Supporting Information for

"Reductive Defluorination of Graphite Monofluoride by Weak, Non-Nucleophilic Reductants Reveals Low-Lying Electron-Accepting Sites"

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Table of Contents

1. General Experimental Methods

Graphite fluoride (>61 wt. %F) was purchased from Sigma-Aldrich. It was washed with deionized water at room temperature and dried at 150 ºC under vacuum for at least 24 hours before use. X-ray photoelectron spectroscopy (XPS) of ground solids shows that it has a stoichiometry of $CF_{1.0}$. Solvents such as acetonitrile (MeCN), dichloromethane (DCM), toluene, and cyclohexane were pre-dried and bubbled with N_2 for 30 min to remove oxygen before use. Unless otherwise noted, reagents were purchased from Aldrich or Alfa and were used as received.

The Raman spectra were taken with an InVia Renishaw Raman Microscope with 514.5 nm excitation. NMR spectra were recorded on a Varian Inova (400 MHz) NMR spectrometer for liquid samples, with NORELL NO. 502-7 5mm NMR sample tubes (made of ASTM Type 1 Class B borosilicate glass). Chemical shifts were reported in ppm δ. The UV-vis spectra were taken with a Varian Cary 5000 spectrometer.

The XPS spectra for all solids studied in this work were obtained after they were ground as slurries in water with an agate pestle and mortar and, unless noted otherwise, dried in vacuum at room temperature. The spectra were recorded with a PHI *Versa Probe* II Scanning X-ray Microprobe instrument with a monochromatic Al Kα X-ray source under ultrahigh vacuum (UHV) conditions. The powder samples were pelletized for XPS measurements. Scotch double-sided tape (6137H-2PC-MP) was used for sample mounting. The C 1s peak of C-F at 290.4 eV was used as an internal standard for binding energy scale calibration.[1] Survey scans were recorded using PHI software *SmartSoft* –XPS v2.0 at the 187.75 eV pass energy with the step of 0.4 eV. High resolution F 1s and C 1s XPS spectra with the 0.1 eV energy step were recorded at 2.95 eV and 11.75 eV pass energies correspondingly. The PHI *MultyPack* v9.0 software was used for data processing. Shirley background was used for quantification. In general multiple spectra were recorded on different sample areas, to quantitatively evaluate reproducibility and avoid artifacts or detect radiation damage.

For a typical reaction of GF with reductants in this study, a mixture of typically 0.2 g GF, 0.05 g reductant and 2 mL MeCN, held in a polypropylene tube, was stirred for various periods of time (ranging from hours to as long as 7 days) at room temperature. The solids were isolated by centrifugation or filtering and then were repetitively washed with MeCN, DCM, toluene, and hexane until the supernatant was colorless. Reactions of GF with vapors of reductants were also

conducted, by putting typically 0.1 g GF and 0.05 g reductant in separate arms of an H-shaped reactor connected to a vacuum line. The reductants were cooled with liquid nitrogen. The reactor was evacuated and then sealed by means of a stopcock so that GF was exposed to only the reductant vapor for up to 48 hour. In all cases XPS showed some incorporation of heteroatoms from the reductants to the solid products, i.e., 0.6 atom % Fe(III) (E_b 710.2 eV and 723.3 eV) in the case of $FeCp_2$*, 1.0 atom % N (E_b 400.8 eV) in the case of TMPD, 1.2 atom % S (E_b 164.2 eV and 165.3 eV) in the case of TTF, and 0.1 atom % Os(III) (E_b 55.7 eV and 53.3 eV) in the case of $OsCp_2$*.

For the aniline polymerization and the battery work, the graphite fluoride was used as received. XPS shows it has a C/F atomic ratio of 1.0/1.1 and thus the material is denote $CF_{1.1}$. $CF_{1.1}$ electrodes were prepared by mixing the graphite fluoride powder and Super P carbon in a mortar for fully milling. Then the polyvinylidene difluoride (PVdF) binder solution in N-methylpyrrolidone (NMP) was added into the mortar. The ratios of $CF_{1.1}$: Super P: PVdF were 85:5:10 wt. %. The mixture was grinded and dispersed for more than 1 hour to prepare a slurry. Before making the electrode, an aluminum foil was cleaned by 0.02 M sodium hydroxide (NaOH) solution in isopropanol (IPL), then cleaned with de-ionized water and acetone, and then dried. The slurry was then coated onto the aluminum foil with a casting knife, followed by evaporating the NMP solvent at 60 °C under vacuum for 12 hrs. The electrodes were then cut into circular disks with 1.1 cm diameter (0.97 cm^2 in area). The electrodes were rolled by a rolling machine before using. The GF-polyaniline electrodes were made following the same procedures with the same weight ratios. Both electrodes have similar thickness and mass loading.

Electrochemical performances of the cells were evaluated within standard CR2032 coin cell casings (D20.0 × H3.2 mm). The coin cells were assembled in the glove box. First, 1.0 M $LiPF_6$ in ethylene carbonate (EC)/diethyl carbonate (DEC) electrolyte (15 μL) was added into the electrode. Then a Celgard 2400 polypropylene separator was placed on the top of the electrode followed by adding 15 μL electrolyte on the top of the separator. Finally, lithium metal anode with a nickel foam spacer was placed on the separator. The cell was crimped and taken out of the glove box. The cell was kept rest for 15 hours before test.

The cells were galvanostatically discharged to 1.5 V on an Arbin battery cycler at a fixed *C*-rate of *C*/50, with 1*C* = 896 mA g^{-1} for GF, and 1*C* = 788 mA g^{-1} for GF-polyaniline. The

theoretical specific capacities were calculated based on the contents of fluorine in GF and GF-polyaniline. The specific capacity values shown in this work are calculated by dividing the capacities obtained by the mass of active materials. Electrochemical impedance spectroscopy (EIS) data were collected with a Bio-Logic VSP impedance analyzer in the frequency range of 200 kHz−0.1 Hz on cells.

2. Reactions of GF with $FeCp_2^*$ and $OsCp_2^*$

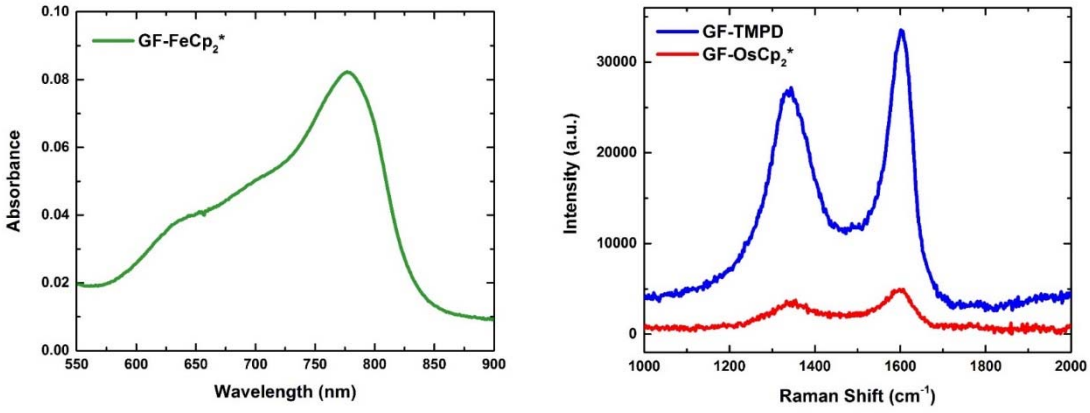

Figure S1. (Left) UV-vis spectrum of GF-$FeCp_2^*$ in MeCN after reaction. The UV-vis spectrum was obtained with the supernatant of GF-$FeCp_2^*$ reaction mixture in MeCN. The strong band at 779 nm is consistent with absorption band of $[FeCp_2^{*+}]$.[2] (Right) Raman spectrum of GF-$OsCp_2^*$ in contrast with a GF-TMPD mixture.

For a typical GF-$OsCp_2^*$ reaction, 0.15 g GF and 0.07 g $OsCp_2^*$ were mixed in 1.5 ml MeCN, contained in a polypropylene tube, stirred at room temperature for 6 days after which the reaction mixture was filtered. The solids were washed with 5 mL MeCN, four 5 mL portions of warm (50˚C) toluene and 5 mL hexane. XPS analysis demonstrated that the product contained 0.1 atom % Os with E_b Os($4f_{5/2}$) 55.7 eV and Os($4f_{7/2}$) 53.3 eV. The Os binding energies are in agreement with literature data for $[OsCp_2^*][BF_4]$.[3] Weak Raman signal from the solid (Figure S1, relative to GF-TMPD reacting at the same mole ratio for the same time) and its gray color (instead of black color as in the cases of $FeCp_2^*$ and TMPD) indicate that GF is barely reduced by $OsCp_2^*$.

3. ^{19}F-NMR of GF-$FeCp_2^*$ and GF-TTF Reactions

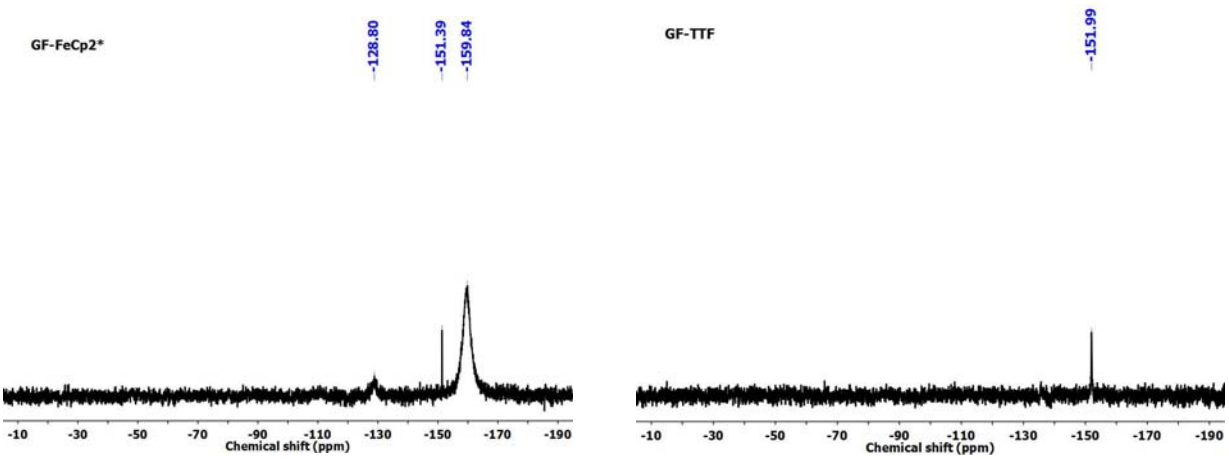

Figure S2. ^{19}F-NMR spectra of GF-FeCp$_2$* in MeCN, and GF-TTF in MeCN after reaction for 24 hours.

