Supplementary Informaion

Synthesis, isolation, and characterization of the products of chlorination of C_{70}

C_{70} fullerene (40 mg) was heated with an excess of $SbCl_5$ in a thick-walled glass ampoule at 440 °C for six days. MALDI MS analysis of the reaction product revealed $C_{70}Cl_n$ compounds as the most abundant components. The product was then dissolved in toluene and subjected to HPLC separation using a semipreparative Buckyprep column (10 mm I.D. × 250 mm, Nacalai Tesque Inc., flow rate of 2.3 mL min^{-1}). The HPLC trace in the range of 5 – 25 min is shown in Figure S1.

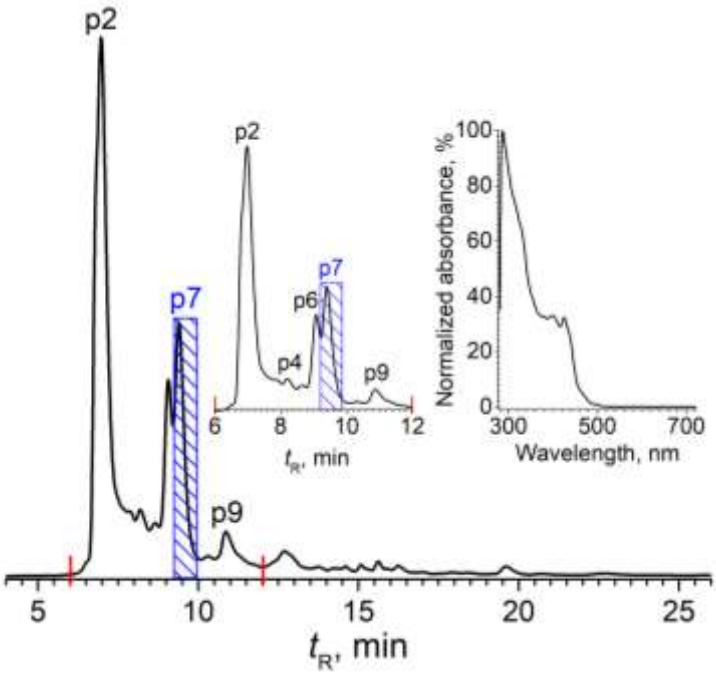

Fig. S1 HPLC separation of the chlorination product of fullerene C_{70} (Cosmosil Buckyprep, 10 mm I.D. x 25 cm, toluene, 2.3 mL·min^{-1}). Insets show an enlarged region of the HPLC plot in the range of 6 - 12 min and the UV/Vis spectrum of fraction p7.

Of the 12 collected HPLC fractions, only fractions p2 and p7 afforded, upon slow evaporation, suitable crystals for an X-ray crystallographic study (the rest of the fractions gave only viscous filmy deposits on the vessel walls). The mid-sized crystals from fraction p2 were identified as the known IPR chlorides $C_{70}Cl_{26/28}$ reported previously in ref. S1. Small orange crystals from fraction p7 studied with the use of synchrotron radiation turned out to be composed of two isostructural derivatives, $C_{68}Cl_{26}(OH)_2$ and $C_{68}Cl_{25}(OH)_3$, distributed over the same crystallographic sites. They are clearly attributable to partial hydrolysis of the initially formed $C_{68}Cl_{28}$ upon exposure to ambient atmosphere. The MALDI mass spectra of the initial fraction p7 in its solution form and of the final crystals (Figure S2) are consistent with the composition established by the X-ray data. Figure S3 further demonstrates good agreement between the experimental and calculated isotopic distributions of the fragment ions. Mass spectra of several minor fractions between p2 and p7 and of the fraction p9 revealed mixed $C_{68}Cl_n(OH)_m$ compositions. Of particular interest was fraction p6 where the signals due to the products of yet deeper skeletal transformations, $C_{66}Cl_n$ and $C_{66}Cl_{n-1}(OH)$, have been detected.

