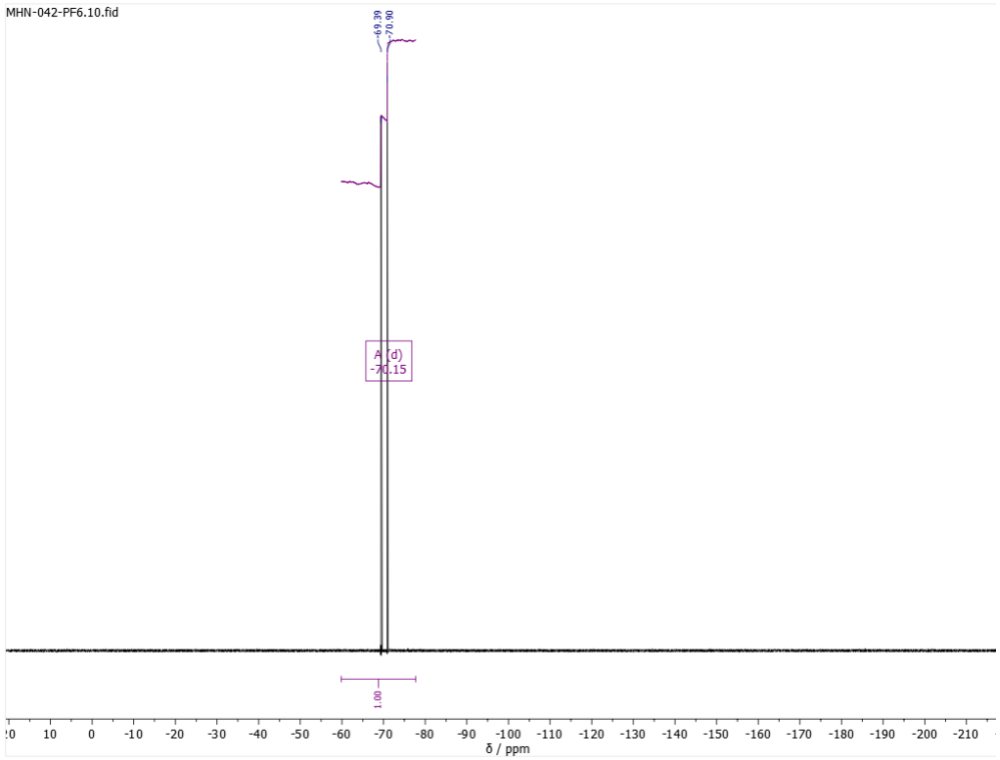

Figure S21. ^{19}F-NMR spectrum (471 MHz, DMSO-d$_6$) of $^{n\text{Pr}}$DMQAPF$_6$**.**

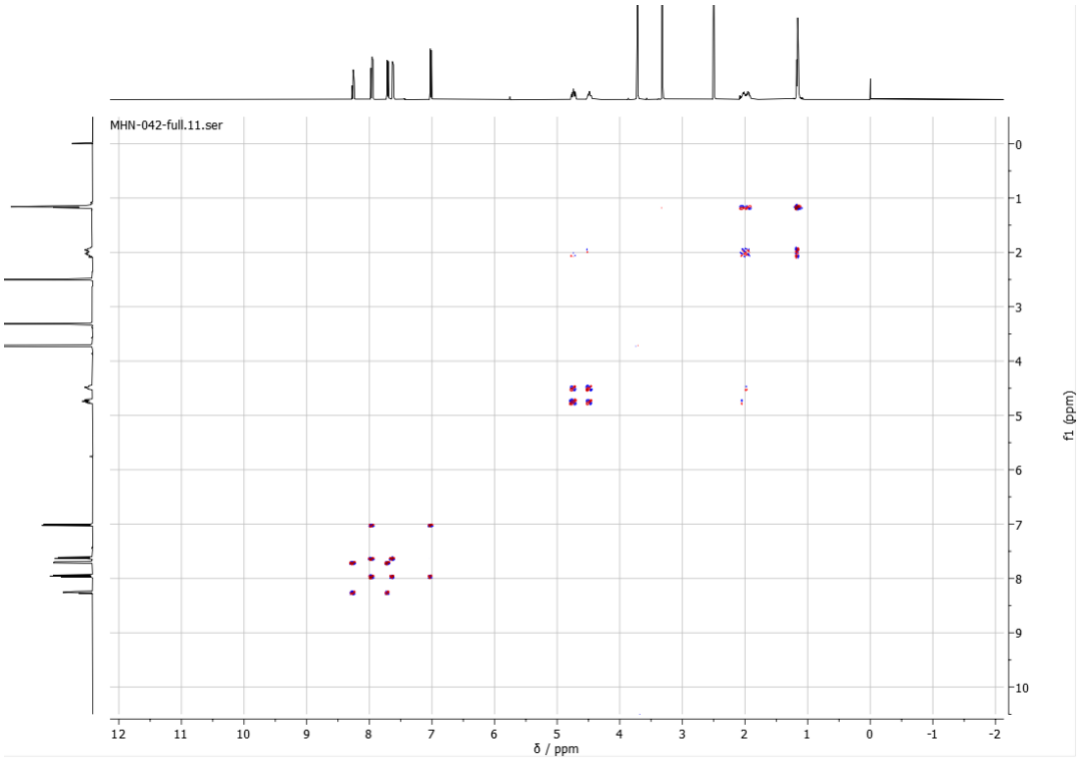

Figure S22. ^{1}H-^{1}H-COSY spectrum (500 MHz, DMSO-d_6) of $^{n\text{Pr}}$DMQAPF$_6$.

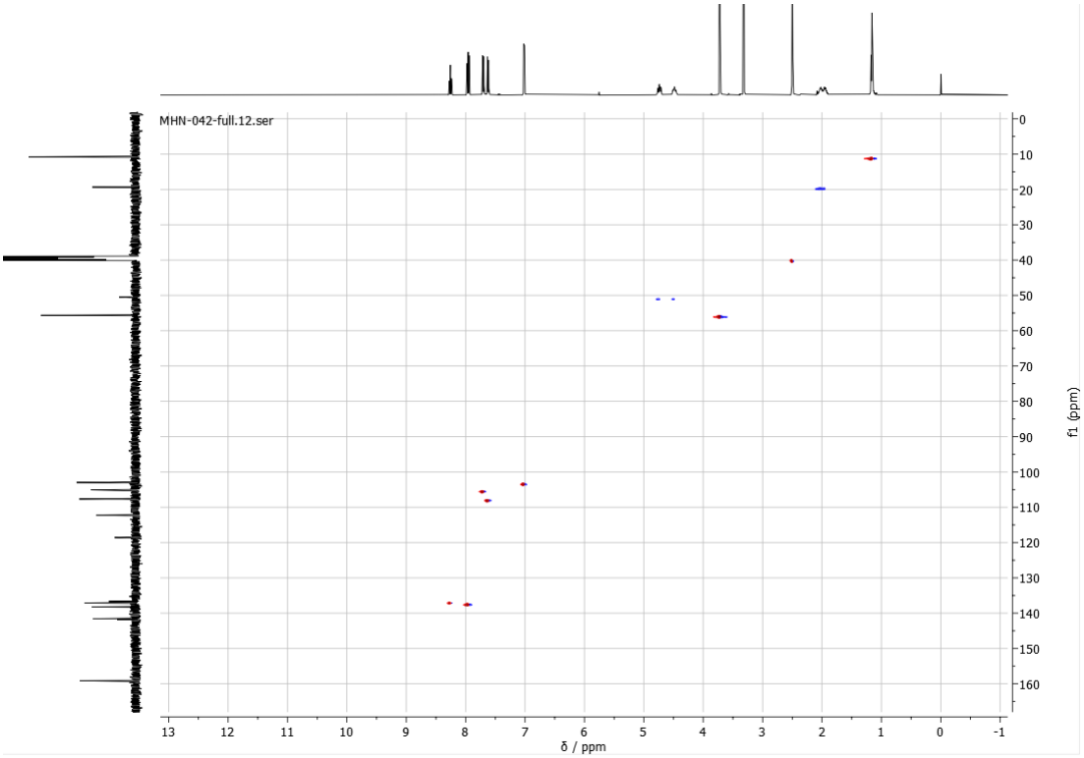

Figure S23. ^{1}H-^{13}C-HSQC spectrum (500 MHz, 126 MHz, DMSO-d_6) of $^{n\text{Pr}}$DMQAPF$_6$.

