Supplementary Information

Regioselective Chlorine-Addition Reaction toward $C_{54}Cl_8$ and Role of Chlorine Atoms in Stone-Wales Rearrangement

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Table S1. Predicted relative energies (↵E, kcal/mol) and addition sites of chlorine for low-lying $^{\#369}C_{54}Cl_x$ species in the radical-addition process.

Step	Addition sites	Precursor	⊿E
1	**C1(A)**	$^{\#369}C_{54}$	0.00
	C2	$^{\#369}C_{54}$	5.90
2	**C1C4(B)**	**B**	0.00
	C1C2	**C**	0.09
3	**C1C4C2(D)/C1C2C4**	**B/C**	0.00
	C1C2C3	C	6.50
4	**C1C4C2C6(E)**	**D**	0.00
	C1C4C2C7	**D**	0.99
5	**C1C4C2C6C8(F)**	**E**	0.92
	C1C4C2C7C5(G)	**D**	0.00
	C1C4C2C6C3	**E**	3.34
6	**C1C4C2C6C8C3(H)/ C1C4C2C7C5C3** [a]	**F/G**	0.00
	C1C4C2C6C8C5	**F**	15.73
7	**C1C4C2C6C8C3C5(I)**	**H**	0.00
	C1C4C2C6C8C3C7	**H**	5.73
8	**C1C4C2C6C8C3C5C7**	**I**	-

[a] The addition pattern C1C4C2C6C8C3 is equal to C1C4C2C7C5C3.

Table S2. Relative energies (in kcal/mol) of each reactant, transition state (TS), and product in the two SW rearrangements.

	AM1	B3LYP/6-31G*		AM1	B3LYP/6-31G*
$^{\#866}C_{56}Cl_2$	0.00	0.00	$^{\#864}C_{56}Cl_2$-2	0.00	0.00
TS I	58.88	72.88	TS II	86.28	96.53
$^{\#864}C_{56}Cl_2$-1	-27.01	-22.59	$^{\#913}C_{56}Cl_2$	-2.40	-0.33

Table S3. Relative energies (↵E, kcal/mol), HOMO-LUMO gaps (eV) of $C_{54}Cl_{10}$ and $C_{54}Cl_{12}$ isomers with lower energies.

	$^{\#540}C_{54}Cl_{10}$			$^{\#540}C_{54}Cl_{12}$	
isomers	↵E	gap	isomers	↵E	gap
$^{\#540}C_{54}Cl_{10}$-1	0.00	2.86	$^{\#540}C_{54}Cl_{12}$-1	0.00	2.74
$^{\#540}C_{54}Cl_{10}$-2	3.18	2.75	$^{\#540}C_{54}Cl_{12}$-2	1.15	2.70
$^{\#540}C_{54}Cl_{10}$-3	4.35	2.84	$^{\#540}C_{54}Cl_{12}$-3	1.91	2.83