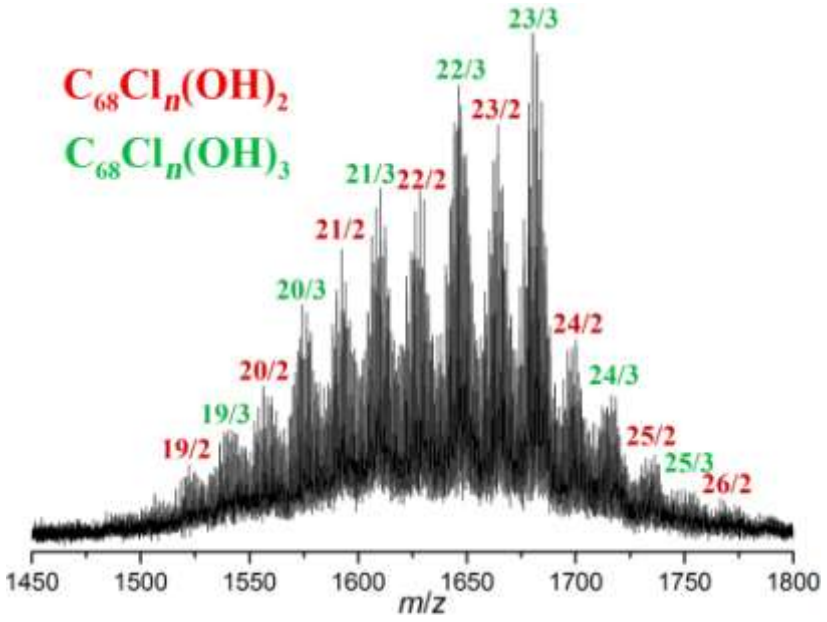

Fig. S2 Negative-ion MALDI TOF mass spectrum of fraction p7 with overlapping fragment progressions due to $C_{68}Cl_{26}(OH)_2$ (red) and $C_{68}Cl_{25}(OH)_3$ (green). The composition of the fragment ions is given as Cl/(OH) ratios, n/2 or n/3, respectively.

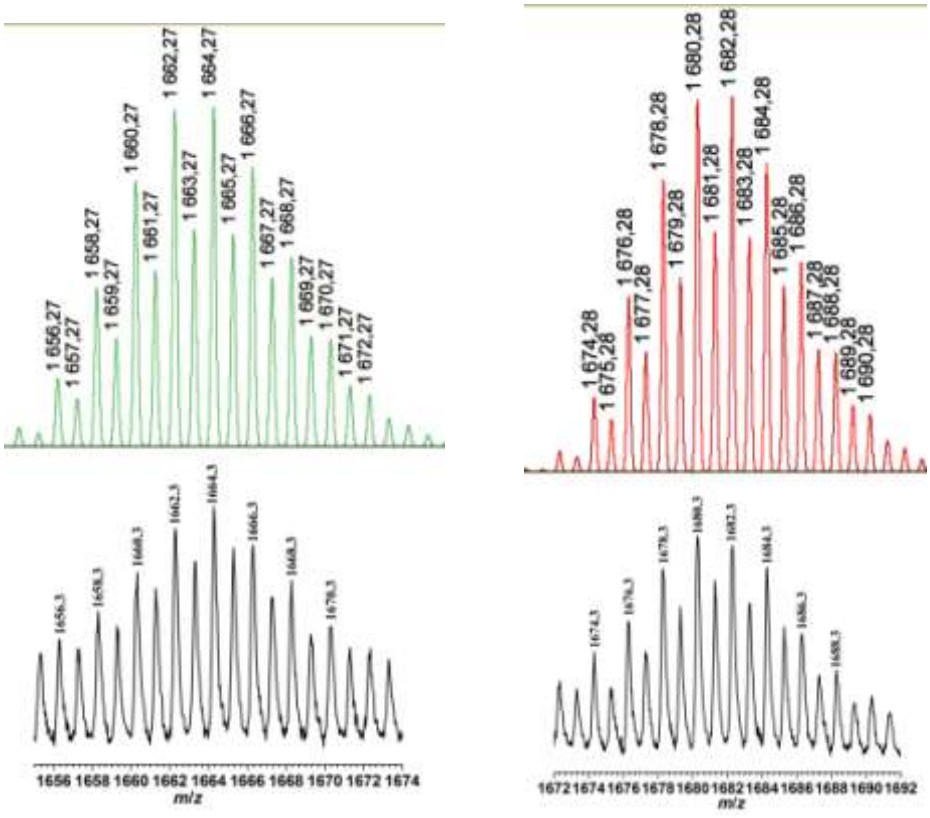

Fig. S3 Experimental (bottom) and theoretical (top) isotopic distribution of $C_{68}Cl_{23}(OH)_2$ (left) and $C_{68}Cl_{23}(OH)_3$ (right) as fragment ions in the spectra of $C_{68}Cl_{26}(OH)_2$ and $C_{68}Cl_{25}(OH)_3$, respectively.