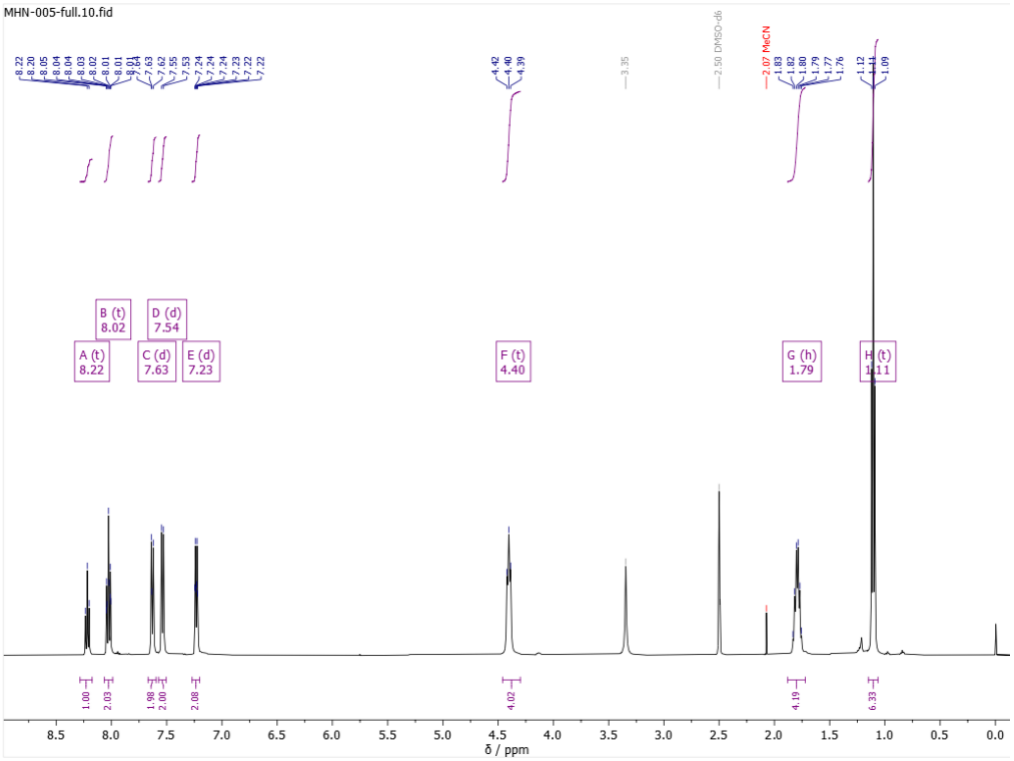

Figure S24. ^{1}H-NMR spectrum (500 MHz, DMSO-d$_6$) of **^{nPr}DAOTAPF$_6$**.

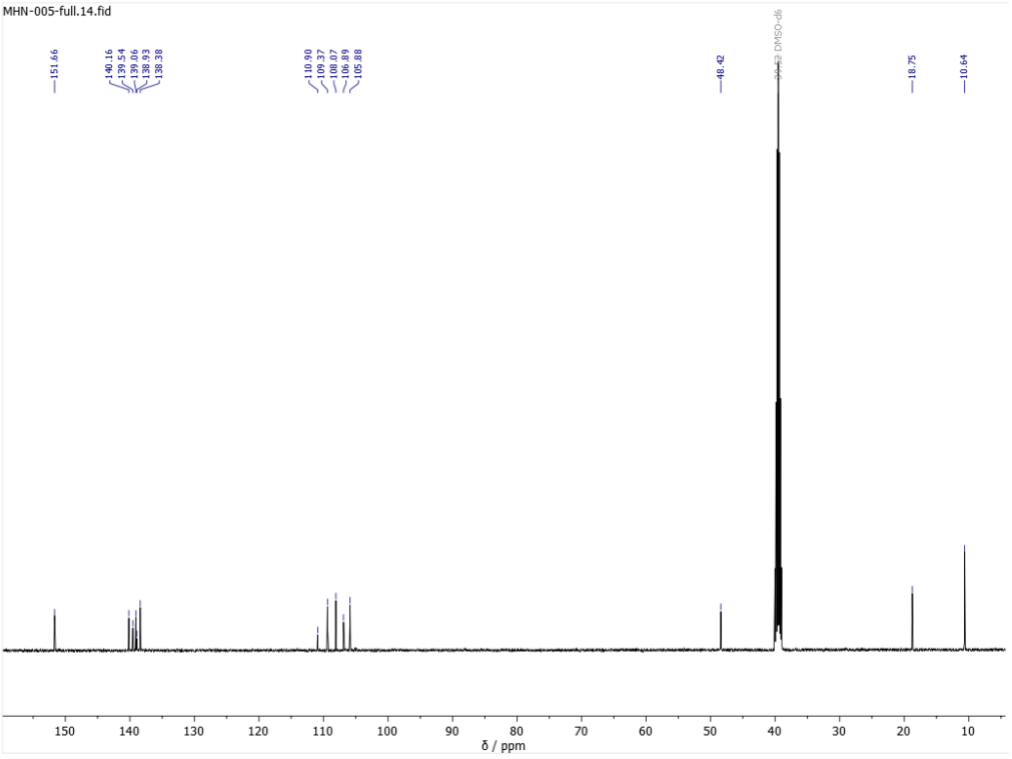

Figure S25. ^{13}C-NMR spectrum (126 MHz, DMSO-d$_6$) of **^{nPr}DAOTAPF$_6$**.

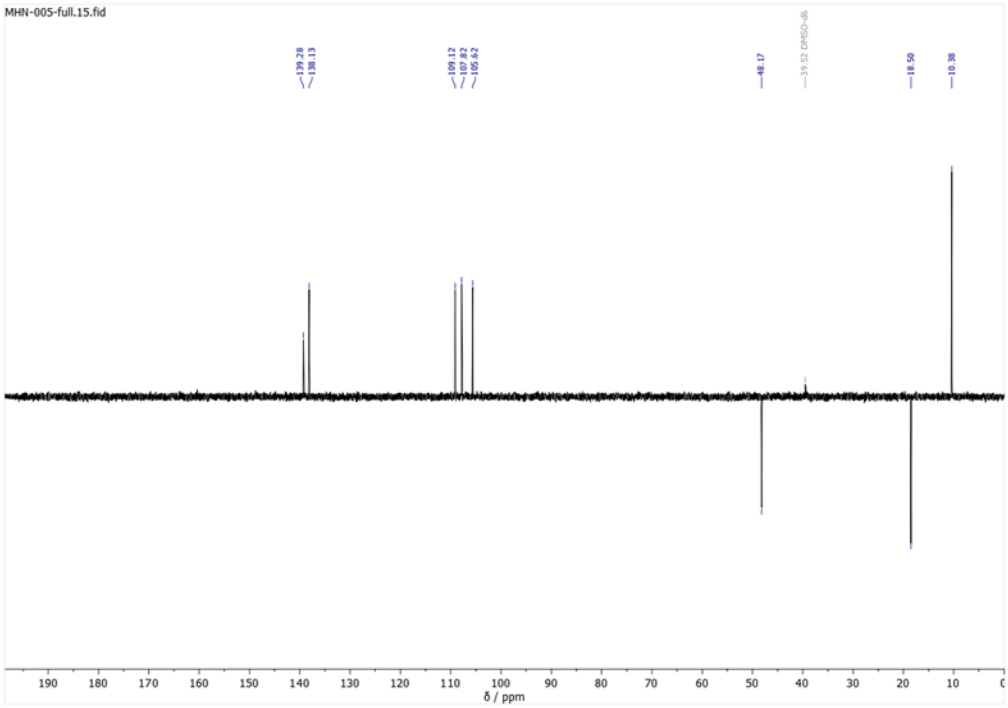

Figure S26. ^{13}C-NMR spectrum (126 MHz, DMSO-d$_6$) of **^{nPr}DAOTAPF$_6$**.