The liquid ^{19}F-NMR spectra above clearly show after the reactions the presence of fluorine-containing species in solution and thus defluorination of GF. The chemical shift of the peaks at ~-130 ppm and ~-152 ppm (relative to $CFCl_3$) indicates these species correspond to SiF_6^{2-} and BF_4^- respectively, presumably the reaction products of F^- with Si and B from the borosilicate glass NMR tube.[4] The peak at ~160 ppm in the GF-FeCp$_2$* reaction mixture is due to HF.[4a]

4. XPS and Fluorine Content Measurement

XPS was used to study fluorine content change after reductive defluorination. The XPS spectra for all solids studied in this work were obtained after they were ground as slurries in water with an agate pestle and mortar and, unless noted otherwise, dried in vacuum at room temperature. For TMPD and TTF, the reactions were conducted with excess reductants in MeCN for 7 days and then the solid products were washed with MeCN, DCM and

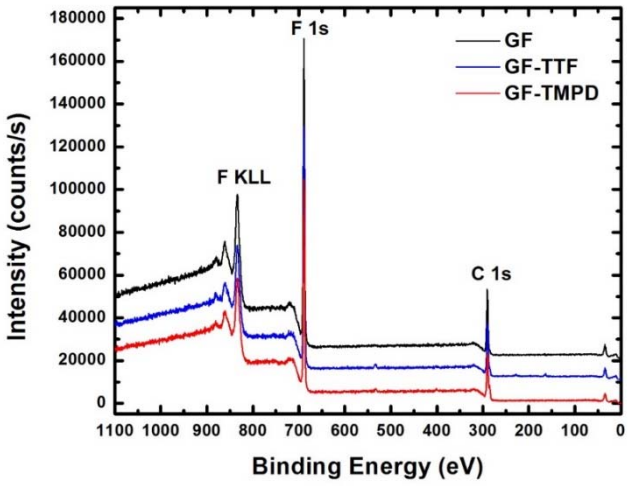

Figure S3. XPS spectra of GF and solid residues after GF reacts with TTF or TMPD.

hexanes. The XPS spectra have been calibrated according to the C 1s peak of C-F (290.4 eV). The integration of the F 1s peak over the integration of the C 1s peak (F/C ratio) shows the decrease in F content from 1.00 for GF to 0.927 for GF-TTF and 0.710 for GF-TMPD after reaction.

Table S1. Fluorine content of GF, GF-TTF and GF-TMPD

Sample	GF	GF-TTF	GF-TMPD
F/C Ratio	1.00	0.927	0.710

For GF-aniline reactions, the high-resolution XPS spectra are normalized according to the C 1s peak (294-284 eV). Figure S4A shows shift of C 1s peak to lower binding energy, due to partial conversion of F-bonded sp^3 C (290.3 eV) to sp^2 C and, to a far less extent, presence of polyaniline (4%). A broad peak with peak position at 285.5 eV appears as a result of the reduction. Note a minor peak at the same position exists in GF before reduction, indicating existence of sp^2 C in the starting material. This is consistent with the gray color of all commercially available GF. Figure S4B shows the decrease of fluorine content from the original 1.1 F/C to 0.8 F/C. Figure S4C shows the increase of nitrogen content by 0.7%, due to presence of aniline oligomers and polymers. Some N atoms are also present in the starting material GF with binding energy (403 eV) corresponding to pyridine N-oxides.[5]

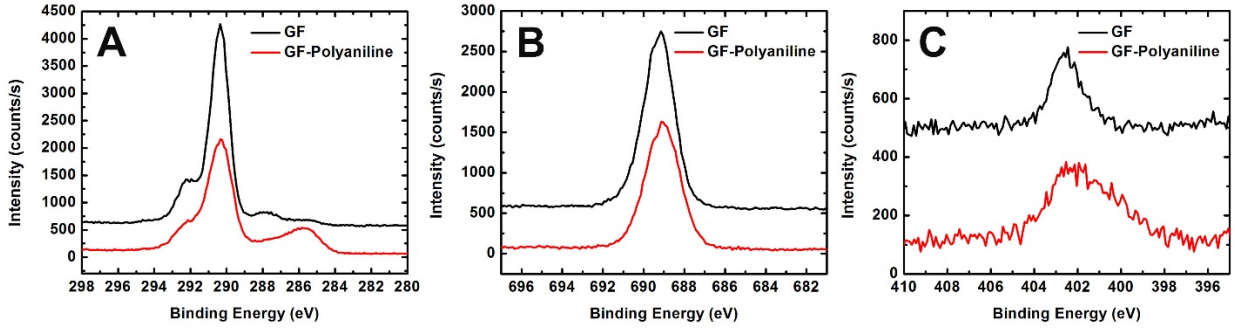

Figure S4. XPS spectra of GF and GF-Polyaniline. A) C 1s peak. B) F 1s peak. C) N 1s peak.

5. IR Characterization of GF-Polyaniline Composite

IR spectra confirmed the presence of polyaniline in the solid products of the GF-aniline reaction. Shown in figure S5, the IR bands at 1594, 1497, 1310, 1259, and 800 cm^{-1} (red curve)

are consistent with emeraldine, i.e., the conductive form of polyaniline. Among these the 1595 and 1497 cm^{-1} bands are assigned to quinonoid and benzenoid ring-stretching vibrations, respectively. The 1310 and 1259 cm^{-1} bands are due to C-N stretching, and the 800 cm^{-1} band due to out-of-plane C-H bending mode of the *p*-disubstituted phenyl rings. Therefore, mixing aniline with GF produces sp^2-carbon from partial reduction of the GF and at the same time conjugated polyaniline due to the oxidative polymerization of aniline, both of which could contribute to electrical conductivity of the composite material.

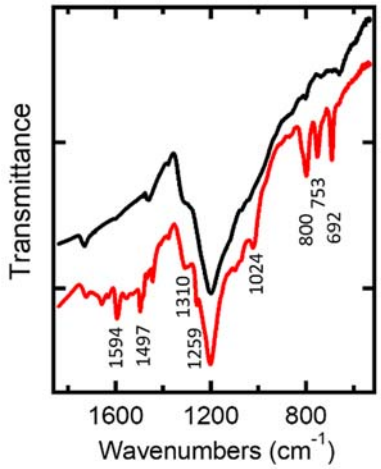

Figure S5. IR spectra of GF (black curve) and the GF-polyaniline composite materials we made (red), both obtained in KBr pellets. The 753 and 692 cm^{-1} bands due to residual aniline. The broad peak at 1200 cm^{-1} is due to C-F stretching.

6. Quantum Chemistry Calculations

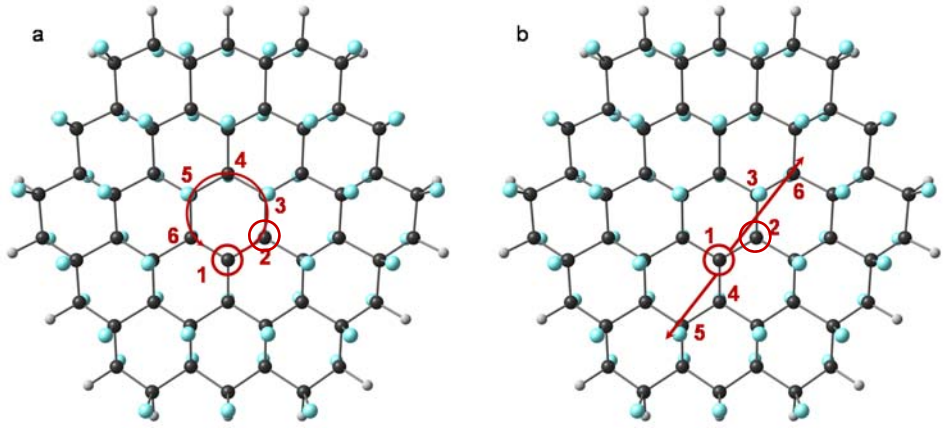

Figure S6. Depiction of how sp^2-carbon propagates along a (a) ring and (b) zigzag path as defluorination proceeds. The carbon atoms labeled as **1** and **2** are the two sp^2 atoms we started with.

Electron affinities of a C=C bond in GF was calculated with a fragment of graphene fluoride with the formula of $C_{54}F_{52}H_{18}$ (figure S6). It is assumed to be terminated by 18 H atoms on the periphery because H has similar electronegativity as C. Possible artifact caused by assuming such H termination as well as the size is excluded by varying the size of the fragment and obtaining converging values (see below). The calculated electron affinities of $C_{54}F_{52}H_{18}$ and possible products after stepwise reduction and defluorination in acetonitrile are shown in Table S2. The two columns (ring and zigzag) are for two examples of defluorination paths (or the growth paths of conjugated sp^2-carbon atoms) shown in Figure S6, starting with the two sp^2-atoms marked by the red circles. Starting from $C_{54}F_{52}H_{18}$, eliminating an odd number of F atoms leads to free radicals which have greater electron affinities and thus exist as reactive intermediates. Eliminating an even number of F atoms leads to conjugated alkenes with increased conjugation length, which also have greater electron affinities unless a benzene ring is formed (Table S2). Thus our calculations so far suggest that the defluorination in principle could proceed like a random walk in the lattice until a fully closed benzene ring is formed. This will be investigated in more detail in the future. Further we note that presence of radical species in GF is well documented,[6] and our samples are no exception (shown by EPR with g=2.003, figure S8). The radical species formed during the making of GF and, as our calculations have suggested, may also serve as electron-accepting sites for the reduction.