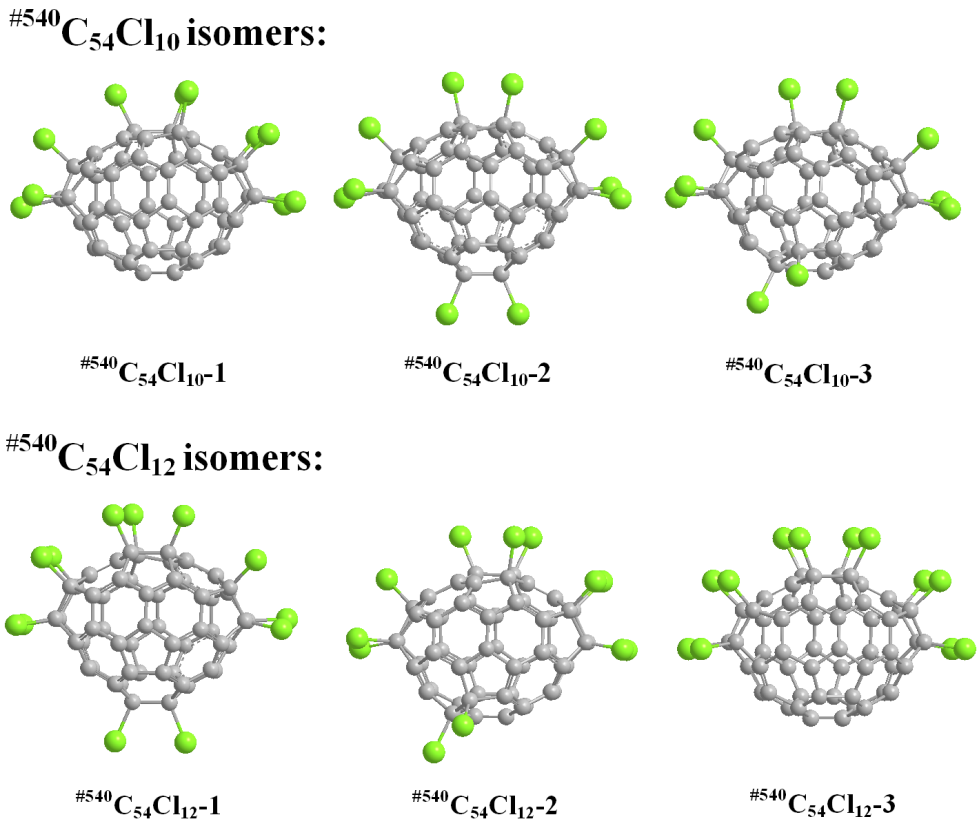

Figure S1. Geometry structures of lowest energy isomers of $^{\#540}C_{54}Cl_{10}$ and $^{\#540}C_{54}Cl_{12}$.

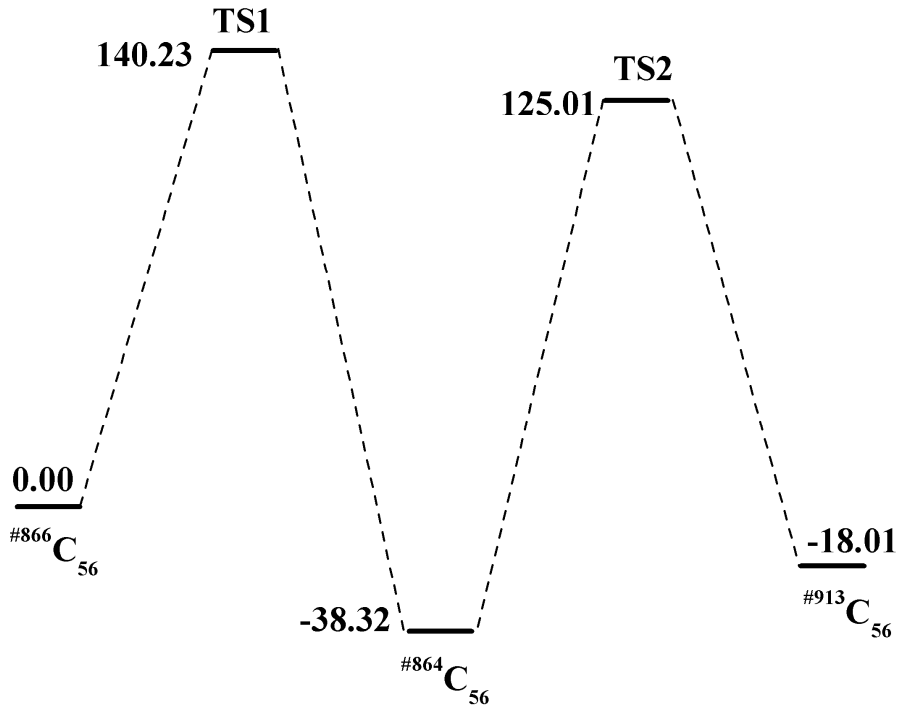

Figure S2. Energy profiles (in kcal/mol) of concerted SW rearrangements from $^{\#866}C_{56}$ to $^{\#913}C_{56}$ (at B3LYP/6-31G* level).

To gain deep insight of C_{54} chlorofullerene, we present the frontier orbitals of $^{\#540}C_{54}Cl_8$ structures in Figure S3, as well as other two exohedral derivatives containing two kinds of most popular exohedral atoms (F and H) with the same addition pattern. The HOMO-LUMO gaps of these three structures are quite similar (ranging 3.12~3.17eV) and their HOMO orbital share alike shapes. The energy levels of frontier orbitals in $^{\#540}C_{54}Cl_8$ and $^{\#540}C_{54}F_8$ are similar, while the orbitals in $^{\#540}C_{54}H_8$ have higher levels than former structures. The exohedral Cl and F atoms can obviously enlarge the HOMO-LUMO gap of pristine $^{\#540}C_{54}$ cage mainly by means of decreasing the energy of HOMO orbital. The H atoms slightly change the HOMO orbital energy but can greatly heighten the energy level of LUMO orbital.