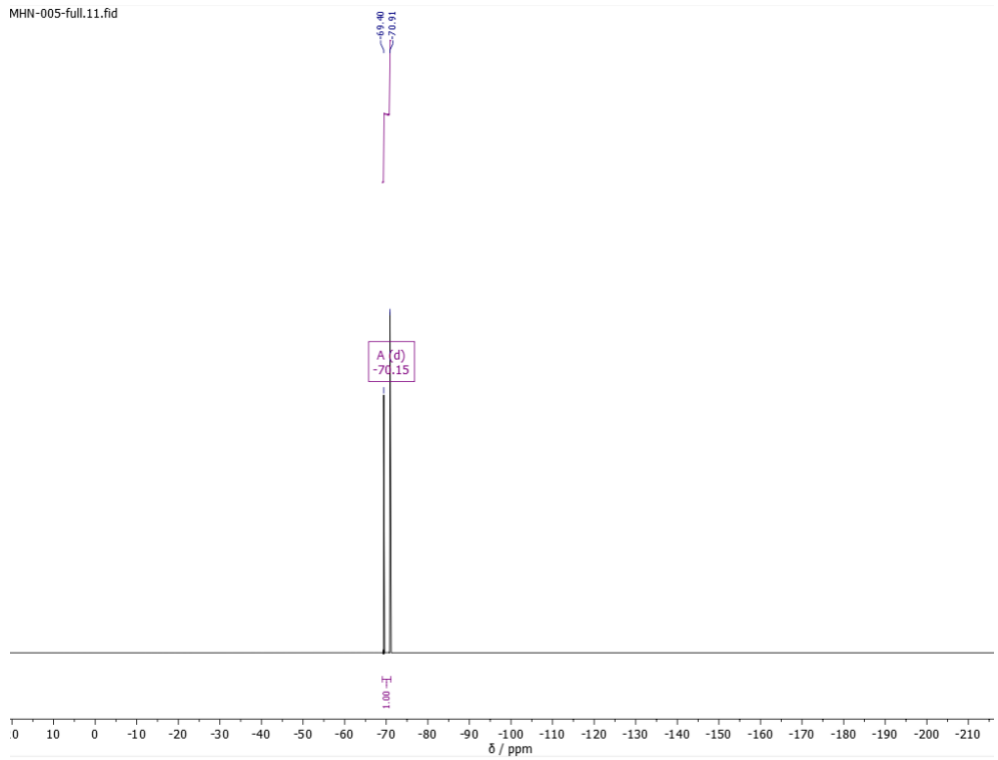

Figure S27. ^{19}F-NMR spectrum (471 MHz, DMSO-d$_6$) of **^{nPr}DAOTAPF$_6$**.

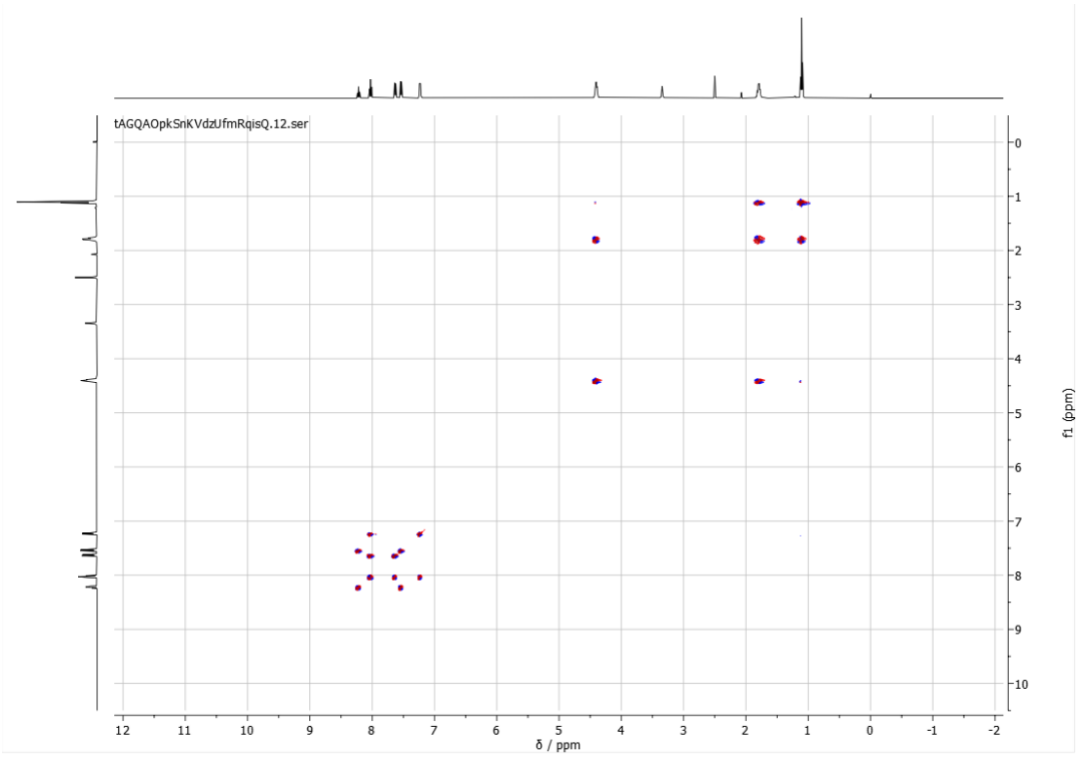

Figure S28. ^{1}H-^{1}H-COSY spectrum (500 MHz, DMSO-d$_6$) of **^{nPr}DAOTAPF$_6$**.

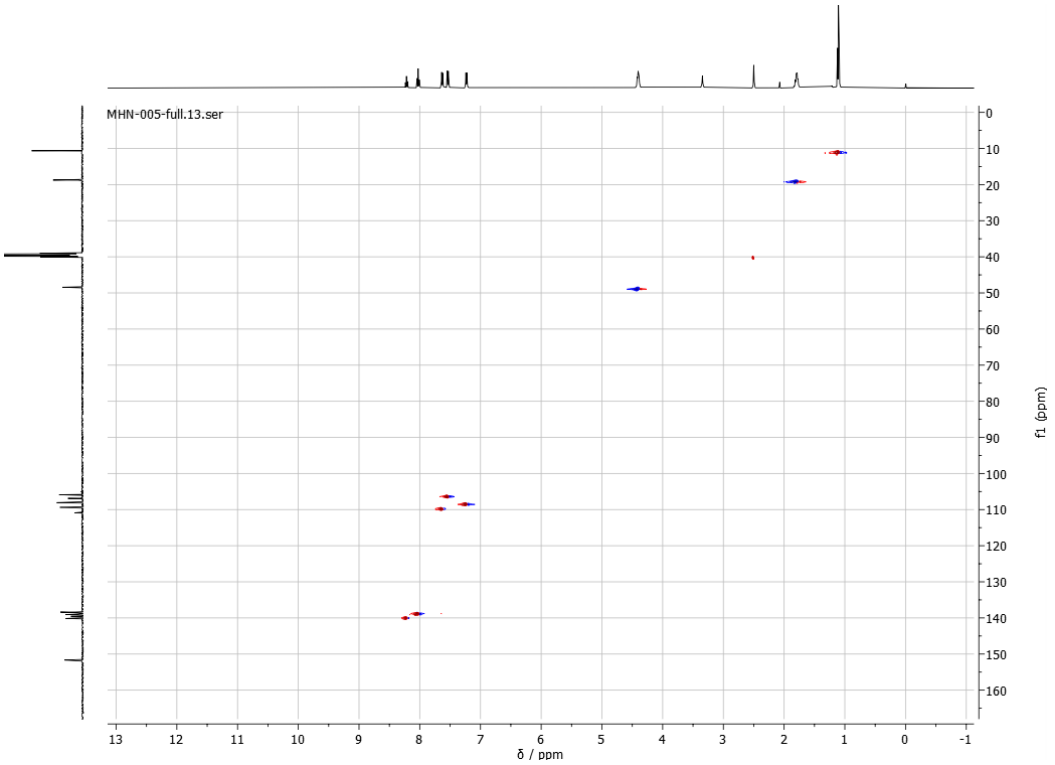

Figure S29. ^{1}H-^{13}C-HSQC spectrum (500 MHz, 126 MHz, DMSO-d$_6$) of **^{nPr}DAOTAPF$_6$**.