Density functional theory calculations were performed with the Gaussian 09 program suite[7] and the M06-2X density functional.[8] Geometries and frequencies were obtained with the 6-31G(d,p) basis set, solvation corrections in acetonitrile (dielectric constant 36.6) were obtained with the 6-31+G(d,p) basis set[9] and SMD solvation model,[10] and gas phase single point energies were obtained with the 6-311+G(2df,p) basis set.[11] Electron affinities are calculated by subtracting the free energy of the neutral species in solvent and that of a free

Table S2

	Electron Affinity in Acetonitrile (eV)	
# of eliminated F	Ring	Zigzag
0	3.82	
1	5.36	
2	4.42	
3	5.49	4.25
4	3.36	5.29

electron in vacuum from the free energy of the anionic species in solvent. A detailed procedure was described elsewhere. [12]

To eliminate possible artifact caused by assuming H termination and finite size of the models we varied the size of the models to obtain converging electron affinity values. A smaller model ($C_{42}F_{40}H_{16}$) gives electron affinities that differ from those of the larger model by less than 0.2 eV. Figure S7 shows the two largest model systems we calculated.

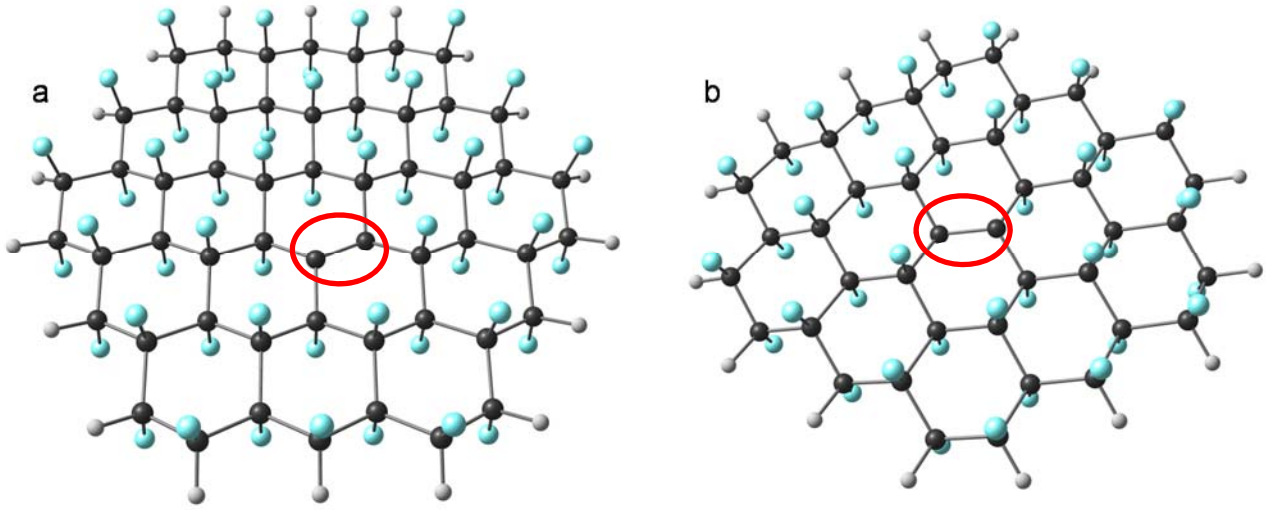

Figure S7. Model systems of two sizes. a) $C_{54}F_{52}H_{18}$. b) $C_{42}F_{40}H_{16}$. Circled are the starting sp^2-carbon atoms.

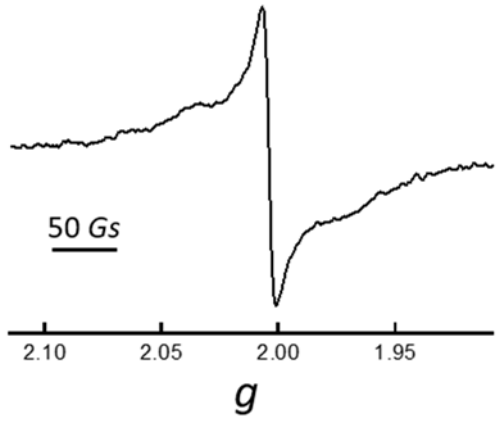

Figure S8. EPR spectrum of GF ($CF_{1.0}$). The spectrum was taken with a Bruker EMX X-band EPR spectrometer with an ER 4119 HS cavity (9.840 GHz at room temperature). A Wilmad quartz EPR sample tubes (outer diameter 4 mm) were used for EPR measurements.

7. Thermodynamics of GF Reduction

By assuming a residual π-bond in GF as an electron acceptor, we can estimate the thermodynamics of electron transfer between the reductants we used and GF. Following the Rehm-Weller equation:[13]

$$\frac{\Delta G}{F} = -(E_A - E_D) - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r R_{DA}},$$

where F is the Faraday constant, E_A and E_D the electron affinity of the oxidant and the standard reduction potential of the reductant, respectively. The third term in the equation is the Coulomb potential between the two ions generated after the electron transfer, with R_{DA} being the distance between them, ε_0 and ε_r the dielectric constant of vacuum and the media around the ion pair, respectively. The standard states for the ΔG calculated are reactants and products in solution with 1M concentration.

With TMPD as an example ($E_D = 4.85\ eV$), and our calculated $E_A = 3.8\ eV$, and assuming $R_{DA} = 5$Å, we get

$$\Delta G\ (\text{in } eV) \approx 1.0 - \frac{2.88}{\varepsilon_r}.$$

Uncertainty in the estimated ΔG arises due to the difficulty in obtaining the dielectric constant at the interface, ε_r, where the electron transfer occurs. The lower limit of ε_r is 2.1 (that of Teflon). The upper limit can be estimated to be 19 (average of 2.1 and that of acetonitrile, 36.6) by applying a continuum dielectric model for charges at the interface between two continuous media.[14] The latter is almost certainly an overestimate because a polar liquid such as acetonitrile near the GF surface with aligned C-F bonds will have restricted orientational dynamics and will have lower dielectric constant than the bulk.[15] We estimate that ΔG has a value between -0.37 and + 0.85 eV, with a median of approximately -0.2 eV, or -5 kcal/mol. Elimination of F^- after reduction of GF will shift the equilibrium in the direction favoring the reduction. In addition, in the experiments we used reductants in large excess, which also favors reduction.

Defluorination produces either radical species or conjugated alkenes with increasing conjugation length, which have increased electron affinities (Table S2) and make further reduction more favorable.

8. Model System Coordinates (Calculated)

$C_{54}F_{52}H_{18}$

	X	Y	Z
0	-1.171690000	-0.218235000	
C	-0.626948000	-1.301484000	0.208432000
C	3.559898000	1.627491000	0.258980000
C	2.913455000	0.297820000	-0.204140000
C	3.790537000	-0.918859000	0.222893000
C	3.162160000	-2.260303000	-0.241314000
C	1.692699000	-2.391771000	0.239920000
F	0.863400000	-1.118285000	-1.582679000
F	2.876785000	0.323223000	-1.569418000
C	-2.918326000	-0.216460000	0.195359000
C	-3.567138000	-1.568104000	-0.232105000
C	-2.715370000	-2.779143000	0.236133000
C	-1.246548000	-2.652448000	-0.246539000
C	-3.146623000	2.313398000	0.189985000
C	-3.791016000	0.978956000	-0.262529000
C	-4.019419000	3.526883000	-0.231821000
C	-3.393174000	4.862822000	0.216603000
C	-1.924565000	4.997183000	-0.236645000
C	1.016913000	5.256277000	0.238750000
C	2.486700000	5.382467000	-0.212119000
C	3.336916000	4.175818000	0.233842000

C	5.014209000	1.755944000	-0.261220000
C	5.881693000	0.547936000	0.146959000
C	5.253885000	-0.792352000	-0.282034000
C	-0.400744000	-3.859546000	0.235634000
C	1.071633000	-3.730101000	-0.237213000
C	4.013585000	-3.467084000	0.220790000
C	1.918040000	-4.936110000	0.233426000
C	3.387409000	-4.807513000	-0.211147000
C	5.476480000	-3.337378000	-0.241659000
C	6.103047000	-1.997274000	0.160226000
F	-0.652125000	-1.250293000	1.572800000
F	1.704263000	-2.418215000	1.605287000
F	3.178792000	-2.287156000	-1.608633000
F	3.877116000	-0.934212000	1.587586000
F	3.639939000	1.636948000	1.622975000
H	-3.958147000	5.664791000	-0.278524000
F	5.277510000	-0.811749000	-1.653710000
C	5.653078000	3.092088000	0.159522000
F	5.013104000	1.779223000	-1.634569000
C	4.801487000	4.301811000	-0.242262000
F	3.412053000	4.237357000	1.603777000
C	0.168962000	6.456951000	-0.207658000
F	-1.942872000	5.066191000	-1.608644000
F	1.087564000	-3.760380000	-1.603909000