X-ray crystallography

Crystal data. X-ray diffraction data were collected at 100 K on beamline BL14.2 at the BESSY II electron storage ring (Berlin, Germany) using a hybrid pixel detector Pilatus3S 2M (λ = 0.8266 Å). The structure was solved and anisotropically refined using the SHELX package. Crystal data: $C_{68}Cl_{25.58}(OH)_{2.42}\cdot 3PhMe$: triclinic, $P\ \bar{1}$, a = 13.388(1) Å, b = 14.084(1) Å, c = 21.734(2) Å, α = 72.78(1)°, β = 74.71(1)° γ = 65.42(1)°, V = 3574.4(6) Å^3, Z = 2, $R_1(F)/wR_2(F^2)$ = 0.139/0.257 for 2788/14265 reflections and 1032 parameters. CCDC 2161470 contains the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

Quantum-chemical calculations

Methods

Initial DFT geometry optimizations and computations of the reaction and binding energy values were carried out with the use of the PRIRODA code.[S2] The PBE exchange–correlation functional[S3] and a built-in TZ2P basis set were used. To our long experience, PBE offers reasonable relative energy of the isomeric fullerene chlorides, with small and random deviations from the results of the hybrid functionals, and comparable in magnitude to the deviations between hybrid functionals themselves.

The geometry of the hypothetic $C_{68}(NC3)Cl_{28}$ and the X-ray identified $C_{68}(NC3)Cl_{26}(OH)_2$ and $C_{68}(NC3)Cl_{25}(OH)_3$ molecules was then refined at the mPW3PBE/Def2-TZVP level of theory with the use of the Firefly 8.2 code[S4] partly based on the GAMESS(US) software.[S5] Geometry optimization of $C_{68}Cl_{26}(OH)_2$ and $C_{68}Cl_{25}(OH)_3$ reveals weak intramolecular hydrogen bonds of the types O–H ···Cl (3.19-3.24 Å) and O–H···O (2.94 Å). The intermolecular hydrogen bond O1–H1 ···Cl is directed towards to a Cl atom of a neighbouring molecule.

References

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Cartesian coordinates (mPW3PBE/Def2-TZVP)

a) $C_{68}Cl_{28}$ (E=-15473.8637 a.u.)

C	-1.319299144	-2.702403169	-0.296287684
C	-2.645341241	-2.400188537	-0.886796586
C	-3.118291675	-1.057447135	-0.416366976
C	-2.752860536	-0.578505810	0.876810436
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C	-1.164001091	-0.628004710	2.755562493
C	0.023698638	-1.159682642	3.313443770
C	0.732859425	-2.136427259	2.700189567
C	0.275605661	-2.677581424	1.483232220
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C	0.991433418	-3.157376557	-0.781447476
C	2.305447540	-3.108000471	-1.546675858
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Cl	4.116973004	3.328895044	-0.532225399
Cl	3.547751572	3.214901085	-3.375955786

a) $C_{68}Cl_{26}(OH)_2$ with two H…Cl intramolecular interactions (E=-14705.2245 a.u.)

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Cl	1.383523810	-4.009964056	-3.124266731
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Cl	3.708577015	0.473040653	0.303553723
Cl	4.386852675	3.449042505	-0.834218110
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Cl	0.564933742	1.159669293	-10.200434969
Cl	0.624860087	-2.094899869	-9.969353478
Cl	9.710690350	-0.840609270	-1.993053744
Cl	10.002019734	2.128578157	-2.218709674
Cl	9.961191409	3.011881598	-5.135693819
Cl	10.375221626	0.932879115	-7.479867566
Cl	2.652443703	-0.854319114	-12.152421375
Cl	4.270199276	-3.445667045	-11.072190875
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C	2.373149821	-2.109391886	-4.634251519
C	2.804719581	-3.022442109	-3.575514178
C	3.153655980	-1.984420939	-2.450338358
C	4.577303845	-1.528618401	-2.567014907
C	4.911404363	-0.312276682	-1.979783944
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C	4.346239385	2.191446758	-3.192177141
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C	1.582394465	-0.522192365	-6.606175373
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C	6.847801490	-1.669207501	-3.381746598