X. DFT Coordinates and Structures:

Structure	Gas Phase Optimized Coordinates			
***C*•**	C	0.00003	0.64621	-0.19163
	C	0.00002	-0.76191	-0.23795
	C	0.00000	-3.51170	-0.22503
	C	1.22738	-1.45087	-0.25365
	C	-1.22731	-1.45087	-0.25353
	C	-1.21238	-2.84158	-0.23537
	C	1.21242	-2.84158	-0.23541
	H	-2.12787	-3.41569	-0.20813
	H	2.12789	-3.41571	-0.20808
	H	-0.00001	-4.59556	-0.19855
	C	1.21761	1.36045	-0.10374
	C	3.55994	2.79692	0.10520
	C	2.44283	0.67619	-0.13913
	C	1.19058	2.74640	0.03140
	C	2.35599	3.47922	0.13069
	C	3.61631	1.41361	-0.02044
	H	2.30487	4.55563	0.23316
	H	4.58372	0.93068	-0.01006
	H	4.48675	3.35224	0.19353
	C	-1.21756	1.36042	-0.10365
	C	-3.55994	2.79684	0.10545
	C	-1.19056	2.74638	0.03150
	C	-2.44277	0.67614	-0.13893
	C	-3.61627	1.41353	-0.02017
	C	-2.35599	3.47917	0.13086
	H	-4.58367	0.93056	-0.00965
	H	-2.30489	4.55559	0.23329
	H	-4.48674	3.35214	0.19382
	O	0.00000	3.42578	0.06828
	N	-2.41908	-0.71341	-0.29851
	C	-3.67197	-1.41377	-0.50432
	H	-3.48175	-2.27160	-1.15266
	H	-4.33574	-0.76217	-1.07676
	C	-4.35175	-1.86141	0.78377
	H	-3.66928	-2.50747	1.34274
	H	-4.52898	-0.98742	1.41654
	C	-5.65884	-2.58716	0.50964
	H	-5.49686	-3.47987	-0.10026
	H	-6.36408	-1.94607	-0.02584
	H	-6.13864	-2.90336	1.43703
	N	2.41913	-0.71340	-0.29875
	C	3.67207	-1.41377	-0.50429
	H	3.48197	-2.27167	-1.15259
	H	4.33593	-0.76223	-1.07668
	C	4.35159	-1.86141	0.78393
	H	3.66890	-2.50731	1.34284
	H	4.52889	-0.98742	1.41668
	C	5.65861	-2.58740	0.51008
	H	5.49658	-3.48014	-0.09976
	H	6.13823	-2.90358	1.43757

	H	6.36402	-1.94646	-0.02535
C^{+}	C	0.00001	0.64578	-0.16062
	C	-0.00006	-0.74105	-0.25792
	C	-0.00021	-3.47352	-0.34429
	C	1.24157	-1.43188	-0.30021
	C	-1.24175	-1.43175	-0.30017
	C	-1.21879	-2.82110	-0.33393
	C	1.21846	-2.82123	-0.33398
	H	-2.12492	-3.40724	-0.32354
	H	2.12451	-3.40747	-0.32365
	H	-0.00026	-4.55797	-0.35331
	C	1.21160	1.35206	-0.09292
	C	3.54256	2.78019	0.07956
	C	2.43666	0.66251	-0.15445
	C	1.18154	2.74915	0.04497
	C	2.34131	3.47645	0.12661
	C	3.61318	1.40768	-0.05382
	H	2.30270	4.55221	0.23356
	H	4.58425	0.93555	-0.05789
	H	4.46898	3.33800	0.15769
	C	-1.21153	1.35216	-0.09293
	C	-3.54237	2.78052	0.07947
	C	-1.18134	2.74925	0.04494
	C	-2.43665	0.66273	-0.15443
	C	-3.61311	1.40801	-0.05387
	C	-2.34105	3.47667	0.12654
	H	-4.58422	0.93598	-0.05795
	H	-2.30233	4.55243	0.23347
	H	-4.46873	3.33842	0.15754
	O	0.00013	3.40881	0.10487
	N	-2.41623	-0.70867	-0.30941
	C	-3.68710	-1.42015	-0.47472
	H	-3.51107	-2.27040	-1.13300
	H	-4.36321	-0.76886	-1.02772
	C	-4.30674	-1.86191	0.84227
	H	-3.60141	-2.50330	1.37800
	H	-4.46718	-0.98655	1.47785
	C	-5.61914	-2.59611	0.61943
	H	-5.47763	-3.49295	0.01174
	H	-6.35041	-1.96289	0.11162
	H	-6.05607	-2.90713	1.56835
	N	2.41612	-0.70888	-0.30947
	C	3.68697	-1.42040	-0.47482
	H	3.51089	-2.27076	-1.13293
	H	4.36301	-0.76919	-1.02799
	C	4.30673	-1.86193	0.84219
	H	3.60149	-2.50337	1.37799
	H	4.46705	-0.98649	1.47769
	C	5.61922	-2.59598	0.61941
	H	5.47776	-3.49309	0.01209
	H	6.05637	-2.90656	1.56838
	H	6.35030	-1.96283	0.11123
$C^{\bullet++}$	C	-0.00000	0.65417	-0.16860
	C	-0.00003	-0.72771	-0.27067

	C	-0.00010	-3.50210	-0.39693
	C	1.23954	-1.41444	-0.32581
	C	-1.23963	-1.41438	-0.32576
	C	-1.21122	-2.83701	-0.37958
	C	1.21106	-2.83707	-0.37968
	H	-2.12292	-3.41644	-0.37828
	H	2.12272	-3.41655	-0.37852
	H	-0.00014	-4.58553	-0.42038
	C	1.20982	1.35633	-0.09983
	C	3.55019	2.76795	0.08022
	C	2.43700	0.66333	-0.16117
	C	1.18006	2.75018	0.04117
	C	2.34992	3.46620	0.12713
	C	3.61702	1.39254	-0.06001
	H	2.32132	4.54319	0.23600
	H	4.58878	0.92161	-0.06928
	H	4.47739	3.32399	0.16032
	C	-1.20980	1.35637	-0.09984
	C	-3.55012	2.76811	0.07996
	C	-1.17999	2.75023	0.04109
	C	-2.43701	0.66342	-0.16122
	C	-3.61700	1.39270	-0.06022
	C	-2.34983	3.46631	0.12695
	H	-4.58880	0.92183	-0.06956
	H	-2.32119	4.54330	0.23579
	H	-4.47731	3.32420	0.15993
	O	0.00004	3.40943	0.10058
	N	-2.40005	-0.72383	-0.31949
	C	-3.69013	-1.43897	-0.46267
	H	-3.53137	-2.29161	-1.11936
	H	-4.35991	-0.78054	-1.01169
	C	-4.28240	-1.85491	0.87623
	H	-3.58583	-2.52062	1.39480
	H	-4.40093	-0.97538	1.51469
	C	-5.62306	-2.54711	0.68286
	H	-5.52943	-3.44681	0.07108
	H	-6.35030	-1.88892	0.20320
	H	-6.03699	-2.84623	1.64521
	N	2.40000	-0.72391	-0.31954
	C	3.69011	-1.43902	-0.46279
	H	3.53138	-2.29165	-1.11949
	H	4.35983	-0.78054	-1.01181
	C	4.28243	-1.85494	0.87609
	H	3.58593	-2.52076	1.39461
	H	4.40083	-0.97544	1.51459
	C	5.62316	-2.54699	0.68269
	H	5.52952	-3.44700	0.07137
	H	6.03740	-2.84557	1.64507
	H	6.35016	-1.88891	0.20251
$C^{+}(PF_6)$	C	-0.00004	0.64139	-1.15505
	C	-0.00006	-0.73821	-1.31191
	C	-0.00010	-3.46749	-1.44709
	C	1.23899	-1.42813	-1.34029
	C	-1.23914	-1.42810	-1.34025
	C	-1.21709	-2.81656	-1.41393