F	2.671934000	2.836510000	-1.560283000
F	1.298200000	2.806191000	1.698581000
F	0.432646000	3.892969000	-1.576083000
F	-1.107905000	3.753930000	1.574253000
F	-1.773415000	2.539142000	-1.702498000
F	-3.126529000	2.322262000	1.557864000
F	-1.253713000	-2.684195000	-1.611824000
C	-1.299805000	6.327204000	0.211872000
H	-1.861190000	7.129518000	-0.283390000
F	1.021172000	5.324545000	1.610942000
F	1.546829000	0.080761000	1.696660000
F	4.072454000	-3.495295000	1.592404000
C	-3.344461000	-4.118361000	-0.218185000
C	-4.807260000	-4.246262000	0.247743000
C	-5.659124000	-3.036864000	-0.154286000
C	-5.024354000	-1.697170000	0.276950000
C	-1.023435000	-5.197034000	-0.229220000
C	-2.492693000	-5.327100000	0.217576000
C	-0.174830000	-6.401497000	0.212978000
C	1.293907000	-6.271710000	-0.206389000
C	-5.887440000	-0.492194000	-0.141308000
C	-5.243991000	0.849677000	0.263167000
C	-6.108765000	2.052542000	-0.154642000
C	-5.482559000	3.392974000	0.246937000

H	1.854421000	-7.068295000	0.299317000
H	-0.586420000	-7.284993000	-0.291472000
H	-2.906489000	-6.209893000	-0.289529000
H	-5.225774000	-5.128581000	-0.252998000
H	-6.618310000	-3.117191000	0.372964000
H	-6.837607000	-0.571403000	0.404876000
H	-7.064472000	1.960295000	0.377000000
H	-6.050597000	4.190817000	-0.247472000
F	-5.242121000	0.874252000	1.636516000
F	-3.400343000	-4.161383000	-1.589588000
F	-1.028683000	-5.252103000	-1.601445000
F	-5.036012000	-1.718722000	1.649817000
H	7.065835000	-1.914648000	-0.360483000
H	6.835520000	0.642152000	-0.390876000
H	6.042044000	-4.131958000	0.261502000
H	3.948904000	-5.602536000	0.299136000
H	6.611133000	3.170177000	-0.370176000
H	5.219943000	5.187001000	0.252738000
H	2.901993000	6.269395000	0.286300000
H	0.581317000	7.344551000	0.288630000
F	-4.107535000	3.577714000	-1.601423000
F	-3.875907000	0.976326000	-1.626254000
F	-3.650919000	-1.599724000	-1.596439000
F	-2.723845000	-2.803365000	1.603541000

F	-0.410818000	-3.887017000	1.602491000
F	1.931194000	-4.985801000	1.605773000
F	1.371266000	-6.437971000	-1.560071000
F	3.486053000	-4.962441000	-1.560865000
F	5.587700000	-3.474936000	-1.596007000
F	4.876008000	4.446239000	-1.598391000
F	2.552761000	5.534891000	-1.563832000
F	0.215318000	6.619002000	-1.563883000
F	-6.327182000	2.064508000	-1.503028000
F	-6.118467000	-0.517274000	-1.483484000
F	-5.865607000	-3.084520000	-1.503074000
F	-2.561481000	-5.492201000	1.567786000
F	-0.222106000	-6.576465000	1.566933000
F	6.306784000	-2.004046000	1.510160000
F	6.103532000	0.561417000	1.490603000
F	5.863281000	3.140500000	1.508378000
F	-1.374061000	6.476795000	1.568239000
F	-3.481797000	4.997617000	1.568804000
F	-5.579362000	3.522515000	1.603058000
F	-2.883803000	-0.185895000	1.560615000
F	-1.536198000	-0.191055000	-1.706800000
F	-4.889949000	-4.398415000	1.602582000

$C_{54}F_{51}H_{18}^{\bullet}$

	X	Y	Z
C	1.233876000	-0.781229000	-0.015743000
C	0.004832000	-1.455673000	0.063098000
C	0.008861000	-2.969940000	0.348872000
C	2.545210000	-1.511182000	-0.287994000
C	2.561931000	-2.968037000	0.242102000
C	1.277712000	-3.706575000	-0.179658000
C	1.268895000	0.701990000	-0.359223000
C	-1.255839000	-3.713716000	-0.179099000
C	-1.228546000	-0.787922000	-0.010458000
C	-1.272887000	0.694488000	-0.356393000
C	-0.003866000	1.421522000	0.145136000
C	-2.544663000	-2.983576000	0.244317000
C	-2.536053000	-1.525254000	-0.280325000
C	-3.813021000	-0.784737000	0.225736000
C	-3.838043000	0.692580000	-0.246068000
C	-2.542025000	1.415311000	0.192910000
F	-1.310256000	0.780148000	-1.727288000
F	-2.641799000	-1.569437000	-1.654875000
C	2.534228000	1.429195000	0.189630000
C	2.550611000	2.927882000	-0.227823000
C	1.263923000	3.655895000	0.244421000
C	-0.008644000	2.923864000	-0.258190000
C	3.819150000	-0.763956000	0.213334000

C	3.834807000	0.715110000	-0.251832000
C	5.119910000	-1.494977000	-0.218541000
C	5.123350000	-2.970695000	0.228415000
C	3.843763000	-3.713231000	-0.212912000
C	1.294520000	-5.191088000	0.270905000
C	0.017831000	-5.937444000	-0.167797000
C	-1.263643000	-5.198831000	0.270184000
C	-3.821097000	-3.735255000	-0.215595000
C	-5.106550000	-3.001635000	0.223623000
C	-5.108553000	-1.520986000	-0.204906000
C	-1.285691000	3.648587000	0.244128000
C	-2.567713000	2.912679000	-0.227919000
C	-5.104384000	1.419247000	0.270480000
C	-3.834795000	3.637181000	0.285372000
C	-5.123523000	2.906091000	-0.134035000
C	-6.391130000	0.688293000	-0.156752000
C	-6.387267000	-0.791387000	0.244912000
F	-0.002488000	1.324869000	1.509289000
F	-2.497180000	1.362575000	1.558175000
F	-3.913970000	0.718434000	-1.610363000
F	-3.808437000	-0.795050000	1.593394000
F	-2.572669000	-2.956931000	1.612262000
H	5.969930000	-3.458146000	-0.274429000
F	-5.190341000	-1.525183000	-1.578677000

C	-3.819012000	-5.208285000	0.228184000
F	-3.851922000	-3.789723000	-1.587874000
C	-2.536872000	-5.941669000	-0.182113000
F	-1.298596000	-5.257768000	1.642479000
C	2.572462000	-5.926376000	-0.179685000
F	3.878228000	-3.768111000	-1.585236000
F	-2.628431000	2.977338000	-1.592462000
F	-1.226514000	-3.717243000	-1.547257000
F	0.008235000	-3.077820000	1.717662000
F	1.247258000	-3.711290000	-1.547791000
F	2.586159000	-2.936947000	1.610046000
F	2.650764000	-1.557078000	-1.662513000
F	3.817211000	-0.775929000	1.581284000
F	-0.008635000	2.988865000	-1.622477000
C	3.849970000	-5.185480000	0.231740000
H	4.695823000	-5.669824000	-0.272065000
F	1.328940000	-5.248965000	1.643253000
F	-5.119625000	1.397406000	1.643930000
C	1.264632000	5.143541000	-0.189293000
C	2.537021000	5.877132000	0.276236000
C	3.819147000	5.143667000	-0.133955000
C	3.812443000	3.659746000	0.288195000
C	-1.295198000	5.135886000	-0.190249000
C	-0.017688000	5.872693000	0.262259000

C	-2.572403000	5.861838000	0.273829000
C	-3.849730000	5.120716000	-0.137521000
C	5.106094000	2.936625000	-0.129138000
C	5.094505000	1.448881000	0.271969000
C	6.386940000	0.726505000	-0.150861000
C	6.391557000	-0.752948000	0.251037000
H	-4.689670000	5.592673000	0.388183000
H	-2.580723000	6.840964000	-0.221467000
H	-0.020344000	6.854290000	-0.231622000
H	2.540039000	6.856298000	-0.219031000
H	4.655743000	5.620213000	0.392938000
H	5.932164000	3.411154000	0.418497000
H	7.214745000	1.215235000	0.378824000
H	7.241158000	-1.234190000	-0.249175000
F	5.104509000	1.425827000	1.645402000
F	1.292735000	5.221641000	-1.560188000
F	-1.322765000	5.213302000	-1.561189000
F	3.807105000	3.675107000	1.661437000
H	-7.227687000	-1.279982000	-0.263313000
H	-5.947969000	-3.487370000	-0.289085000
H	-7.223147000	1.170588000	0.372193000
H	-5.953700000	3.377164000	0.410386000
H	-4.661598000	-5.697113000	-0.276791000
H	-2.532647000	-6.916462000	0.321485000

H	0.020500000	-6.911230000	0.341006000
H	2.573188000	-6.901371000	0.323576000
F	5.210977000	-1.503139000	-1.588849000
F	3.913753000	0.745444000	-1.615855000
F	2.612426000	2.995125000	-1.592206000
F	1.255365000	3.658559000	1.612095000
F	-1.277526000	3.651765000	1.611800000
F	-3.831681000	3.652830000	1.658643000
F	-4.012727000	5.255541000	-1.486435000
F	-5.319936000	3.026791000	-1.476666000
F	-6.588977000	0.772583000	-1.505419000
F	-2.554755000	-6.117190000	-1.536762000
F	0.018887000	-6.115832000	-1.518072000
F	2.593111000	-6.101282000	-1.534412000
F	6.586519000	0.809979000	-1.499498000
F	5.305631000	3.061071000	-1.471076000
F	3.982775000	5.280207000	-1.482622000
F	-0.018747000	6.031907000	1.614678000
F	-2.589279000	6.026359000	1.629760000
F	-6.553202000	-0.866293000	1.599447000
F	-5.262713000	-3.099164000	1.573805000
F	-3.960197000	-5.319140000	1.582935000
F	3.991152000	-5.293395000	1.586751000
F	5.271448000	-3.055734000	1.579673000