C	7.165662026	-0.523163463	-2.694657479
C	6.196916191	0.180207918	-2.040701002
C	6.327666893	1.613498291	-1.687142039
C	7.261991745	2.324695520	-2.727379646
C	6.588416936	2.455559702	-4.052893360
C	7.401385081	2.213526307	-5.108321813
C	6.897480585	2.015293156	-6.418071776
C	5.540125520	2.277944560	-6.680325644
C	4.943337568	1.796863285	-7.898301501
C	3.526986489	1.766039886	-8.035269062
C	2.963506123	0.992473611	-9.014256881
C	1.600200902	0.373400977	-8.980898205
C	1.992067886	-1.117458725	-9.430511639
C	2.739326456	-1.820677766	-8.323543581
C	3.977034153	-2.253435417	-8.679897599
C	5.048169945	-2.587398131	-7.749362068
C	4.879505317	-3.129762380	-6.466693965
C	5.863775023	-2.996014040	-5.505314175
C	7.045631226	-2.266838815	-5.722067980
C	7.890118066	-1.937864987	-4.498271615
C	8.580815941	-0.561553820	-4.460616313
C	8.498206543	-0.012616493	-3.060603881
C	8.625023663	1.544862073	-3.129020575
C	8.766931824	1.766624822	-4.700866684
C	8.867482832	0.382191984	-5.352190052
C	8.790783123	0.329554704	-6.845690224
C	7.632365063	1.178737832	-7.297800467
C	7.071396472	0.683937084	-8.428508286
C	5.742833806	1.004659226	-8.778390262
C	5.113879403	0.220768747	-9.752376924
C	3.766324571	0.292278524	-9.904425295
C	3.141797820	-0.934176305	-10.468274386
C	4.286866347	-1.951403617	-10.131835631
C	5.625632071	-1.097249729	-10.262635512
C	6.777465128	-1.611859265	-9.367669785
C	6.316198614	-2.069740451	-8.016245772
C	7.271079868	-1.824023802	-7.020952340
C	8.444181700	-1.025270472	-7.581086482
C	7.805362549	-0.526410491	-8.953935114

b) $C_{68}Cl_{26}(OH)_2$ with one H…Cl intramolecular interaction and the second hydrogen atom free for intermolecular hydrogen bonding (E=-14705.2196 a.u.)

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Cl	-0.346935261	2.867557456	-0.510450026
Cl	-1.129856244	1.218310263	-3.399601573
Cl	2.099671479	-2.507355125	0.329612919
Cl	2.476436889	0.100481843	1.962941957
Cl	1.735120385	3.431766689	1.696506650
Cl	1.570279274	5.791867987	-0.541983181
Cl	-0.669857776	1.283078034	-6.431904260
Cl	-0.148524127	-1.638223361	-5.612023780
Cl	4.830712130	-4.006688245	-2.430455334
Cl	4.981759934	-3.125413495	0.486362957