	C	1.21691	-2.81660	-1.41399
	H	-2.12025	-3.40579	-1.39332
	H	2.12006	-3.40584	-1.39341
	H	-0.00012	-4.55174	-1.47819
	C	1.21012	1.34456	-1.05448
	C	3.53544	2.75734	-0.73543
	C	2.43211	0.65462	-1.09058
	C	1.17808	2.72897	-0.84273
	C	2.33528	3.45225	-0.69813
	C	3.60696	1.39205	-0.92185
	H	2.28935	4.51921	-0.52782
	H	4.57586	0.91736	-0.89551
	H	4.45975	3.30681	-0.59548
	C	-1.21017	1.34459	-1.05443
	C	-3.53544	2.75742	-0.73526
	C	-1.17809	2.72899	-0.84267
	C	-2.43218	0.65468	-1.09047
	C	-3.60700	1.39213	-0.92169
	C	-2.33527	3.45230	-0.69801
	H	-4.57591	0.91746	-0.89530
	H	-2.28930	4.51926	-0.52770
	H	-4.45974	3.30691	-0.59526
	O	0.00000	3.38976	-0.78038
	N	-2.41358	-0.71017	-1.28373
	C	-3.68062	-1.43654	-1.25923
	H	-3.59062	-2.30231	-1.91426
	H	-4.44022	-0.80989	-1.72500
	C	-4.08551	-1.84366	0.14957
	H	-3.28468	-2.43912	0.59414
	H	-4.15903	-0.94862	0.77205
	C	-5.39652	-2.61167	0.15578
	H	-5.32650	-3.52950	-0.43426
	H	-6.21395	-2.01407	-0.25670
	H	-5.67495	-2.89380	1.17159
	P	0.00011	0.02333	2.46579
	F	0.00014	-1.42519	3.17833
	F	0.00009	1.46681	1.67708
	F	-1.15330	-0.50604	1.40823
	F	-1.15617	0.55702	3.45385
	F	1.15345	-0.50607	1.40813
	F	1.15649	0.55701	3.45376
	N	2.41346	-0.71024	-1.28382
	C	3.68048	-1.43666	-1.25935
	H	3.59041	-2.30245	-1.91433
	H	4.44008	-0.81006	-1.72518
	C	4.08541	-1.84369	0.14946
	H	3.28462	-2.43917	0.59409
	H	4.15890	-0.94862	0.77190
	C	5.39645	-2.61165	0.15568
	H	5.32643	-3.52955	-0.43425
	H	5.67494	-2.89366	1.17151
	H	6.21385	-2.01407	-0.25690
$C^{\bullet++}(PF_6)_2$	C	0.83951	0.69967	0.61672
	C	0.93112	-0.58645	1.13565
	C	1.18901	-3.16912	1.98992

C	-0.11018	-1.51008	0.87160
C	2.10360	-0.95942	1.81740
C	2.21112	-2.28985	2.24693
C	0.02817	-2.80971	1.31205
H	3.09716	-2.65552	2.74279
H	-0.71556	-3.56598	1.11702
H	1.29715	-4.19790	2.31333
C	-0.28317	1.07111	-0.13384
C	-2.43996	1.84408	-1.70736
C	-1.32284	0.14002	-0.37618
C	-0.32419	2.32745	-0.69486
C	-1.41702	2.73574	-1.48798
C	-2.41905	0.55957	-1.18074
H	-1.42228	3.73723	-1.89864
H	-3.26239	-0.08899	-1.36526
H	-3.30629	2.14542	-2.28075
C	1.87400	1.61145	0.79378
C	3.91321	3.41848	1.01230
C	1.77058	2.88185	0.20102
C	3.03702	1.23436	1.49101
C	4.06618	2.17381	1.58806
C	2.77388	3.80392	0.31463
H	5.00145	1.94260	2.07456
H	2.68308	4.77504	-0.15212
H	4.73196	4.12439	1.09437
O	0.65593	3.20838	-0.50361
N	3.09840	-0.03320	2.02266
C	4.33438	-0.45049	2.68929
H	4.07836	-1.16884	3.46659
H	4.73406	0.40975	3.22432
C	5.34954	-1.01971	1.70992
H	4.90299	-1.86418	1.17907
H	5.56165	-0.27397	0.93984
C	6.62764	-1.44257	2.41451
H	6.43694	-2.21449	3.16454
H	7.10567	-0.59940	2.91973
H	7.34473	-1.84768	1.70035
P	2.41104	-0.48512	-2.41532
F	1.72164	-0.39223	-3.86294
F	3.05495	-0.55092	-0.89077
F	2.84914	-2.01336	-2.65814
F	3.81042	0.06736	-2.97849
F	0.97473	-1.00680	-1.77042
F	1.92909	1.06087	-2.08522
P	-5.30218	0.44082	0.88368
F	-5.07933	-0.59797	-0.40413
F	-4.94509	1.67726	-0.12588
F	-5.44050	1.45595	2.11991
F	-6.85858	0.55802	0.52108
F	-5.56345	-0.83706	1.83328
F	-3.67069	0.29410	1.19262
N	-1.23529	-1.08860	0.15018
C	-2.31155	-2.06625	-0.09852
H	-2.38460	-2.69948	0.78236
H	-3.25418	-1.52816	-0.12748
C	-2.06451	-2.86503	-1.36943

	H	-1.10012	-3.37708	-1.31763
	H	-1.99021	-2.17612	-2.21491
	C	-3.19641	-3.85477	-1.59398
	H	-3.25406	-4.58665	-0.78452
	H	-3.04905	-4.40144	-2.52576
	H	-4.15984	-3.34376	-1.64755
	C	0.00002	0.65896	-0.49890
	C	-0.00005	-0.75377	-0.35411
	C	-0.00031	-3.52380	-0.05527
	C	1.21328	-1.45444	-0.26821
	C	-1.21349	-1.45424	-0.26805
	C	-1.20454	-2.83507	-0.11583
	C	1.20404	-2.83528	-0.11594
	H	-2.13098	-3.39243	-0.04731
	H	2.13033	-3.39288	-0.04742
	H	-0.00039	-4.60327	0.05171
	C	1.20786	1.36577	-0.24311
	C	3.54518	2.78283	0.31938
	C	2.43281	0.68663	-0.14372
	C	1.18916	2.74170	-0.04360
	C	2.33841	3.45599	0.23803
	C	3.58874	1.39894	0.14215
	H	2.26872	4.52973	0.37308
	H	4.54330	0.89313	0.22625
	H	4.46064	3.32641	0.52689
	C	-1.20764	1.36596	-0.24288
	C	-3.54462	2.78334	0.32023
	C	-1.18868	2.74188	-0.04335
	C	-2.43270	0.68698	-0.14330
	C	-3.58844	1.39945	0.14293
***C*$^-$**	C	-2.33776	3.45631	0.23860
	H	-4.54305	0.89378	0.22717
	H	-2.26788	4.53003	0.37368
	H	-4.45993	3.32705	0.52804
	O	0.00027	3.44592	-0.18502
	N	-2.41480	-0.70634	-0.38805
	C	-3.66044	-1.40144	-0.54891
	H	-3.48808	-2.26949	-1.19467
	H	-4.34685	-0.74805	-1.09888
	C	-4.32847	-1.85909	0.74942
	H	-3.63990	-2.50745	1.29691
	H	-4.49743	-0.98995	1.39003
	C	-5.63895	-2.58328	0.48588
	H	-5.48088	-3.47010	-0.13502
	H	-6.34704	-1.93700	-0.04123
	H	-6.11466	-2.90880	1.41375
	N	2.41470	-0.70670	-0.38837
	C	3.66036	-1.40187	-0.54882
	H	3.48829	-2.26992	-1.19464
	H	4.34695	-0.74853	-1.09862
	C	4.32788	-1.85938	0.74982
	H	3.63899	-2.50768	1.29699
	H	4.49655	-0.99017	1.39043
	C	5.63844	-2.58365	0.48698
	H	5.48061	-3.47074	-0.13359