F	6.544403000	-0.827989000	1.606211000
F	2.491486000	1.373628000	1.554863000
F	1.305926000	0.789463000	-1.730025000
F	2.551493000	6.041727000	1.632176000

$C_{54}F_{50}H_{18}$ Ring

	X	Y	Z
C	0.010135000	1.450553000	0.084664000
C	-0.026790000	0.748719000	1.236038000
C	-0.314089000	1.470507000	2.563782000
C	0.279063000	2.952489000	0.047744000
C	-0.246603000	3.686795000	1.303823000
C	0.186711000	2.943514000	2.581969000
C	0.283784000	0.722589000	-1.225098000
C	0.211081000	0.742448000	3.838478000
C	0.026790000	-0.748719000	1.236038000
C	-0.010135000	-1.450553000	0.084664000
C	-0.283784000	-0.722589000	-1.225098000
C	-0.211081000	-0.742448000	3.838478000
C	0.314089000	-1.470507000	2.563782000
C	-0.186711000	-2.943514000	2.581969000
C	0.246603000	-3.686795000	1.303823000
C	-0.279063000	-2.952489000	0.047744000
F	1.686194000	-1.492372000	2.658772000

C	-0.214801000	1.474975000	-2.500017000
C	0.232534000	0.740643000	-3.797741000
C	-0.232534000	-0.740643000	-3.797741000
C	0.214801000	-1.474975000	-2.500017000
C	-0.224188000	3.678684000	-1.234677000
C	0.246746000	2.953134000	-2.521338000
C	0.206120000	5.169339000	-1.247627000
C	-0.246304000	5.904153000	0.029476000
C	0.196951000	5.169385000	1.311462000
C	-0.278679000	3.687030000	3.860832000
C	0.163046000	2.954755000	5.144374000
C	-0.255094000	1.468432000	5.134013000
C	0.255094000	-1.468432000	5.134013000
C	-0.163046000	-2.954755000	5.144374000
C	0.278679000	-3.687030000	3.860832000
C	-0.246746000	-2.953134000	-2.521338000
C	0.224188000	-3.678684000	-1.234677000
C	-0.196951000	-5.169385000	1.311462000
C	-0.206120000	-5.169339000	-1.247627000
C	0.246304000	-5.904153000	0.029476000
C	0.258771000	-5.900417000	2.584238000
C	-0.156651000	-5.165171000	3.864167000
F	-1.655897000	-0.652439000	-1.300459000
F	-1.651790000	-3.061971000	0.026760000

F	1.615036000	-3.682074000	1.270252000
F	-1.554547000	-2.937631000	2.607926000
F	-1.578285000	-0.781971000	3.838128000
H	0.250563000	6.884307000	0.031118000
F	1.651844000	-3.728298000	3.888851000
C	-0.197219000	-0.740788000	6.418691000
F	1.627503000	-1.450327000	5.196969000
C	0.197219000	0.740788000	6.418691000
F	-1.627503000	1.450327000	5.196969000
C	0.156651000	5.165171000	3.864167000
F	1.568839000	5.235038000	1.343953000
F	1.592401000	-3.678792000	-1.226304000
F	1.578285000	0.781971000	3.838128000
F	-1.686194000	1.492372000	2.658772000
F	1.554547000	2.937631000	2.607926000
F	-1.615036000	3.682074000	1.270252000
F	1.651790000	3.061971000	0.026760000
F	-1.592401000	3.678792000	-1.226304000
F	1.581270000	-1.492085000	-2.480526000
C	-0.258771000	5.900417000	2.584238000
H	0.235513000	6.880331000	2.587064000
F	-1.651844000	3.728298000	3.888851000
F	-1.568839000	-5.235038000	1.343953000
C	0.254338000	-1.471230000	-5.075814000

C	-0.196951000	-0.740697000	-6.359659000
C	0.196951000	0.740697000	-6.359659000
C	-0.254338000	1.471230000	-5.075814000
C	0.259823000	-3.683021000	-3.793320000
C	-0.163506000	-2.954801000	-5.085462000
C	-0.155645000	-5.165460000	-3.804971000
C	0.259012000	-5.900430000	-2.525229000
C	0.163506000	2.954801000	-5.085462000
C	-0.259823000	3.683021000	-3.793320000
C	0.155645000	5.165460000	-3.804971000
C	-0.259012000	5.900430000	-2.525229000
H	-0.235483000	-6.879985000	-2.526688000
H	0.369181000	-5.638734000	-4.644628000
H	0.371228000	-3.434642000	-5.916860000
H	0.322561000	-1.222874000	-7.197563000
H	-0.322561000	1.222874000	-7.197563000
H	-0.371228000	3.434642000	-5.916860000
H	-0.369181000	5.638734000	-4.644628000
H	0.235483000	6.879985000	-2.526688000
F	-1.633389000	3.702107000	-3.797087000
F	1.626803000	-1.459458000	-5.121172000
F	1.633389000	-3.702107000	-3.797087000
F	-1.626803000	1.459458000	-5.121172000
H	0.353411000	-5.646844000	4.708092000

H	0.357729000	-3.431250000	5.986239000
H	-0.235513000	-6.880331000	2.587064000
H	-0.250563000	-6.884307000	0.031118000
H	0.317322000	-1.226779000	7.257243000
H	-0.317322000	1.226779000	7.257243000
H	-0.357729000	3.431250000	5.986239000
H	-0.353411000	5.646844000	4.708092000
F	1.576491000	5.254221000	-1.280866000
F	1.611684000	2.993404000	-2.570631000
F	1.598815000	0.764182000	-3.858218000
F	-1.598815000	-0.764182000	-3.858218000
F	-1.611684000	-2.993404000	-2.570631000
F	-1.576491000	-5.254221000	-1.280866000
F	1.615035000	-6.063889000	-2.543754000
F	1.598641000	-6.067723000	0.026481000
F	1.615209000	-6.064872000	2.603700000
F	1.549879000	0.826627000	6.587505000
F	1.511166000	3.061426000	5.307287000
F	1.509771000	5.284289000	4.008346000
F	1.505343000	5.302955000	-3.964454000
F	1.508381000	3.067790000	-5.269335000
F	1.547838000	0.827969000	-6.538883000
F	-1.508381000	-3.067790000	-5.269335000
F	-1.505343000	-5.302955000	-3.964454000

F	-1.509771000	-5.284289000	4.008346000
F	-1.511166000	-3.061426000	5.307287000
F	-1.549879000	-0.826627000	6.587505000
F	-1.615209000	6.064872000	2.603700000
F	-1.598641000	6.067723000	0.026481000
F	-1.615035000	6.063889000	-2.543754000
F	-1.581270000	1.492085000	-2.480526000
F	1.655897000	0.652439000	-1.300459000
F	-1.547838000	-0.827969000	-6.538883000

$C_{54}F_{49}H_{18}^{\bullet}$ Ring

	X	Y	Z
C	-1.424559000	0.155221000	-0.102741000
C	-0.646719000	1.278436000	0.020025000
C	-1.296090000	2.639728000	0.318365000
C	-2.936116000	0.223172000	-0.324852000
C	-3.582695000	1.522185000	0.226662000
C	-2.760993000	2.752159000	-0.196048000
C	-0.789205000	-1.182941000	-0.455680000
C	-0.484652000	3.864895000	-0.199193000
C	0.792451000	1.186614000	0.030500000
C	1.429167000	-0.106580000	0.019042000
C	0.690387000	-1.256052000	-0.103196000
C	0.992513000	3.771245000	0.237537000

C	1.629876000	2.441255000	-0.259996000
C	3.104800000	2.367990000	0.234031000
C	3.756061000	1.037997000	-0.200955000
C	2.935391000	-0.181996000	0.316828000
F	1.673826000	2.507640000	-1.637317000
C	-1.592355000	-2.386406000	0.143391000
C	-0.971814000	-3.758245000	-0.251076000
C	0.504783000	-3.834159000	0.209729000
C	1.333328000	-2.625506000	-0.325632000
C	-3.734383000	-1.005741000	0.210206000
C	-3.097271000	-2.339990000	-0.250934000
C	-5.236728000	-0.927376000	-0.188027000
C	-5.883061000	0.398429000	0.268264000
C	-5.070820000	1.627403000	-0.196076000
C	-3.421514000	4.074748000	0.270918000
C	-2.607159000	5.307998000	-0.169357000
C	-1.127432000	5.205456000	0.255391000
C	1.806182000	5.009412000	-0.239253000
C	3.288590000	4.928671000	0.184862000
C	3.939834000	3.598970000	-0.242902000
C	2.780648000	-2.723395000	0.226461000
C	3.601329000	-1.492427000	-0.196454000
C	5.239629000	0.957309000	0.255284000
C	5.075597000	-1.595026000	0.271244000

C	5.902055000	-0.369835000	-0.168601000
C	6.063873000	2.179495000	-0.202763000
C	5.411696000	3.507834000	0.197987000
F	3.031414000	-0.169726000	1.688230000
F	3.766242000	1.013297000	-1.568868000
F	3.105735000	2.405077000	1.601824000
F	1.025651000	3.785235000	1.605126000
H	-6.867718000	0.459931000	-0.215297000
F	3.986666000	3.612444000	-1.615516000
C	1.161516000	6.343555000	0.197574000
F	1.798928000	5.056425000	-1.612287000
C	-0.315249000	6.436050000	-0.203314000
F	-1.111605000	5.274901000	1.627557000
C	-4.896080000	4.173465000	-0.161700000
F	-5.157045000	1.660334000	-1.566809000
F	3.620240000	-1.468985000	-1.564785000
F	-0.510825000	3.863594000	-1.567037000
F	-1.322918000	2.732775000	1.689745000
F	-2.745765000	2.778401000	-1.564351000
F	-3.568071000	1.480999000	1.594955000
F	-3.097374000	0.211942000	-1.692693000
F	-3.706551000	-0.984347000	1.578122000
F	1.385427000	-2.778462000	-1.693495000
C	-5.714294000	2.947630000	0.260128000