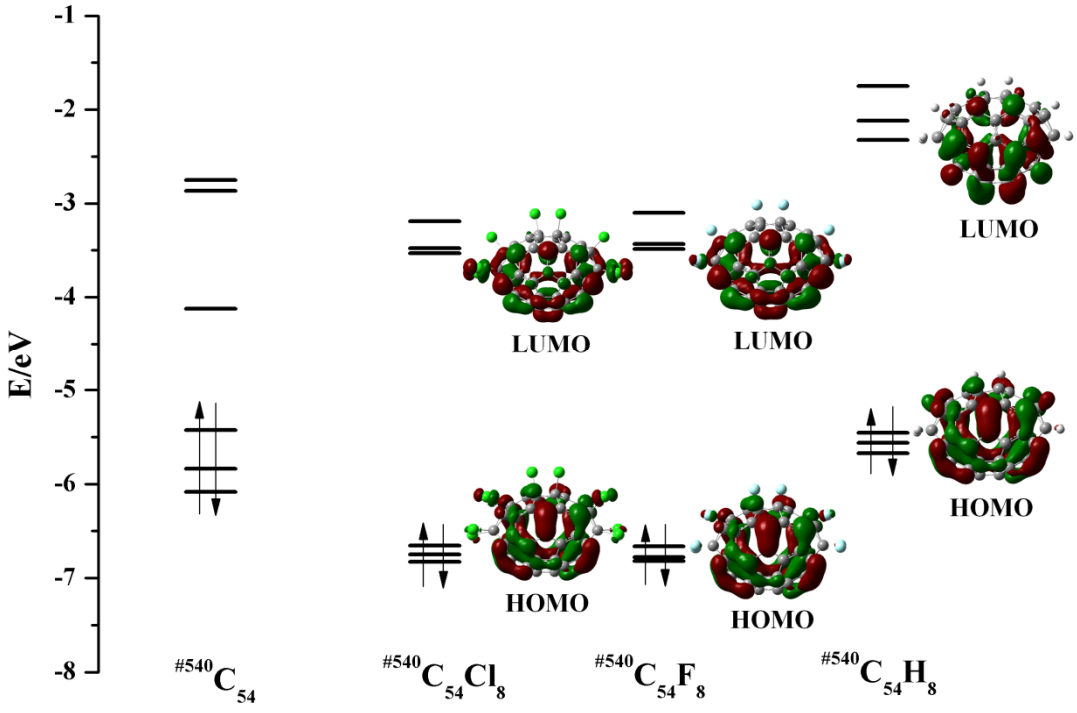

Figure S3. Frontier orbital energies and HOMO/LUMO orbital maps of $^{\#540}C_{54}$ cage and $^{\#540}C_{54}X_8$ structures.

The charge populations of $^{\#540}C_{54}X_8$ structures present different influence of three

kinds of exohedral atoms to fullerene electronic property (Figure S4). Ca and Cb atoms having little positive charges (in black color) in pristine cage will turn red when bonding with Cl/H atoms. All carbon atoms of addition sites have large negative charges in $^{\#540}C_{54}Cl_8$ and $^{\#540}C_{54}H_8$. The Cl atoms are slightly positive charged (in black color), revealing little charge transfer to the cage. The F atoms with red color show obvious electronegativity leading all carbon atoms bonding with them turn green. Hence, since fullerene cage is a kind of electron-deficient structure like Cl and F atom, an electronegativity sequence of $^{\#540}C_{54}$ cage and two halogen elements could be concluded as:

$$Cl< {}^{\#540}C_{54}<F$$

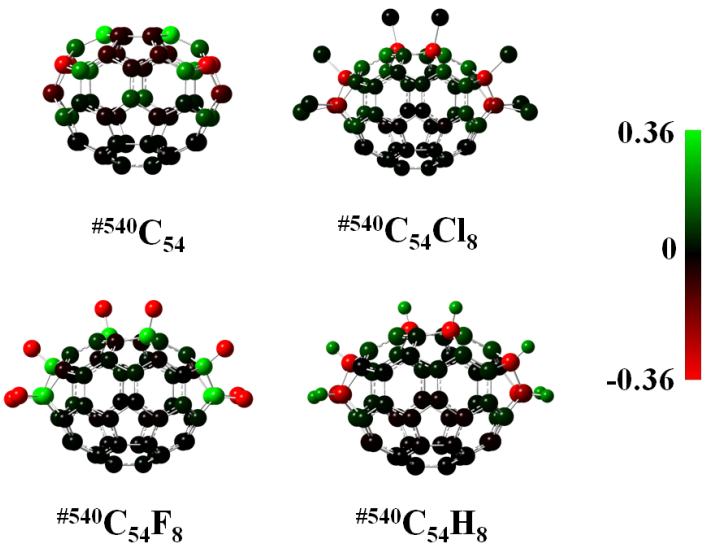

Figure S4. Mulliken atomic charge populations of $^{\#540}C_{54}$ cage and $^{\#540}C_{54}X_8$ structures.

The calculated excitation energies show very good accordance to experimental results (Table S4) with relative differences of -0.20~0.20 eV. The first excitation at 2.56 eV (486 nm), which is very near to optical gap of 2.47 eV (504 nm), mainly

stems from electronic transition of HOMO→LUMO. Second lowest-energy excitation at 2.77 eV (449 nm) corresponds to electronic transition from HOMO-1 orbital to LUMO+1 orbital. Other peaks with higher energies composed of integrated π→π* transitions among frontier cage orbitals.