	H	6.11388	-2.90876	1.41513
	H	6.34668	-1.93757	-0.04020
$C^{-\bullet\bullet}$	C	0.01855	0.63415	-0.16808
	C	-0.00647	-0.75349	-0.25076
	C	-0.00366	-3.54686	-0.27039
	C	1.24807	-1.47550	-0.28019
	C	-1.24100	-1.47127	-0.27490
	C	-1.24098	-2.84215	-0.27507
	C	1.21582	-2.85406	-0.27475
	H	-2.16155	-3.41175	-0.25253
	H	2.13176	-3.43368	-0.25597
	H	-0.00517	-4.63065	-0.25033
	C	1.20430	1.35261	-0.10496
	C	3.58967	2.81004	0.06381
	C	2.46735	0.66722	-0.16479
	C	1.20296	2.76192	0.03117
	C	2.34669	3.49317	0.11150
	C	3.62798	1.41558	-0.06590
	H	2.28670	4.56999	0.21907
	H	4.59899	0.93338	-0.07169
	H	4.51667	3.36619	0.14208
	C	-1.21477	1.35764	-0.08335
	C	-3.55856	2.79739	0.11189
	C	-1.18266	2.74132	0.04930
	C	-2.43805	0.67242	-0.13415
	C	-3.61859	1.41753	-0.01820
	C	-2.35522	3.47779	0.14367
	H	-4.58720	0.93613	-0.01026
	H	-2.29924	4.55429	0.24770
	H	-4.48629	3.35453	0.19931
	O	-0.01076	3.42967	0.09014
	N	-2.43176	-0.70713	-0.30077
	C	-3.68680	-1.39173	-0.49866
	H	-3.49791	-2.25678	-1.13823
	H	-4.35604	-0.74099	-1.06849
	C	-4.35927	-1.83566	0.79555
	H	-3.66068	-2.47032	1.34659
	H	-4.54033	-0.95786	1.42272
	C	-5.66101	-2.57665	0.53627
	H	-5.49004	-3.47119	-0.06928
	H	-6.37496	-1.94674	-0.00275
	H	-6.13557	-2.89274	1.46775
	N	2.43594	-0.72562	-0.32177
	C	3.68470	-1.42409	-0.48805
	H	3.50896	-2.29802	-1.12076
	H	4.36730	-0.78183	-1.05133
	C	4.33576	-1.85160	0.82371
	H	3.63436	-2.48636	1.37159
	H	4.49743	-0.96342	1.44042
	C	5.64815	-2.58459	0.59688
	H	5.49719	-3.48667	-0.00340
	H	6.10871	-2.88742	1.54001
	H	6.36585	-1.95295	0.06501

	C	0.00011	0.62950	0.56556
	C	-0.00003	-0.66259	-0.19160
	C	-0.00029	-3.10622	-1.45216
	C	1.21169	-1.26886	-0.50731
	C	-1.21187	-1.26869	-0.50716
	C	-1.20734	-2.50772	-1.14609
	C	1.20689	-2.50792	-1.14621
	H	-2.13207	-3.00296	-1.40967
	H	2.13152	-3.00331	-1.40988
	H	-0.00039	-4.06792	-1.95388
	C	1.22226	1.42520	0.22268
	C	3.48128	2.92998	-0.27090
	C	2.41672	0.77871	-0.09410
	C	1.17222	2.80497	0.24311
	C	2.29767	3.57834	0.01631
	C	3.55020	1.54816	-0.34831
	H	2.22022	4.65725	0.05507
	H	4.48591	1.08868	-0.63569
	H	4.37434	3.51262	-0.46841
	C	-1.22194	1.42539	0.22276
	C	-3.48078	2.93049	-0.27064
	C	-1.17168	2.80515	0.24317
	C	-2.41653	0.77908	-0.09390
	C	-3.54992	1.54868	-0.34802
	C	-2.29704	3.57868	0.01644
	H	-4.48574	1.08932	-0.63525
C-H	H	-2.21943	4.65758	0.05516
	H	-4.37377	3.51326	-0.46809
	O	0.00032	3.46364	0.50733
	N	-2.40687	-0.62037	-0.16033
	C	-3.63909	-1.38500	-0.10752
	H	-3.86046	-1.84382	-1.07928
	H	-4.45403	-0.69371	0.09397
	C	-3.63964	-2.43432	0.99805
	H	-2.78366	-3.10265	0.88332
	H	-3.50684	-1.92073	1.95419
	C	-4.92977	-3.23842	1.00475
	H	-5.06448	-3.78045	0.06499
	H	-4.93267	-3.97262	1.81179
	H	-5.80132	-2.59293	1.14213
	N	2.40683	-0.62073	-0.16069
	C	3.63885	-1.38565	-0.10763
	H	3.85999	-1.84498	-1.07920
	H	4.45400	-0.69450	0.09343
	C	3.63916	-2.43452	0.99836
	H	2.78295	-3.10260	0.88390
	H	3.50657	-1.92052	1.95431
	C	4.92903	-3.23902	1.00530
	H	4.93176	-3.97285	1.81269
	H	5.80080	-2.59376	1.14230
	H	5.06347	-3.78154	0.06579
	H	0.00011	0.41137	1.64510

Structure	Solvated Phase Optimized Coordinates			
	C	0.00000	0.64857	-0.19867
	C	0.00001	-0.76045	-0.24915
	C	0.00002	-3.50954	-0.24731
	C	1.22887	-1.44872	-0.26673
	C	-1.22885	-1.44873	-0.26672
	C	-1.21383	-2.84026	-0.25468
	C	1.21386	-2.84025	-0.25468
	H	-2.12843	-3.41591	-0.23227
	H	2.12846	-3.41589	-0.23227
	H	0.00002	-4.59358	-0.22645
	C	1.21851	1.36162	-0.10725
	C	3.56308	2.79629	0.10735
	C	2.44403	0.67542	-0.14401
	C	1.19305	2.74784	0.03208
	C	2.35822	3.48071	0.13484
	C	3.61876	1.41336	-0.02282
	H	2.31211	4.55742	0.24091
	H	4.58647	0.93120	-0.01546
	H	4.49040	3.35042	0.19758
	C	-1.21852	1.36160	-0.10725
	C	-3.56309	2.79626	0.10736
	C	-1.19307	2.74783	0.03208
	C	-2.44403	0.67540	-0.14401
***C*•**	C	-3.61876	1.41333	-0.02281
	C	-2.35824	3.48069	0.13484
	H	-4.58647	0.93116	-0.01545
	H	-2.31214	4.55740	0.24091
	H	-4.49042	3.35038	0.19760
	O	-0.00001	3.42826	0.06927
	N	-2.42113	-0.71205	-0.30720
	C	-3.67884	-1.41608	-0.49828
	H	-3.49529	-2.27427	-1.14682
	H	-4.34979	-0.76709	-1.06393
	C	-4.34139	-1.86190	0.79867
	H	-3.65261	-2.50710	1.35107
	H	-4.51872	-0.98730	1.43082
	C	-5.64818	-2.59289	0.53780
	H	-5.48549	-3.48573	-0.07130
	H	-6.35866	-1.95342	0.00778
	H	-6.11634	-2.90781	1.47162
	N	2.42115	-0.71203	-0.30720
	C	3.67886	-1.41605	-0.49828
	H	3.49532	-2.27422	-1.14685
	H	4.34983	-0.76705	-1.06389
	C	4.34137	-1.86193	0.79867
	H	3.65258	-2.50715	1.35103
	H	4.51868	-0.98735	1.43087

	C	5.64817	-2.59289	0.53781
	H	5.48550	-3.48572	-0.07133
	H	6.11631	-2.90785	1.47163
	H	6.35867	-1.95340	0.00784
	C	-0.00000	0.64601	-0.16106
	C	-0.00001	-0.73923	-0.26072
	C	-0.00003	-3.47107	-0.35439
	C	1.24154	-1.42992	-0.30469
	C	-1.24157	-1.42990	-0.30468
	C	-1.21927	-2.81923	-0.34233
	C	1.21922	-2.81925	-0.34234
	H	-2.12446	-3.40673	-0.33603
	H	2.12439	-3.40677	-0.33604
	H	-0.00004	-4.55527	-0.36698
	C	1.21163	1.35238	-0.09309
	C	3.54437	2.77869	0.07849
	C	2.43562	0.66264	-0.15654
	C	1.18219	2.74876	0.04583
	C	2.34199	3.47563	0.12782
	C	3.61436	1.40746	-0.05704
	H	2.30579	4.55128	0.23676
	H	4.58546	0.93581	-0.06561
	H	4.47112	3.33560	0.15637
	C	-1.21162	1.35239	-0.09307
	C	-3.54435	2.77874	0.07852
	C	-1.18217	2.74878	0.04584
C^+	C	-2.43562	0.66267	-0.15652
	C	-3.61436	1.40751	-0.05700
	C	-2.34195	3.47566	0.12785
	H	-4.58546	0.93587	-0.06557
	H	-2.30574	4.55131	0.23679
	H	-4.47108	3.33565	0.15641
	O	0.00002	3.41000	0.10705
	N	-2.41566	-0.70681	-0.31098
	C	-3.68600	-1.41905	-0.47310
	H	-3.51205	-2.26874	-1.13160
	H	-4.36666	-0.76843	-1.02000
	C	-4.29445	-1.86216	0.84818
	H	-3.58351	-2.50264	1.37688
	H	-4.45578	-0.98665	1.48293
	C	-5.60481	-2.60112	0.63158
	H	-5.45740	-3.49476	0.02044
	H	-6.33699	-1.96657	0.12658
	H	-6.03511	-2.91487	1.58338
	N	2.41565	-0.70684	-0.31100
	C	3.68598	-1.41908	-0.47313
	H	3.51203	-2.26879	-1.13161
	H	4.36663	-0.76847	-1.02005
	C	4.29447	-1.86215	0.84815