H	-6.693435000	3.012856000	-0.230733000
F	-3.460451000	4.104697000	1.644098000
F	5.297107000	0.998009000	1.627459000
C	1.153828000	-5.191582000	-0.187688000
C	0.334170000	-6.407594000	0.302634000
C	-1.142612000	-6.314846000	-0.098202000
C	-1.779186000	-4.963942000	0.302636000
C	3.449237000	-4.057587000	-0.195501000
C	2.626012000	-5.279332000	0.269011000
C	4.915142000	-4.144962000	0.261040000
C	5.733040000	-2.918912000	-0.160774000
C	-3.269466000	-4.899719000	-0.085122000
C	-3.900867000	-3.548246000	0.302526000
C	-5.392596000	-3.479008000	-0.098571000
C	-6.045159000	-2.150927000	0.302088000
H	6.704810000	-2.973995000	0.345910000
H	5.351489000	-5.024367000	-0.229001000
H	3.060928000	-6.165113000	-0.214106000
H	0.762007000	-7.293497000	-0.182718000
H	-1.685049000	-7.096673000	0.448690000
H	-3.788662000	-5.677874000	0.490897000
H	-5.906389000	-4.280044000	0.448152000
H	-7.027262000	-2.095869000	-0.183554000
F	-3.891869000	-3.508619000	1.675851000

F	1.161891000	-5.314252000	-1.555703000
F	3.512962000	-4.125244000	-1.566209000
F	-1.746463000	-4.940390000	1.675993000
H	5.949463000	4.313847000	-0.317079000
H	3.819923000	5.734975000	-0.339139000
H	7.035154000	2.116096000	0.303528000
H	6.869855000	-0.427853000	0.348210000
H	1.702656000	7.143812000	-0.322471000
H	-0.747423000	7.308818000	0.301962000
H	-3.032300000	6.179748000	0.346768000
H	-5.320389000	5.050021000	0.343961000
F	-5.352658000	-0.967193000	-1.556066000
F	-3.186589000	-2.424200000	-1.612600000
F	-1.015456000	-3.873212000	-1.612727000
F	0.513487000	-3.799166000	1.577586000
F	2.735848000	-2.724984000	1.594702000
F	5.116964000	-1.619691000	1.644455000
F	5.911080000	-2.964478000	-1.514766000
F	6.090837000	-0.390448000	-1.517593000
F	6.242576000	2.179777000	-1.557060000
F	-0.383076000	6.599700000	-1.557862000
F	-2.697914000	5.473539000	-1.518474000
F	-5.005568000	4.318940000	-1.515935000
F	-5.554745000	-3.655470000	-1.442667000

F	-3.420532000	-5.126305000	-1.419970000
F	-1.243336000	-6.532735000	-1.442270000
F	2.694868000	-5.404857000	1.623121000
F	5.006618000	-4.275143000	1.618361000
F	5.534878000	3.656152000	1.550634000
F	3.399335000	5.093741000	1.532591000
F	1.253099000	6.519294000	1.549224000
F	-5.871028000	2.982060000	1.617272000
F	-6.026012000	0.413749000	1.622281000
F	-6.193508000	-2.142217000	1.659997000
F	-1.503841000	-2.253711000	1.503789000
F	-0.867002000	-1.299622000	-1.837480000
F	0.398964000	-6.540907000	1.660622000

$C_{54}F_{48}H_{18}$ Ring

	X	Y	Z
C	0.000000000	1.409800000	-0.000295000
C	1.220923000	0.704900000	0.000295000
C	2.533509000	1.462722000	0.279927000
C	0.000000000	2.925444000	-0.279927000
C	1.267363000	3.672754000	0.222430000
C	2.547017000	2.933945000	-0.222430000
C	-1.220923000	0.704900000	0.000295000
C	3.814380000	0.738809000	-0.222430000

C	1.220923000	-0.704900000	-0.000295000
C	0.000000000	-1.409800000	0.000295000
C	-1.220923000	-0.704900000	-0.000295000
C	3.814380000	-0.738809000	0.222430000
C	2.533509000	-1.462722000	-0.279927000
C	2.547017000	-2.933945000	0.222430000
C	1.267363000	-3.672754000	-0.222430000
C	0.000000000	-2.925444000	0.279927000
F	2.613650000	-1.508992000	-1.653918000
C	-2.533509000	1.462722000	0.279927000
C	-3.814380000	0.738809000	-0.222430000
C	-3.814380000	-0.738809000	0.222430000
C	-2.533509000	-1.462722000	-0.279927000
C	-1.267363000	3.672754000	0.222430000
C	-2.547017000	2.933945000	-0.222430000
C	-1.279100000	5.157094000	-0.239526000
C	0.000000000	5.904900000	0.189727000
C	1.279100000	5.157094000	-0.239526000
C	3.826625000	3.686280000	0.239526000
C	5.113793000	2.952450000	-0.189727000
C	5.105725000	1.470814000	0.239526000
C	5.105725000	-1.470814000	-0.239526000
C	5.113793000	-2.952450000	0.189727000
C	3.826625000	-3.686280000	-0.239526000

C	-2.547017000	-2.933945000	0.222430000
C	-1.267363000	-3.672754000	-0.222430000
C	1.279100000	-5.157094000	0.239526000
C	-1.279100000	-5.157094000	0.239526000
C	0.000000000	-5.904900000	-0.189727000
C	2.555395000	-5.903605000	-0.206070000
C	3.834974000	-5.164839000	0.206070000
F	0.000000000	-3.017983000	1.653918000
F	1.248601000	-3.689854000	-1.590303000
F	2.571206000	-2.926248000	1.590303000
F	3.819808000	-0.763606000	1.590303000
H	0.000000000	6.873153000	-0.329266000
F	3.851747000	-3.740130000	-1.612167000
C	6.390369000	-0.738765000	0.206070000
F	5.164921000	-1.465646000	-1.612167000
C	6.390369000	0.738765000	-0.206070000
F	5.164921000	1.465646000	1.612167000
C	3.834974000	5.164839000	-0.206070000
F	1.313174000	5.205776000	-1.612167000
F	-1.248601000	-3.689854000	-1.590303000
F	3.819808000	0.763606000	-1.590303000
F	2.613650000	1.508992000	1.653918000
F	2.571206000	2.926248000	-1.590303000
F	1.248601000	3.689854000	1.590303000

F	0.000000000	3.017983000	-1.653918000
F	-1.248601000	3.689854000	1.590303000
F	-2.613650000	-1.508992000	-1.653918000
C	2.555395000	5.903605000	0.206070000
H	2.549507000	6.875872000	-0.302265000
F	3.851747000	3.740130000	1.612167000
F	1.313174000	-5.205776000	1.612167000
C	-5.105725000	-1.470814000	-0.239526000
C	-6.390369000	-0.738765000	0.206070000
C	-6.390369000	0.738765000	-0.206070000
C	-5.105725000	1.470814000	0.239526000
C	-3.826625000	-3.686280000	-0.239526000
C	-5.113793000	-2.952450000	0.189727000
C	-3.834974000	-5.164839000	0.206070000
C	-2.555395000	-5.903605000	-0.206070000
C	-5.113793000	2.952450000	-0.189727000
C	-3.826625000	3.686280000	0.239526000
C	-3.834974000	5.164839000	-0.206070000
C	-2.555395000	5.903605000	0.206070000
H	-2.549507000	-6.875872000	0.302265000
H	-4.679926000	-5.645874000	-0.302265000
H	-5.952325000	-3.436576000	-0.329266000
H	-7.229433000	-1.229998000	-0.302265000
H	-7.229433000	1.229998000	0.302265000

H	-5.952325000	3.436576000	0.329266000
H	-4.679926000	5.645874000	0.302265000
H	-2.549507000	6.875872000	-0.302265000
F	-3.851747000	3.740130000	1.612167000
F	-5.164921000	-1.465646000	-1.612167000
F	-3.851747000	-3.740130000	-1.612167000
F	-5.164921000	1.465646000	1.612167000
H	4.679926000	-5.645874000	-0.302265000
H	5.952325000	-3.436576000	-0.329266000
H	2.549507000	-6.875872000	0.302265000
H	0.000000000	-6.873153000	0.329266000
H	7.229433000	-1.229998000	-0.302265000
H	7.229433000	1.229998000	0.302265000
H	5.952325000	3.436576000	0.329266000
H	4.679926000	5.645874000	0.302265000
F	-1.313174000	5.205776000	-1.612167000
F	-2.571206000	2.926248000	-1.590303000
F	-3.819808000	0.763606000	-1.590303000
F	-3.819808000	-0.763606000	1.590303000
F	-2.571206000	-2.926248000	1.590303000
F	-1.313174000	-5.205776000	1.612167000
F	-2.578830000	-6.084975000	-1.559779000
F	0.000000000	-6.096725000	-1.538679000
F	2.578830000	-6.084975000	-1.559779000

F	6.559158000	0.809155000	-1.559779000
F	5.279919000	3.048362000	-1.538679000
F	3.980328000	5.275820000	-1.559779000
F	-3.980328000	5.275820000	-1.559779000
F	-5.279919000	3.048362000	-1.538679000
F	-6.559158000	0.809155000	-1.559779000
F	-5.279919000	-3.048362000	1.538679000
F	-3.980328000	-5.275820000	1.559779000
F	3.980328000	-5.275820000	1.559779000
F	5.279919000	-3.048362000	1.538679000
F	6.559158000	-0.809155000	1.559779000
F	2.578830000	6.084975000	1.559779000
F	0.000000000	6.096725000	1.538679000
F	-2.578830000	6.084975000	1.559779000
F	-2.613650000	1.508992000	1.653918000
F	-6.559158000	-0.809155000	1.559779000