Cl	6.998658506	-1.050409901	0.732538659
Cl	4.314127942	5.794269175	1.100370664
Cl	4.603211948	7.137664409	-1.736156847
Cl	1.290740978	-1.073008996	-8.316656694
Cl	2.446165318	-3.670647235	-6.716596817
Cl	8.142516964	4.127193941	0.709127259
Cl	7.440828418	6.614772826	-0.784656072
Cl	7.823747062	6.267515399	-3.781521341
Cl	9.525649580	3.887438988	-4.956105032
Cl	4.374500367	-2.546560725	-9.047211895
Cl	6.482546674	-3.629588708	-6.839305101
Cl	7.484868496	-1.077880560	-8.557292107
Cl	9.079664665	-1.526296278	-5.896204474
Cl	10.182889800	1.048896882	-3.929064168
Cl	9.305751658	1.432051495	-7.115282994
O	1.395832647	2.928993993	-6.848528588
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C	1.380211028	2.374213426	-3.527038742
C	0.563241417	1.171859286	-3.916254661
C	1.339404226	0.053056035	-3.299658601
C	1.755810774	-0.053604511	-1.974584685
C	2.688491302	-1.037208352	-1.761232880
C	3.135630322	-1.235243000	-0.382311068
C	2.798433411	0.175546242	0.217864102
C	3.947199544	1.121886016	0.037508126
C	3.669240603	2.483847836	0.074022304
C	2.319793934	3.131061897	0.054652723
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C	1.903689516	2.042845381	-5.865370545
C	0.779868918	0.975299067	-5.495304900
C	1.263548223	-0.523903626	-5.612830865
C	1.908170829	-0.753983495	-4.279505511
C	3.026194360	-1.566144742	-4.053347291
C	3.395847965	-1.708341924	-2.722572400
C	4.654670631	-2.258402246	-2.146135298
C	4.620904406	-1.790531525	-0.590611299
C	5.724804835	-0.667651223	-0.520262028
C	5.262071294	0.727132445	-0.232170936
C	6.247653172	1.688994704	-0.448321493
C	5.956504982	3.022024595	-0.289245377
C	4.668034201	3.421121047	-0.083937860
C	4.185856350	4.793832869	-0.367938214
C	5.035887449	5.412002324	-1.532212270
C	4.715201248	4.758339100	-2.834743173
C	5.798714711	4.525369286	-3.612405759

C	5.743875951	3.681079041	-4.748321747
C	4.493992351	3.226726541	-5.208323639
C	4.431274730	2.142121426	-6.152577034
C	3.197023086	1.464134145	-6.380736935
C	3.212926975	0.234221577	-6.984666515
C	2.196924754	-0.849897681	-6.798866032
C	3.192412434	-2.081896851	-6.536119520
C	3.838460357	-1.954575171	-5.177761051
C	5.196206477	-1.915568009	-5.214359445
C	6.046434424	-1.406687005	-4.146530573
C	5.763365243	-1.470963483	-2.774315451
C	6.353754438	-0.587633864	-1.890602643
C	7.209962905	0.450041820	-2.296934306
C	7.558599202	1.511711706	-1.253041960
C	7.698414548	2.963583464	-1.733856821
C	7.072736530	3.888464854	-0.713045938
C	6.642037043	5.206167478	-1.448349255
C	7.084165451	4.882004592	-2.943103710
C	7.831540993	3.542878630	-2.923643877
C	8.154336262	2.936082636	-4.255870552
C	6.923066246	2.987634974	-5.122974287
C	6.876984099	1.938403153	-5.980975776
C	5.654448464	1.514302667	-6.544394579
C	5.610029905	0.248960426	-7.140763546
C	4.408397637	-0.320159916	-7.420359722
C	4.422401311	-1.807326923	-7.455808900
C	5.731050639	-2.046276936	-6.625495524
C	6.666605328	-0.810434699	-6.996574281
C	7.663601805	-0.430150652	-5.876338462
C	7.072589830	-0.529958958	-4.501655123
C	7.592566818	0.438611142	-3.633407378
C	8.508170489	1.401956658	-4.377549733
C	8.100180979	1.059067049	-5.880196972

c) $C_{68}Cl_{25}(OH)_3$ with one H…Cl and one H…O intramolecular interactions and the third hydrogen atom free for intermolecular hydrogen bonding (E=-14320.9080 a.u.)

Cl	0.052102777	0.001659118	0.057909627
Cl	-0.335918842	2.870755573	-0.500134878
Cl	-1.116883443	1.204669734	-3.373870278
Cl	2.190265472	-2.497671143	0.375388597
Cl	2.514777157	0.143001678	1.972537864
Cl	1.748101610	3.475063240	1.693777234
Cl	1.567768088	5.817834813	-0.564834004
Cl	-0.673435155	1.261446456	-6.407901683
Cl	-0.134291861	-1.653602319	-5.577219020
Cl	4.879023072	-3.983461447	-2.381242517
Cl	5.116254493	-3.025235453	0.524323711
Cl	4.316283369	5.849299671	1.071004959
Cl	4.603777999	7.166293268	-1.777669929
Cl	1.283871249	-1.090228978	-8.293498343
Cl	2.459926411	-3.677827325	-6.694750771
Cl	8.152805188	4.179033354	0.684333650
Cl	7.447173641	6.656539029	-0.831257994