	H	3.58355	-2.50263	1.37688
	H	4.45580	-0.98663	1.48287
	C	5.60483	-2.60111	0.63153
	H	5.45740	-3.49478	0.02046
	H	6.03517	-2.91479	1.58333
	H	6.33697	-1.96658	0.12647
$C^{\bullet++}$	C	0.00000	0.65165	-0.16279
	C	0.00000	-0.72607	-0.26318
	C	0.00001	-3.49921	-0.39464
	C	1.23760	-1.41304	-0.32013
	C	-1.23759	-1.41304	-0.32012
	C	-1.21026	-2.83582	-0.37637
	C	1.21028	-2.83581	-0.37639
	H	-2.12036	-3.41595	-0.37813
	H	2.12039	-3.41593	-0.37817
	H	0.00002	-4.58118	-0.42009
	C	1.20941	1.35495	-0.09626
	C	3.54963	2.76232	0.07588
	C	2.43161	0.66258	-0.16029
	C	1.18015	2.74789	0.04268
	C	2.34970	3.46180	0.12605
	C	3.61472	1.38931	-0.06419
	H	2.32259	4.53786	0.23538
	H	4.58462	0.91618	-0.07988
	H	4.47748	3.31611	0.15320
	C	-1.20941	1.35493	-0.09624
	C	-3.54964	2.76230	0.07593
	C	-1.18017	2.74788	0.04269
	C	-2.43161	0.66257	-0.16026
	C	-3.61473	1.38928	-0.06414
	C	-2.34972	3.46178	0.12608
	H	-4.58463	0.91615	-0.07982
	H	-2.32262	4.53784	0.23541
	H	-4.47749	3.31608	0.15326
	O	-0.00001	3.41021	0.10359
	N	-2.39467	-0.72325	-0.31547
	C	-3.68048	-1.43590	-0.46593
	H	-3.51766	-2.28824	-1.12004
	H	-4.34848	-0.77778	-1.01599
	C	-4.27138	-1.85042	0.87235
	H	-3.57352	-2.51583	1.38697
	H	-4.39065	-0.97016	1.50860
	C	-5.61000	-2.54385	0.67878
	H	-5.50633	-3.44180	0.06597
	H	-6.33142	-1.88359	0.19279
	H	-6.02515	-2.84209	1.64158
	N	2.39468	-0.72323	-0.31549
	C	3.68049	-1.43588	-0.46597
	H	3.51767	-2.28821	-1.12010

	H	4.34848	-0.77775	-1.01602
	C	4.27139	-1.85043	0.87230
	H	3.57352	-2.51585	1.38691
	H	4.39066	-0.97018	1.50857
	C	5.61000	-2.54385	0.67871
	H	5.50633	-3.44182	0.06593
	H	6.02518	-2.84207	1.64152
	H	6.33141	-1.88360	0.19270
$C^+(PF_6)$	C	-0.00000	0.37303	-1.22638
	C	0.00000	-1.01055	-1.11357
	C	0.00001	-3.72213	-0.76599
	C	1.24051	-1.69761	-1.03709
	C	-1.24051	-1.69761	-1.03708
	C	-1.21872	-3.07607	-0.85520
	C	1.21874	-3.07606	-0.85520
	H	-2.12317	-3.65529	-0.75103
	H	2.12318	-3.65528	-0.75104
	H	0.00001	-4.79484	-0.60708
	C	1.21096	1.08106	-1.26849
	C	3.54274	2.52037	-1.29360
	C	2.43421	0.39235	-1.20896
	C	1.18109	2.48125	-1.33747
	C	2.34009	3.21453	-1.36032
	C	3.61292	1.14471	-1.21550
	H	2.30203	4.29435	-1.41338
	H	4.58415	0.67941	-1.13963
	H	4.46905	3.08365	-1.29426
	C	-1.21096	1.08106	-1.26849
	C	-3.54275	2.52036	-1.29361
	C	-1.18110	2.48124	-1.33747
	C	-2.43421	0.39234	-1.20896
	C	-3.61292	1.14470	-1.21550
	C	-2.34010	3.21452	-1.36032
	H	-4.58415	0.67940	-1.13963
	H	-2.30204	4.29434	-1.41339
	H	-4.46906	3.08363	-1.29427
	O	0.00000	3.14395	-1.38250
	N	-2.41472	-0.98393	-1.14431
	C	-3.68729	-1.70762	-1.13137
	H	-3.53919	-2.66145	-1.63510
	H	-4.39158	-1.16201	-1.75732
	C	-4.23809	-1.90428	0.27247
	H	-3.50166	-2.44127	0.87616
	H	-4.37115	-0.92757	0.74544
	C	-5.55482	-2.66257	0.25092
	H	-5.43278	-3.65355	-0.19294
	H	-6.31015	-2.12652	-0.32879
	H	-5.94262	-2.79550	1.26162
	P	0.00001	0.65066	2.60884

	F	-0.00006	-0.59263	3.65806
	F	0.00003	1.89426	1.55156
	F	-1.15351	-0.09527	1.72704
	F	-1.15223	1.39533	3.48282
	F	1.15349	-0.09534	1.72704
	F	1.15227	1.39527	3.48284
	N	2.41472	-0.98393	-1.14431
	C	3.68729	-1.70761	-1.13137
	H	3.53919	-2.66144	-1.63511
	H	4.39159	-1.16200	-1.75732
	C	4.23809	-1.90428	0.27247
	H	3.50166	-2.44128	0.87615
	H	4.37114	-0.92758	0.74544
	C	5.55482	-2.66257	0.25092
	H	5.43279	-3.65354	-0.19295
	H	5.94262	-2.79550	1.26162
	H	6.31015	-2.12650	-0.32878
$C^{\bullet++}(PF_6)_2$	C	-1.41210	0.63248	-1.05701
	C	-1.51956	-0.73324	-1.22507
	C	-1.75227	-3.49254	-1.41909
	C	-0.35048	-1.52923	-1.15640
	C	-2.80023	-1.30393	-1.40891
	C	-2.89364	-2.72235	-1.50132
	C	-0.49664	-2.94178	-1.25602
	H	-3.84624	-3.21798	-1.60771
	H	0.35376	-3.60153	-1.17910
	H	-1.84514	-4.56934	-1.47602
	C	-0.16166	1.21808	-0.82665
	C	2.25861	2.39359	-0.32140
	C	0.99326	0.41899	-0.77736
	C	-0.08479	2.59844	-0.61444
	C	1.12533	3.19806	-0.36800
	C	2.21753	1.02723	-0.51620
	H	1.17862	4.26665	-0.20607
	H	3.13847	0.47042	-0.44285
	H	3.22197	2.84627	-0.12018
	C	-2.55645	1.43860	-1.07521
	C	-4.77359	3.04237	-1.04044
	C	-2.42214	2.81487	-0.85548
	C	-3.82144	0.86164	-1.27445
	C	-4.94275	1.68844	-1.25035
	C	-3.52765	3.62769	-0.84497
	H	-5.94436	1.30539	-1.37070
	H	-3.41909	4.69076	-0.67523
	H	-5.65343	3.67413	-1.02026
	O	-1.20277	3.36463	-0.64619
	N	-3.89041	-0.51528	-1.47473
	C	-5.22048	-1.11368	-1.69895
	H	-5.10200	-1.97129	-2.35572