Table S4. Simulated electronic excitation energies of $^{\#540}C_{54}Cl_8$.

Exp.[a]	TDDFT	Characterization
288	302	π→π*
341	345	π→π*
406	381	π→π*
465	449	π→π*
504	486	π→π*

[a] The data comes from ref. 24.

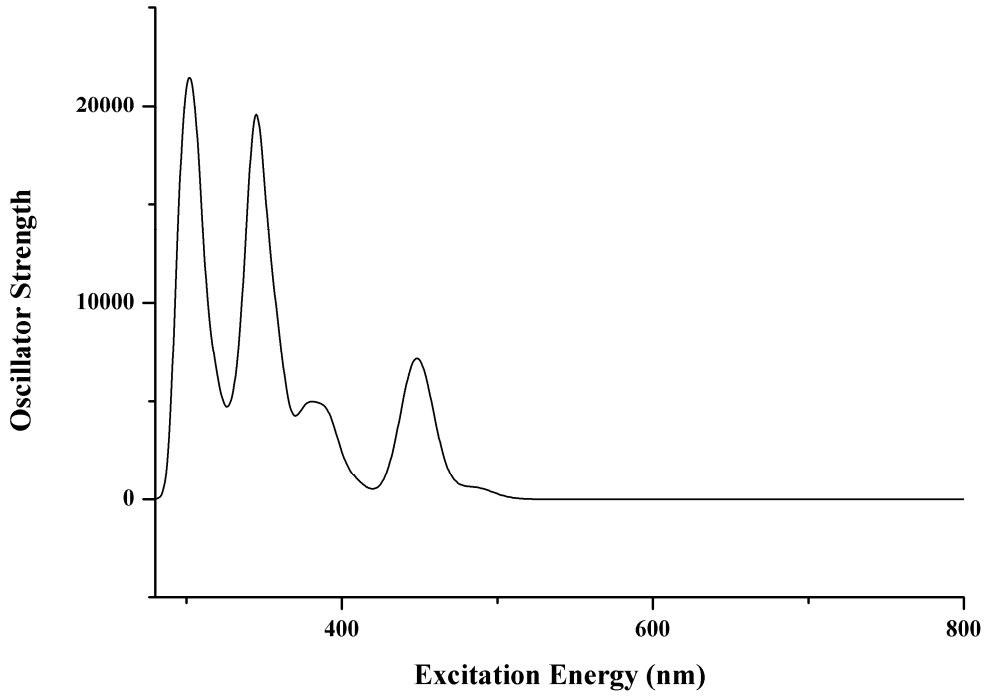

Figure S5. Simulated UV-Vis-NIR spectrum of $^{\#540}C_{54}Cl_8$.

Coordinates of C_{54} chlorofullerenes, $C_{54}F_8$, and $C_{54}H_8$ structures. The three isomers are predicted at B3LYP/6-311G** level, while other structures are predicted at B3LYP/6-31G* level.

$^{\#540}C_{54}Cl_8$:

C	-0.000003	3.258234	0.534877
C	-0.000001	2.954669	-0.831941

C	-1.161902	2.365081	-1.440702
C	-0.692029	1.243736	-2.278236
C	-1.458610	0.000007	-2.239575
C	-0.692027	-1.243724	-2.278242
C	-1.161902	-2.365071	-1.440711
C	0.000001	-2.954663	-0.831953
C	0.000000	-3.258236	0.534862
C	1.169904	-2.927771	1.314663
C	0.723936	-2.292896	2.529747
C	1.424992	-1.175884	2.999516
C	0.693789	-0.000009	3.439907
C	1.424992	1.175870	2.999522
C	0.723935	2.292884	2.529758
C	1.169901	2.927765	1.314677
C	-1.169906	2.927765	1.314674
C	-0.723939	2.292882	2.529758
C	-1.424994	1.175868	2.999517
C	-0.693792	-0.000009	3.439906
C	-1.424995	-1.175886	2.999518
C	-0.723938	-2.292898	2.529748
C	-1.169904	-2.927771	1.314662
C	-2.329913	-2.461355	0.676348
C	-2.338680	-2.260266	-0.744532
C	-3.371438	-1.239299	-1.141063
C	-2.702487	0.000003	-1.660742
C	-3.371448	1.239311	-1.141065
C	-2.338681	2.260271	-0.744518
C	-2.329912	2.461351	0.676358
C	-3.117503	1.416978	1.256542
C	-2.633705	0.741004	2.353210
C	-2.633708	-0.741023	2.353218
C	-3.117497	-1.416992	1.256537
C	-4.048224	-0.798675	0.227648
C	-4.048224	0.798674	0.227652
C	1.161904	2.365079	-1.440699
C	0.692033	1.243736	-2.278235
C	1.458615	0.000005	-2.239572
C	0.692034	-1.243724	-2.278241
C	1.161906	-2.365075	-1.440710
C	2.338681	-2.260266	-0.744525
C	2.329911	-2.461355	0.676351
C	3.117500	-1.416989	1.256538
C	2.633704	-0.741019	2.353213
C	2.633704	0.741009	2.353220