$C_{54}F_{50}H_{18}$ Linear

	X	Y	Z
C	-1.382324000	-0.386156000	-0.092387000
C	-1.154464000	0.946380000	0.002702000
C	-2.307320000	1.903605000	0.337202000
C	-2.785649000	-0.966849000	-0.317108000
C	-3.921195000	-0.056675000	0.215795000

C	-3.676391000	1.403369000	-0.202557000
C	-0.257360000	-1.377043000	-0.402455000
C	-2.054269000	3.349763000	-0.161078000
C	0.207896000	1.556955000	-0.055049000
C	1.361741000	0.600992000	-0.388027000
C	1.100503000	-0.843964000	0.116893000
C	-0.689018000	3.882391000	0.333729000
C	0.435344000	2.889782000	0.034941000
C	1.837933000	3.482539000	0.241009000
C	2.978066000	2.557891000	-0.253566000
C	2.721099000	1.102468000	0.173972000
F	1.435053000	0.552524000	-1.756428000
C	-0.504020000	-2.815725000	0.172992000
C	0.641218000	-3.793828000	-0.229005000
C	2.019836000	-3.258492000	0.242089000
C	2.265012000	-1.810383000	-0.270743000
C	-3.011251000	-2.422614000	0.204788000
C	-1.881527000	-3.379518000	-0.255531000
C	-4.404698000	-2.972460000	-0.215578000
C	-5.545921000	-2.034275000	0.225252000
C	-5.308635000	-0.578696000	-0.231961000
C	-4.831337000	2.336427000	0.230951000
C	-4.589800000	3.788619000	-0.229059000
C	-3.211922000	4.315170000	0.222706000

C	-0.445524000	5.309539000	-0.237101000
C	0.934727000	5.880195000	0.135491000
C	2.078682000	4.937117000	-0.285438000
C	3.637877000	-1.290398000	0.231337000
C	3.886895000	0.164079000	-0.247419000
C	4.358117000	3.072890000	0.221765000
C	5.254985000	0.680564000	0.249345000
C	5.505073000	2.133804000	-0.190947000
C	4.599251000	4.522127000	-0.235938000
C	3.455210000	5.463504000	0.158263000
F	1.011072000	-0.776138000	1.479509000
F	2.641390000	1.106623000	1.539163000
F	2.993850000	2.599162000	-1.621908000
F	1.937525000	3.617870000	1.611732000
F	-0.737340000	4.041118000	1.699194000
H	-6.460943000	-2.383768000	-0.272763000
F	2.097942000	4.944867000	-1.656717000
C	-1.586684000	6.289805000	0.139091000
F	-0.450943000	5.247536000	-1.611177000
C	-2.968580000	5.762780000	-0.264385000
F	-3.269470000	4.413576000	1.592556000
C	-6.205475000	1.809792000	-0.219609000
F	-5.375350000	-0.582304000	-1.604224000
F	3.960146000	0.164312000	-1.613636000

F	-1.997679000	3.304283000	-1.529461000
F	-2.365283000	1.962685000	1.707728000
F	-3.638251000	1.431632000	-1.571069000
F	-3.911892000	-0.091096000	1.584136000
F	-2.900269000	-1.046899000	-1.687451000
F	-3.016566000	-2.402298000	1.572302000
F	2.320049000	-1.864749000	-1.634547000
C	-6.445467000	0.356841000	0.206295000
H	-7.358893000	0.008376000	-0.292150000
F	-4.895466000	2.363324000	1.603134000
F	4.391234000	3.116049000	1.594324000
C	3.167851000	-4.215223000	-0.181006000
C	2.927580000	-5.663355000	0.298595000
C	1.545764000	-6.190473000	-0.104892000
C	0.405004000	-5.231186000	0.305277000
C	4.789635000	-2.235890000	-0.199712000
C	4.548655000	-3.689119000	0.263391000
C	6.164588000	-1.710364000	0.253798000
C	6.404255000	-0.257370000	-0.172035000
C	-0.975906000	-5.780337000	-0.101057000
C	-2.114624000	-4.815537000	0.287435000
C	-3.496168000	-5.363851000	-0.123908000
C	-4.640430000	-4.422759000	0.270107000
H	7.306227000	0.093677000	0.345774000

H	6.922935000	-2.332255000	-0.238400000
H	5.306464000	-4.314538000	-0.228369000
H	3.682819000	-6.289834000	-0.192397000
H	1.378175000	-7.130643000	0.435959000
H	-1.133615000	-6.710293000	0.462283000
H	-3.640135000	-6.306800000	0.418948000
H	-5.553211000	-4.775459000	-0.225880000
F	-2.135392000	-4.789335000	1.660758000
F	3.208298000	-4.300431000	-1.551314000
F	4.860979000	-2.272176000	-1.570992000
F	0.421233000	-5.220288000	1.678512000
H	3.614118000	6.409679000	-0.375563000
H	1.062866000	6.813576000	-0.430433000
H	5.506204000	4.872669000	0.272992000
H	6.407911000	2.480950000	0.330540000
H	-1.408599000	7.214895000	-0.423878000
H	-3.727849000	6.393374000	0.214231000
H	-5.351092000	4.417056000	0.253091000
H	-6.964223000	2.432093000	0.271620000
F	-4.475432000	-3.055207000	-1.584735000
F	-1.913295000	-3.476379000	-1.618356000
F	0.656425000	-3.903785000	-1.591793000
F	2.024085000	-3.242515000	1.609567000
F	3.634008000	-1.290936000	1.598865000

F	5.272596000	0.681782000	1.622388000
F	6.604886000	-0.228308000	-1.522327000
F	5.696745000	2.189907000	-1.539287000
F	4.768935000	4.597034000	-1.589605000
F	-3.072600000	5.851374000	-1.624119000
F	-4.701078000	3.874542000	-1.584250000
F	-6.344639000	1.890720000	-1.576406000
F	-3.561996000	-5.587837000	-1.469558000
F	-1.009951000	-6.032986000	-1.439384000
F	1.546014000	-6.422158000	-1.450354000
F	4.674532000	-3.779079000	1.616259000
F	6.306652000	-1.788699000	1.610132000
F	3.515989000	5.679414000	1.503830000
F	0.989673000	6.136444000	1.472375000
F	-1.589947000	6.553901000	1.478249000
F	-6.616569000	0.329956000	1.561939000
F	-5.703579000	-2.082340000	1.577069000
F	-4.793327000	-4.480204000	1.626051000
F	-0.517650000	-2.730896000	1.537091000
F	-0.200185000	-1.494521000	-1.767788000
F	3.045927000	-5.766166000	1.655406000

$C_{54}F_{49}H_{18}^{\bullet}$ Linear

X	Y	Z

C	0.857570000	-1.278466000	0.100480000
C	1.530974000	-0.001073000	0.039397000
C	3.011615000	-0.005422000	-0.336761000
C	1.517946000	-2.486668000	-0.009914000
C	3.012046000	-2.550604000	-0.309573000
C	3.733187000	-1.274743000	0.178181000
C	-0.649457000	-1.282993000	0.410790000
C	3.738182000	1.260314000	0.179017000
C	0.862948000	1.278635000	0.108207000
C	-0.644498000	1.285897000	0.416459000
C	-1.354097000	0.003175000	-0.102454000
C	3.020258000	2.538557000	-0.306909000
C	1.528460000	2.485647000	0.004596000
C	0.813350000	3.822655000	-0.228610000
C	-0.657239000	3.835783000	0.258677000
C	-1.374196000	2.540561000	-0.162435000
F	-0.757541000	1.309880000	1.782213000
C	-1.386375000	-2.534480000	-0.169222000
C	-2.887390000	-2.554112000	0.245672000
C	-3.610937000	-1.267556000	-0.230074000
C	-2.874664000	0.004848000	0.278839000
C	0.795927000	-3.816739000	-0.249818000
C	-0.672580000	-3.831087000	0.248386000
C	1.522405000	-5.090418000	0.269589000

C	3.008543000	-5.121061000	-0.119950000
C	3.718969000	-3.810239000	0.262815000
C	5.242942000	-1.288993000	-0.178523000
C	5.964604000	-0.012137000	0.301605000
C	5.247375000	1.267365000	-0.179581000
C	3.732242000	3.795737000	0.259138000
C	3.028152000	5.108108000	-0.128081000
C	1.543069000	5.109400000	0.284932000
C	-3.605466000	1.279503000	-0.230223000
C	-2.877399000	2.563992000	0.246133000
C	-1.396431000	5.107532000	-0.235790000
C	-3.607178000	3.829840000	-0.266514000
C	-2.883109000	5.118929000	0.165287000
C	-0.667352000	6.389032000	0.210668000
C	0.816487000	6.386323000	-0.175841000
F	-1.235853000	0.005146000	-1.464388000
F	-1.299474000	2.486978000	-1.526678000
F	-0.651459000	3.891383000	1.626468000
F	0.825236000	3.975714000	-1.602591000
F	3.154730000	2.624000000	-1.674833000
H	3.478430000	-5.929171000	0.457256000
F	1.527009000	5.143736000	1.656072000
C	5.235588000	3.823364000	-0.107796000
F	3.685977000	3.747395000	1.633190000