	H	-5.80629	-0.39755	-2.26930
	C	-5.90198	-1.48539	-0.39150
	H	-5.28390	-2.20878	0.14639
	H	-5.96832	-0.60099	0.24664
	C	-7.28609	-2.05873	-0.64522
	H	-7.23552	-2.95969	-1.26041
	H	-7.92625	-1.33614	-1.15592
	H	-7.76629	-2.32374	0.29698
	P	-1.89649	-0.05784	2.60699
	F	-0.82852	0.34916	3.75717
	F	-2.96354	-0.46469	1.43124
	F	-2.10375	-1.51416	3.29238
	F	-3.11069	0.54949	3.49480
	F	-0.68084	-0.66509	1.69257
	F	-1.68742	1.39688	1.89331
	P	6.13636	0.14259	-0.18914
	F	5.02910	-0.19481	0.96207
	F	5.46660	1.61928	-0.38247
	F	7.21969	0.47977	-1.35120
	F	7.13905	0.73695	0.94037
	F	6.78292	-1.33745	-0.00296
	F	5.11233	-0.45470	-1.32339
	N	0.85339	-0.95164	-0.98466
	C	2.07129	-1.78728	-0.94875
	H	1.93499	-2.60835	-1.64799
	H	2.89175	-1.19736	-1.34824
	C	2.37950	-2.27889	0.45729
	H	1.50489	-2.79216	0.86586
	H	2.57361	-1.41992	1.10318
	C	3.58404	-3.20522	0.44909
	H	3.40257	-4.08588	-0.17163
	H	3.80402	-3.54826	1.46062
	H	4.46722	-2.68983	0.07122
	C	0.00000	0.67148	-0.62032
	C	0.00005	-0.74911	-0.42659
	C	0.00016	-3.51119	-0.09247
	C	1.21394	-1.44499	-0.32202
	C	-1.21378	-1.44509	-0.32203
	C	-1.20559	-2.82689	-0.15720
	C	1.20586	-2.82679	-0.15715
C^-	H	-2.13017	-3.38523	-0.08525
	H	2.13048	-3.38504	-0.08515
	H	0.00021	-4.58973	0.02152
	C	1.20594	1.36921	-0.29462
	C	3.52559	2.76793	0.38368
	C	2.42635	0.68318	-0.16547
	C	1.18555	2.73885	-0.05921
	C	2.32452	3.44778	0.28123
	C	3.57367	1.38820	0.17398

	H	2.25785	4.51858	0.43991
	H	4.52510	0.88098	0.27359
	H	4.43514	3.30315	0.63251
	C	-1.20599	1.36912	-0.29464
	C	-3.52576	2.76764	0.38369
	C	-1.18572	2.73876	-0.05922
	C	-2.42635	0.68300	-0.16553
	C	-3.57373	1.38791	0.17397
	C	-2.32475	3.44759	0.28122
	H	-4.52510	0.88059	0.27362
	H	-2.25816	4.51840	0.43992
	H	-4.43535	3.30278	0.63256
	O	-0.00011	3.44562	-0.23954
	N	-2.41604	-0.70139	-0.44566
	C	-3.67428	-1.40543	-0.53621
	H	-3.53185	-2.27553	-1.18402
	H	-4.38533	-0.75961	-1.06043
	C	-4.28018	-1.85369	0.79347
	H	-3.57244	-2.50212	1.31605
	H	-4.42795	-0.98361	1.43828
	C	-5.59953	-2.58045	0.58846
	H	-5.46611	-3.47090	-0.03183
	H	-6.33014	-1.93718	0.09060
	H	-6.03084	-2.89932	1.53901
	N	2.41614	-0.70121	-0.44562
	C	3.67441	-1.40519	-0.53618
	H	3.53206	-2.27514	-1.18420
	H	4.38552	-0.75926	-1.06016
	C	4.28010	-1.85383	0.79347
	H	3.57230	-2.50246	1.31572
	H	4.42773	-0.98396	1.43858
	C	5.59952	-2.58048	0.58846
	H	5.46625	-3.47073	-0.03215
	H	6.03067	-2.89964	1.53898
	H	6.33019	-1.93702	0.09093
	C	0.00954	0.63892	-0.16993
	C	-0.00394	-0.74545	-0.23831
	C	0.00235	-3.52753	-0.25644
	C	1.24548	-1.45460	-0.27160
	C	-1.23789	-1.46022	-0.26458
	C	-1.22836	-2.83787	-0.26022
$C^{-\bullet}$	C	1.21296	-2.84724	-0.26420
	H	-2.14625	-3.41013	-0.23987
	H	2.12817	-3.42563	-0.24665
	H	0.00154	-4.61166	-0.23790
	C	1.21086	1.36560	-0.11117
	C	3.60233	2.82344	0.05738
	C	2.48079	0.67456	-0.16605
	C	1.20491	2.77554	0.03058

	C	2.34360	3.51242	0.11082
	C	3.63812	1.41570	-0.07141
	H	2.28510	4.58949	0.22175
	H	4.60820	0.93149	-0.07885
	H	4.52944	3.37876	0.13589
	C	-1.21961	1.35678	-0.08186
	C	-3.56527	2.79631	0.11929
	C	-1.18809	2.74287	0.05375
	C	-2.44642	0.67257	-0.13048
	C	-3.62368	1.41047	-0.01320
	C	-2.36395	3.47661	0.15148
	H	-4.59193	0.92920	-0.00939
	H	-2.31695	4.55389	0.25653
	H	-4.49312	3.35149	0.20629
	O	-0.01261	3.43712	0.09466
	N	-2.42986	-0.70947	-0.30297
	C	-3.68723	-1.40456	-0.50539
	H	-3.49937	-2.26300	-1.15315
	H	-4.35509	-0.75203	-1.07198
	C	-4.36183	-1.85642	0.78359
	H	-3.67468	-2.50233	1.33706
	H	-4.54541	-0.98399	1.41739
	C	-5.66553	-2.58839	0.51043
	H	-5.49653	-3.47852	-0.10122
	H	-6.37267	-1.94826	-0.02365
	H	-6.14215	-2.90822	1.43855
	N	2.43779	-0.72168	-0.31938
	C	3.68708	-1.43476	-0.48695
	H	3.51148	-2.30052	-1.12951
	H	4.37341	-0.79269	-1.04316
	C	4.33524	-1.87666	0.81996
	H	3.63778	-2.51699	1.36752
	H	4.50704	-0.99603	1.44500
	C	5.64324	-2.61314	0.58096
	H	5.48575	-3.50948	-0.02499
	H	6.10223	-2.92420	1.52108
	H	6.36127	-1.97926	0.05379
	C	0.00000	0.63008	0.56510
	C	0.00000	-0.66349	-0.18988
	C	-0.00001	-3.11601	-1.43392
	C	1.21339	-1.27156	-0.50173
	C	-1.21340	-1.27156	-0.50173
C-H	C	-1.20846	-2.51552	-1.13287
	C	1.20844	-2.51553	-1.13288
	H	-2.13208	-3.01651	-1.38919
	H	2.13207	-3.01652	-1.38919
	H	-0.00001	-4.08257	-1.92628
	C	1.22249	1.42412	0.21901
	C	3.48457	2.92877	-0.27002

C	2.41835	0.77542	-0.09461
C	1.17407	2.80447	0.23928
C	2.29890	3.57917	0.01265
C	3.55372	1.54665	-0.34493
H	2.22578	4.65884	0.04976
H	4.49290	1.08827	-0.62212
H	4.37896	3.51040	-0.46443
C	-1.22250	1.42412	0.21901
C	-3.48457	2.92878	-0.27004
C	-1.17407	2.80447	0.23927
C	-2.41835	0.77543	-0.09462
C	-3.55372	1.54666	-0.34494
C	-2.29890	3.57917	0.01264
H	-4.49290	1.08828	-0.62213
H	-2.22577	4.65885	0.04975
H	-4.37896	3.51041	-0.46445
O	-0.00000	3.46309	0.50615
N	-2.40969	-0.62174	-0.16239
C	-3.64541	-1.38840	-0.11792
H	-3.84997	-1.85648	-1.08750
H	-4.46489	-0.69796	0.06365
C	-3.65827	-2.42501	0.99878
H	-2.80480	-3.09924	0.89895
H	-3.53614	-1.90259	1.95177
C	-4.95079	-3.22536	0.99825
H	-5.07363	-3.77489	0.06145
H	-4.96360	-3.95104	1.81299
H	-5.82029	-2.57403	1.11856
N	2.40969	-0.62174	-0.16238
C	3.64541	-1.38839	-0.11793
H	3.84996	-1.85646	-1.08752
H	4.46488	-0.69794	0.06363
C	3.65828	-2.42500	0.99877
H	2.80482	-3.09925	0.89894
H	3.53615	-1.90259	1.95176
C	4.95081	-3.22534	0.99823
H	4.96364	-3.95102	1.81297
H	5.82031	-2.57400	1.11854
H	5.07366	-3.77486	0.06143
H	0.00000	0.41575	1.64507