C	3.117495	1.416984	1.256544
C	2.329910	2.461353	0.676363
C	2.338681	2.260273	-0.744518
C	3.371442	1.239307	-1.141051
C	2.702491	0.000005	-1.660736
C	3.371448	-1.239305	-1.141062
C	4.048231	-0.798680	0.227654
C	4.048226	0.798679	0.227657
Cl	-5.670626	1.542260	0.506079
Cl	-4.518014	1.911327	-2.402929
Cl	-4.518018	-1.911307	-2.402949
Cl	-5.670616	-1.542269	0.506075
Cl	5.670614	-1.542303	0.506060
Cl	4.518021	-1.911322	-2.402924
Cl	5.670607	1.542312	0.506072
Cl	4.518030	1.911321	-2.402919

$^{\#540}C_{54}Cl_8$-2:

C	0.384797	-0.668104	3.176129
C	0.362366	0.693939	2.846055
C	-0.872101	1.285992	2.394082
C	-0.595115	2.127426	1.271665
C	-1.460922	2.152730	0.186673
C	-0.913751	2.393022	-1.210890
C	-1.452434	1.317487	-2.168340
C	-0.362366	0.693938	-2.846055
C	-0.384797	-0.668105	-3.176129
C	0.820356	-1.469348	-3.027068
C	0.444896	-2.692127	-2.355836
C	1.278378	-3.182208	-1.341741
C	0.691345	-3.605424	-0.087068
C	1.557398	-3.157412	0.986485
C	0.990843	-2.677957	2.173096
C	1.501144	-1.447718	2.727365
C	-0.820356	-1.469347	3.027068
C	-0.444896	-2.692126	2.355836
C	-1.278378	-3.182208	1.341742
C	-0.691344	-3.605424	0.087069
C	-1.557398	-3.157412	-0.986484
C	-0.990843	-2.677957	-2.173095
C	-1.501144	-1.447719	-2.727365
C	-2.598696	-0.813645	-2.129883
C	-2.601715	0.608715	-1.929445
C	-3.555306	0.997074	-0.831997

C	-2.732725	1.511424	0.329043
C	-3.027161	0.804088	1.465146
C	-2.060591	0.565929	2.458023
C	-2.038574	-0.867718	2.728559
C	-2.973100	-1.478121	1.813891
C	-2.548514	-2.550420	1.065272
C	-2.713752	-2.522020	-0.410442
C	-3.265404	-1.414668	-1.018447
C	-4.141582	-0.406352	-0.306282
C	-3.904134	-0.398437	1.254569
C	1.452434	1.317488	2.168340
C	0.913751	2.393022	1.210890
C	1.460922	2.152730	-0.186674
C	0.595115	2.127425	-1.271665
C	0.872101	1.285992	-2.394082
C	2.060591	0.565928	-2.458023
C	2.038574	-0.867718	-2.728559
C	2.973100	-1.478122	-1.813891
C	2.548515	-2.550421	-1.065271
C	2.713752	-2.522019	0.410443
C	3.265405	-1.414667	1.018448
C	2.598696	-0.813645	2.129883
C	2.601715	0.608715	1.929444
C	3.555306	0.997074	0.831997
C	2.732725	1.511424	-0.329044
C	3.027161	0.804087	-1.465146
C	3.904134	-0.398438	-1.254569
C	4.141582	-0.406351	0.306282
Cl	-1.276260	4.108600	-1.788218
Cl	4.784533	2.212066	1.381900
Cl	-5.838180	-0.740814	-0.813093
Cl	-5.421130	-0.323198	2.261620
Cl	-4.784533	2.212065	-1.381901
Cl	5.421130	-0.323198	-2.261621
Cl	5.838180	-0.740814	0.813093
Cl	1.276260	4.108601	1.788217

$^{\#369}C_{54}Cl_8$:

C	-2.017292	-1.168070	2.893138
C	-2.030347	-2.293745	2.068247
C	-0.786535	-3.031029	1.838016
C	-0.783799	-3.436152	0.493277
C	0.298114	-3.088884	-0.324499
C	-0.244354	-2.324272	-1.452047