C	5.966593000	2.542612000	0.312149000
F	5.373926000	1.292831000	-1.547789000
C	5.957211000	-2.566788000	0.315677000
F	3.675189000	-3.757059000	1.636600000
F	-2.946085000	2.623514000	1.611140000
F	3.650458000	1.245656000	1.547620000
F	3.079523000	-0.006585000	-1.709590000
F	3.643902000	-1.259979000	1.546653000
F	3.153387000	-2.642644000	-1.676558000
F	0.803138000	-3.972843000	-1.622794000
F	-2.956361000	0.005204000	1.642276000
C	5.221500000	-3.845614000	-0.102566000
H	5.665996000	-4.680064000	0.454919000
F	5.371206000	-1.316235000	-1.546551000
F	-1.387271000	5.146181000	-1.608919000
C	-5.105116000	-1.270523000	0.196771000
C	-5.840924000	-2.545331000	-0.267793000
C	-5.110432000	-3.826180000	0.151654000
C	-3.621764000	-3.819481000	-0.262152000
C	-5.100298000	1.287340000	0.195348000
C	-5.839412000	0.009285000	-0.256908000
C	-5.831516000	2.563905000	-0.271377000
C	-5.096266000	3.842654000	0.146231000
C	-2.901869000	-5.110608000	0.172752000

C	-1.415825000	-5.105866000	-0.234131000
C	-0.691028000	-6.389011000	0.219462000
C	0.793029000	-6.392048000	-0.166729000
H	-5.564125000	4.682729000	-0.382836000
H	-6.813315000	2.565882000	0.218476000
H	-6.821295000	0.011660000	0.235901000
H	-6.822755000	-2.542741000	0.222009000
H	-5.581930000	-4.665406000	-0.375514000
H	-3.378782000	-5.946068000	-0.357843000
H	-1.171935000	-7.229350000	-0.296948000
H	1.274965000	-7.214956000	0.376253000
F	-1.408961000	-5.153299000	-1.606991000
F	-5.186554000	-1.298034000	1.567729000
F	-5.182532000	1.316701000	1.566237000
F	-3.628003000	-3.821464000	-1.635386000
H	1.292654000	7.223614000	0.351004000
H	3.517421000	5.916451000	0.433532000
H	-1.144628000	7.228345000	-0.310795000
H	-3.355189000	5.954427000	-0.369579000
H	5.684592000	4.657142000	0.447089000
H	6.960423000	2.550522000	-0.152220000
H	6.968470000	-0.014016000	-0.144329000
H	6.950772000	-2.578933000	-0.149182000
F	1.499845000	-5.106784000	1.643612000

F	-0.664183000	-3.879890000	1.616335000
F	-2.952606000	-2.610759000	1.610919000
F	-3.604381000	-1.259291000	-1.597520000
F	-3.597816000	1.271002000	-1.597676000
F	-3.613070000	3.828370000	-1.639668000
F	-5.240585000	4.004748000	1.494180000
F	-3.005684000	5.297402000	1.510935000
F	-0.759405000	6.569004000	1.561950000
F	6.084702000	2.548795000	1.673561000
F	6.053937000	-0.011434000	1.661241000
F	6.076134000	-2.570679000	1.676940000
F	-0.782255000	-6.559916000	1.571972000
F	-3.021068000	-5.283497000	1.519151000
F	-5.253908000	-3.985402000	1.500040000
F	-5.994254000	0.008740000	-1.609738000
F	-5.986891000	2.581392000	-1.628221000
F	0.912687000	6.576316000	-1.523239000
F	3.156701000	5.330072000	-1.465969000
F	5.413114000	4.009386000	-1.448481000
F	5.401509000	-4.034759000	-1.442486000
F	3.149530000	-5.357374000	-1.454585000
F	0.890584000	-6.602615000	-1.510940000
F	-1.316317000	-2.478284000	-1.533491000
F	-0.759127000	-1.307020000	1.776862000

F	-5.996322000	-2.564432000	-1.624627000

$C_{54}F_{48}H_{18}$ Linear

	X	Y	Z
C	-1.008251000	-1.127623000	-0.060473000
C	-1.498789000	0.281198000	0.032904000
C	-2.983645000	0.443978000	0.388982000
C	-1.816960000	-2.214300000	0.036389000
C	-3.314395000	-2.091827000	0.326682000
C	-3.857932000	-0.725543000	-0.152732000
C	0.480155000	-1.320307000	-0.387217000
C	-3.534610000	1.792962000	-0.130394000
C	-0.686090000	1.379591000	-0.038605000
C	0.794966000	1.214385000	-0.403528000
C	1.347176000	-0.137461000	0.117155000
C	-2.664440000	2.979399000	0.368026000
C	-1.171420000	2.789545000	0.061823000
C	-0.358709000	3.877301000	-0.030637000
C	1.133790000	3.748954000	-0.339702000
C	1.670047000	2.381541000	0.140368000
F	0.879173000	1.241000000	-1.771644000
C	1.051470000	-2.654865000	0.177869000
C	2.535090000	-2.859289000	-0.243045000
C	3.417188000	-1.679218000	0.239185000

C	2.851032000	-0.322913000	-0.264531000
C	-1.281116000	-3.640396000	0.245704000
C	0.173994000	-3.841117000	-0.251792000
C	-2.165760000	-4.802170000	-0.293530000
C	-3.645819000	-4.648912000	0.091954000
C	-4.175988000	-3.246514000	-0.269743000
C	-5.367483000	-0.559852000	0.189031000
C	-5.922789000	0.800698000	-0.281531000
C	-5.042459000	1.977674000	0.214424000
C	-3.223167000	4.302636000	-0.197788000
C	-2.355132000	5.498630000	0.200507000
C	-0.881711000	5.313142000	-0.209290000
C	3.731914000	0.848364000	0.254671000
C	3.176705000	2.214875000	-0.225420000
C	1.998739000	4.901821000	0.253590000
C	4.054534000	3.374208000	0.316234000
C	3.509423000	4.755000000	-0.088389000
C	1.474507000	6.298637000	-0.122395000
C	0.001917000	6.482449000	0.261308000
F	1.236318000	-0.113011000	1.480260000
F	1.549568000	2.371698000	1.504120000
F	1.283672000	3.846854000	-1.702728000
F	-2.787351000	3.043123000	1.735970000
H	-4.213844000	-5.377663000	-0.502012000

F	-0.865929000	5.493334000	-1.594976000
C	-4.709208000	4.506994000	0.165610000
F	-3.175427000	4.253516000	-1.571197000
C	-5.597041000	3.334550000	-0.266878000
F	-5.172560000	2.007239000	1.582708000
C	-6.241980000	-1.733762000	-0.321075000
F	-4.116677000	-3.177118000	-1.642319000
F	3.285034000	2.269443000	-1.588079000
F	-3.435229000	1.770255000	-1.497616000
F	-3.079021000	0.427867000	1.758017000
F	-3.750559000	-0.708452000	-1.519411000
F	-3.478755000	-2.184765000	1.689385000
F	-1.316750000	-3.815213000	1.614796000
F	2.931005000	-0.320950000	-1.628199000
C	-5.677092000	-3.100022000	0.085023000
H	-6.216107000	-3.866238000	-0.486647000
F	-5.508355000	-0.586067000	1.556163000
F	1.892721000	4.861362000	1.625110000
C	4.898285000	-1.867536000	-0.183909000
C	5.460324000	-3.228926000	0.271444000
C	4.572877000	-4.401587000	-0.161201000
C	3.098690000	-4.211249000	0.252036000
C	5.220121000	0.670229000	-0.158952000
C	5.786493000	-0.695227000	0.285596000

C	6.105250000	1.839221000	0.325472000
C	5.540821000	3.205454000	-0.080170000
C	2.218280000	-5.392474000	-0.196696000
C	0.745259000	-5.204844000	0.213495000
C	-0.138376000	-6.376611000	-0.257597000
C	-1.611020000	-6.193128000	0.127357000
H	6.103441000	3.974256000	0.464623000
H	7.082544000	1.721480000	-0.159050000
H	6.764090000	-0.813985000	-0.201428000
H	6.436681000	-3.350284000	-0.214367000
H	4.934486000	-5.299270000	0.356629000
H	2.584883000	-6.288502000	0.322981000
H	0.228171000	-7.278898000	0.248151000
H	-2.194111000	-6.939824000	-0.426399000
F	0.730845000	-5.268037000	1.585559000
F	4.980557000	-1.892613000	-1.554810000
F	5.317209000	0.698713000	-1.528948000
F	3.101847000	-4.228728000	1.625241000
H	-0.377797000	7.380176000	-0.239090000
H	-2.730327000	6.387568000	-0.323424000
H	2.058607000	7.029724000	0.450877000
H	4.048601000	5.503381000	0.508126000
H	-5.052901000	5.397415000	-0.376817000
H	-6.582356000	3.464792000	0.197145000

H	-6.918664000	0.927428000	0.163467000
H	-7.228400000	-1.619579000	0.144842000
F	-2.141055000	-4.804004000	-1.667564000
F	0.162341000	-3.874348000	-1.620276000
F	2.590702000	-2.909456000	-1.609089000
F	3.407944000	-1.676148000	1.606842000
F	3.709044000	0.838159000	1.621908000
F	4.039902000	3.354794000	1.690058000
F	5.719052000	3.363197000	-1.424611000
F	3.709215000	4.980805000	-1.415615000
F	1.615908000	6.536588000	-1.459997000
F	-5.709851000	3.367703000	-1.628293000
F	-6.003901000	0.824694000	-1.641001000
F	-6.358629000	-1.708190000	-1.681970000
F	-0.067003000	-6.541065000	-1.612050000
F	2.314296000	-5.563973000	-1.545125000
F	4.696819000	-4.563623000	-1.511392000
F	5.930730000	-0.726945000	1.639354000
F	6.251352000	1.822625000	1.683574000
F	-0.060750000	6.642131000	1.619000000
F	-2.435282000	5.686536000	1.551798000
F	-4.862174000	4.697944000	1.509792000
F	-5.889863000	-3.280847000	1.421301000
F	-3.823763000	-4.887167000	1.421617000

F	-1.737111000	-6.406659000	1.468698000
F	0.992682000	-2.600876000	1.542957000
F	0.572556000	-1.345026000	-1.755176000
F	5.605170000	-3.279251000	1.628825000

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