C	0.480017	-1.243249	-1.977211
C	-0.220329	-0.000067	-2.244360
C	0.480012	1.243142	-1.977278
C	-0.244372	2.324186	-1.452173
C	0.298084	3.088870	-0.324679
C	-0.783840	3.436170	0.493083
C	-0.786575	3.031139	1.837838
C	-2.030383	2.293848	2.068115
C	-2.017311	1.168224	2.893070
C	-2.760360	0.000060	2.506667
C	-0.777854	-0.728533	3.517455
C	-0.777862	0.728737	3.517414
C	0.403528	1.426836	3.307270
C	0.417968	2.587920	2.422517
C	1.613811	2.534108	1.647936
C	1.549898	2.720872	0.243452
C	2.405387	1.899738	-0.586322
C	1.882016	1.193890	-1.632096
C	2.714333	-0.000047	-1.991491
C	1.882026	-1.193966	-1.632035
C	2.405403	-1.899741	-0.586228
C	1.549928	-2.720834	0.243607
C	1.613843	-2.533976	1.648071
C	0.417999	-2.587765	2.422666
C	0.403548	-1.426629	3.307347
C	1.641098	-0.704878	3.114301
C	1.641088	0.705090	3.114266
C	2.419258	1.403781	2.146666
C	3.273161	0.701017	1.301593
C	3.657515	1.266279	-0.042435
C	3.930347	-0.000014	-0.972593
C	3.657513	-1.266215	-0.042375
C	3.273174	-0.700884	1.301629
C	2.419281	-1.403614	2.146743
C	-2.808040	-2.290137	0.858922
C	-2.113629	-3.157325	-0.177668
C	-1.667570	-2.292999	-1.344307
C	-2.351402	-1.162761	-1.688000
C	-1.638404	-0.000070	-2.108410
C	-2.351411	1.162643	-1.688064
C	-1.667595	2.292905	-1.344437
C	-2.113667	3.157296	-0.177852
C	-2.808072	2.290163	0.858790
C	-3.504019	1.171525	0.479040

C	-3.479396	0.000021	1.295022
C	-3.504002	-1.171533	0.479108
C	-3.659366	-0.796857	-0.993846
C	-3.659374	0.796763	-0.993891
Cl	5.011855	-2.476644	0.104840
Cl	3.124548	-0.000100	-3.768887
Cl	5.011746	2.476835	0.104840
Cl	-3.035300	-4.659699	-0.652284
Cl	-5.089095	-1.590727	-1.762079
Cl	5.521445	-0.000221	-1.744975
Cl	-5.089104	1.590576	-1.762182
Cl	-3.035338	4.659636	-0.652557

$^{\#540}C_{54}Cl_{10}$-1:

C	-0.426704	0.127766	-3.149532
C	-0.307548	1.318556	-2.399112
C	0.938147	1.689997	-1.820057
C	0.730710	2.479433	-0.526173
C	1.443247	1.690262	0.597946
C	0.812564	1.558648	1.973771
C	1.199370	0.218414	2.617058
C	0.021369	-0.477821	3.022676
C	-0.078610	-1.876116	2.923831
C	-1.329811	-2.479480	2.483881
C	-1.000915	-3.471201	1.482346
C	-1.800465	-3.549773	0.331121
C	-1.162284	-3.622214	-0.970922
C	-1.923605	-2.795788	-1.892977
C	-1.246765	-2.030089	-2.853481
C	-1.627268	-0.647036	-3.018806
C	0.690749	-0.770566	-3.200581
C	0.195092	-2.106902	-2.966357
C	0.923249	-2.945558	-2.110315
C	0.227761	-3.693443	-1.077570
C	1.051770	-3.676348	0.117994
C	0.443856	-3.535081	1.373696
C	1.007831	-2.583536	2.304585
C	2.190177	-1.896980	1.975928
C	2.303724	-0.486799	2.220909
C	3.315837	0.139316	1.302481
C	2.596566	1.043063	0.327345
C	3.193147	0.913744	-1.054324
C	2.055705	0.922281	-2.042378
C	1.918627	-0.369463	-2.654667

C	2.725648	-1.296674	-1.923616
C	2.202294	-2.529287	-1.590592
C	2.284759	-2.991526	-0.185638
C	2.881995	-2.177848	0.754242
C	3.860704	-1.064921	0.415163
C	3.774057	-0.570654	-1.102560
C	-1.398328	1.810044	-1.624466
C	-0.899766	2.582755	-0.397969
C	-1.487364	1.879291	0.830850
C	-0.704287	1.432447	1.883006
C	-1.126473	0.330835	2.700151
C	-2.370184	-0.258202	2.503110
C	-2.479010	-1.704473	2.332683
C	-3.395776	-1.919897	1.234101
C	-3.001574	-2.752244	0.210123
C	-3.064902	-2.261108	-1.194677
C	-3.491658	-0.972556	-1.452640
C	-2.704791	-0.124964	-2.294448
C	-2.616897	1.169385	-1.672145
C	-3.620568	1.291102	-0.554016
C	-2.821629	1.345809	0.731764
C	-3.243714	0.358567	1.586797
C	-4.203852	-0.636663	0.992913
C	-4.339990	-0.152883	-0.504661
Cl	1.253497	3.014133	3.028604
Cl	-4.746528	2.699849	-0.744531
Cl	5.493938	-1.650368	0.915980
Cl	5.323855	-0.716551	-2.018946
Cl	4.583989	1.076070	2.208983
Cl	-5.772494	-0.721164	1.918167
Cl	-6.021651	-0.176937	-1.156688
Cl	-1.516655	4.302858	-0.406775
Cl	4.424579	2.213139	-1.363053
Cl	1.525395	4.121223	-0.615549

$^{\#540}C_{54}Cl_{12}$-1:

C	0.394522	0.041479	-3.042582
C	0.192593	-1.260423	-2.536597
C	-1.084255	-1.653767	-2.045454
C	-0.941738	-2.672907	-0.913231
C	-1.619184	-2.050520	0.330000
C	-0.998064	-2.203319	1.708892
C	-1.309230	-0.971601	2.574251
C	-0.091414	-0.431847	3.090528

C	0.098719	0.953871	3.216311
C	1.389456	1.538560	2.891504
C	1.146725	2.699629	2.072625
C	1.971577	2.952614	0.995396
C	1.488116	3.593628	-0.312981
C	2.070421	2.590480	-1.316837
C	1.353069	2.043684	-2.360990
C	1.639661	0.698007	-2.776646
C	-0.665867	0.997984	-2.943753
C	-0.102671	2.234564	-2.466350
C	-0.789878	2.963354	-1.519641
C	-0.110120	3.792920	-0.419843
C	-0.898793	3.293234	0.797570
C	-0.313172	2.877070	1.974034
C	-0.935304	1.822943	2.730973
C	-2.160790	1.278095	2.303770
C	-2.365455	-0.144558	2.309227
C	-3.403813	-0.534408	1.293695
C	-2.727338	-1.293911	0.175348
C	-3.299647	-0.888762	-1.162184
C	-2.151873	-0.794995	-2.133856
C	-1.928484	0.577174	-2.498170
C	-2.682502	1.404136	-1.623574
C	-2.076891	2.524512	-1.078139
C	-2.145787	2.733850	0.378060
C	-2.816392	1.807190	1.159287
C	-3.861904	0.839653	0.630631
C	-3.787520	0.615948	-0.948348
C	1.243269	-1.955720	-1.870211
C	0.678816	-2.901124	-0.802696
C	1.293578	-2.465131	0.532049
C	0.525392	-2.159936	1.643814
C	1.008150	-1.246967	2.642016
C	2.289837	-0.718445	2.556205
C	2.495858	0.727498	2.631589
C	3.432479	1.071584	1.601761
C	3.096319	2.099948	0.739250
C	3.141615	1.858090	-0.720193
C	3.502003	0.607016	-1.201844
C	2.679669	-0.021212	-2.173009
C	2.501344	-1.400846	-1.802061
C	3.481750	-1.783623	-0.722342
C	2.662937	-2.012644	0.532125
C	3.135135	-1.221852	1.548982

C	4.163176	-0.198496	1.141095
C	4.289154	-0.417702	-0.415997
Cl	-1.544847	-3.785878	2.493651
Cl	4.519949	-3.203542	-1.158326
Cl	-5.461290	1.431675	1.225173
Cl	-5.312974	1.020660	-1.827321
Cl	-4.737559	-1.533727	2.018851
Cl	5.720814	-0.380711	2.069942
Cl	5.977102	-0.385026	-1.049977
Cl	1.187366	-4.627858	-1.116617
Cl	-4.603746	-2.033436	-1.696301
Cl	-1.836368	-4.219217	-1.292495
Cl	2.423333	5.168397	-0.526856
Cl	-0.601398	5.548429	-0.690356

$^{540}C_{54}F_8$:

C	-0.339069	-0.428532	-3.188222
C	-0.322839	0.935983	-2.856882
C	0.908818	1.530896	-2.387712
C	0.615394	2.375097	-1.267762
C	1.469098	2.401502	-0.170289
C	0.903328	2.650983	1.229484
C	1.426349	1.560867	2.197167
C	0.322839	0.935983	2.856882
C	0.339069	-0.428533	3.188222
C	-0.866039	-1.229388	3.020994
C	-0.480917	-2.452800	2.352148
C	-1.300195	-2.944130	1.323039
C	-0.693656	-3.369202	0.076412
C	-1.546105	-2.922792	-1.012082
C	-0.959957	-2.440610	-2.192277
C	-1.464390	-1.211396	-2.758667
C	0.866039	-1.229388	-3.020994
C	0.480917	-2.452800	-2.352148
C	1.300195	-2.944130	-1.323039
C	0.693656	-3.369202	-0.076412
C	1.546105	-2.922792	1.012082
C	0.959957	-2.440610	2.192277
C	1.464390	-1.211396	2.758667
C	2.576316	-0.579270	2.178814
C	2.579237	0.847607	1.974074
C	3.546202	1.226296	0.879584
C	2.746552	1.765700	-0.295932
C	3.062586	1.057640	-1.434609

C	2.103228	0.812216	-2.437580
C	2.083412	-0.627513	-2.706081
C	3.005805	-1.238145	-1.777379
C	2.566210	-2.309929	-1.028324
C	2.714181	-2.286795	0.455428
C	3.271170	-1.185772	1.081803
C	4.120879	-0.158052	0.360821
C	3.924649	-0.159319	-1.190992
C	-1.426349	1.560867	-2.197167
C	-0.903328	2.650983	-1.229484
C	-1.469098	2.401502	0.170289
C	-0.615394	2.375097	1.267762
C	-0.908818	1.530896	2.387712
C	-2.103228	0.812216	2.437580
C	-2.083412	-0.627513	2.706081
C	-3.005805	-1.238145	1.777379
C	-2.566210	-2.309929	1.028324
C	-2.714181	-2.286795	-0.455428
C	-3.271170	-1.185772	-1.081803
C	-2.576316	-0.579270	-2.178814
C	-2.579237	0.847607	-1.974074
C	-3.546202	1.226296	-0.879584
C	-2.746552	1.765700	0.295932
C	-3.062586	1.057640	1.434609
C	-3.924649	-0.159319	1.190992
C	-4.120879	-0.158052	-0.360821
F	1.184900	3.944834	1.662412
F	-4.551207	2.072135	-1.303398
F	5.451062	-0.296210	0.676929
F	5.154851	-0.134853	-1.821304
F	4.551207	2.072135	1.303398
F	-5.154851	-0.134853	1.821304
F	-5.451062	-0.296210	-0.676929
F	-1.184900	3.944834	-1.662411

$^{540}C_{54}H_8$:

C	0.152337	3.202293	0.159683
C	0.155367	2.865385	-1.204770
C	-1.042451	2.326219	-1.803334
C	-0.685667	1.233693	-2.655252
C	-1.480927	0.087013	-2.679610
C	-0.831446	-1.283180	-2.930331
C	-1.296482	-2.273705	-1.832855
C	-0.155367	-2.865385	-1.204770

C	-0.152337	-3.202293	0.159683
C	1.041391	-2.960848	0.960808
C	0.619601	-2.318034	2.184182
C	1.379705	-1.242918	2.675415
C	0.697932	-0.034530	3.098173
C	1.484968	1.102015	2.653799
C	0.828713	2.243691	2.173032
C	1.299076	2.837097	0.941372
C	-1.041391	2.960848	0.960808
C	-0.619601	2.318034	2.184182
C	-1.379705	1.242918	2.675415
C	-0.697932	0.034530	3.098173
C	-1.484968	-1.102015	2.653799
C	-0.828713	-2.243691	2.173032
C	-1.299076	-2.837097	0.941372
C	-2.440696	-2.319405	0.307718
C	-2.460356	-2.117229	-1.119536
C	-3.501405	-1.088531	-1.500622
C	-2.759949	0.137235	-2.041514
C	-3.142884	1.256119	-1.329634
C	-2.241386	2.306322	-1.083810
C	-2.235721	2.569528	0.355143
C	-3.106434	1.589503	0.964160
C	-2.629063	0.873681	2.045412
C	-2.689147	-0.615448	2.019904
C	-3.206344	-1.268179	0.913104
C	-4.102921	-0.604010	-0.116432
C	-3.993894	0.956593	-0.111508
C	1.296482	2.273705	-1.832855
C	0.831446	1.283180	-2.930331
C	1.480927	-0.087013	-2.679610
C	0.685667	-1.233693	-2.655252
C	1.042451	-2.326219	-1.803334
C	2.241386	-2.306322	-1.083810
C	2.235721	-2.569528	0.355143
C	3.106434	-1.589503	0.964160
C	2.629063	-0.873681	2.045412
C	2.689147	0.615448	2.019904
C	3.206344	1.268179	0.913104
C	2.440696	2.319405	0.307718
C	2.460356	2.117229	-1.119536
C	3.501405	1.088531	-1.500622
C	2.759949	-0.137235	-2.041514
C	3.142884	-1.256119	-1.329634

C	3.993894	-0.956593	-0.111508
C	4.102921	0.604010	-0.116432
H	-1.036362	-1.646485	-3.948704
H	4.264838	1.477030	-2.186268
H	-5.144723	-0.917737	0.007425
H	-4.991114	1.414990	-0.128643
H	-4.264838	-1.477030	-2.186268
H	4.991114	-1.414990	-0.128643
H	5.144723	0.917737	0.007425
H	1.036362	1.646485	-3.948704