Cl	7.811699126	6.288763838	-3.827423347
Cl	9.519536668	3.916775803	-4.994966574
Cl	4.367232268	-2.551668262	-9.040636810
Cl	6.495835537	-3.619785285	-6.844529964
Cl	7.475212582	-1.068238869	-8.577314926
Cl	9.093002542	-1.500637300	-5.927682212
Cl	10.195000908	1.082570887	-3.967451245
Cl	9.296388679	1.457123087	-7.154374552
O	1.381675293	2.915144969	-6.842908168
H	2.095116158	3.494839335	-7.135962552
O	8.668936305	1.157557216	-0.500145904
H	8.385426649	0.400285571	0.035953742
O	6.781177991	-0.816898805	0.448834631
H	6.882533097	-1.771610799	0.586633351
C	1.518889625	0.710525570	-0.663644265
C	1.330519129	2.335352824	-0.842057763
C	1.690467123	2.853352204	-2.226585727
C	1.385827938	2.375913847	-3.519799763
C	0.573993654	1.166770199	-3.898840021
C	1.358906429	0.054012516	-3.281720786
C	1.780289331	-0.045522415	-1.957636791
C	2.716897876	-1.025682112	-1.742690934
C	3.182740073	-1.205596965	-0.365500709
C	2.828172177	0.208394955	0.225566168
C	3.963258895	1.165423606	0.027601671
C	3.682729331	2.525751641	0.069658354
C	2.331150835	3.164790280	0.053146143
C	2.698628430	4.472754651	-0.756071725
C	2.574976932	3.909901462	-2.140334895
C	3.474802454	4.190839145	-3.176972841
C	3.340475572	3.508837773	-4.403880004
C	2.170467028	2.757804381	-4.580298502
C	1.899507790	2.035885718	-5.858566539
C	0.782914220	0.964620615	-5.477868896
C	1.272672200	-0.532670355	-5.591690660
C	1.925951065	-0.755270246	-4.260929371
C	3.047993806	-1.563323451	-4.037300121
C	3.421646247	-1.698791995	-2.705802991
C	4.690203576	-2.228520062	-2.132619192
C	4.670495682	-1.727955385	-0.589446590
C	5.774758278	-0.606806075	-0.526997621
C	5.270567510	0.778638121	-0.265181642
C	6.248983326	1.738830682	-0.485144890
C	5.966721529	3.070677693	-0.314098073
C	4.679004980	3.465822597	-0.096736404
C	4.190540655	4.834186132	-0.387118470
C	5.038837915	5.443089196	-1.558991917
C	4.715020448	4.776938682	-2.854358050
C	5.796472889	4.540062628	-3.633744345
C	5.739018118	3.691841461	-4.766118069
C	4.488567875	3.232512523	-5.219490075
C	4.425181434	2.145163803	-6.160149927
C	3.192388265	1.461300838	-6.378874581
C	3.209523778	0.229450795	-6.978363578

C	2.199455872	-0.858523768	-6.782444273
C	3.201083762	-2.085381761	-6.521886131
C	3.855116042	-1.952258467	-5.167401665
C	5.212667969	-1.907002026	-5.216584045
C	6.066482544	-1.388925298	-4.158663220
C	5.784994048	-1.439831853	-2.785875753
C	6.365687994	-0.540148106	-1.918996231
C	7.222084418	0.491389565	-2.327427163
C	7.558929220	1.544139400	-1.271061633
C	7.722120103	2.997293844	-1.751041019
C	7.086929062	3.930427364	-0.738507395
C	6.648981065	5.240984954	-1.480704695
C	7.084367730	4.905094774	-2.973804845
C	7.839670149	3.568645931	-2.948495838
C	8.156548258	2.960398648	-4.284410488
C	6.919574812	3.003942962	-5.145463605
C	6.873325588	1.953941969	-6.003071690
C	5.648957342	1.522208529	-6.557698208
C	5.605632729	0.254714133	-7.150237081
C	4.404519651	-0.320750654	-7.419900117
C	4.423906472	-1.807948898	-7.451406461
C	5.738865541	-2.038899463	-6.630458004
C	6.667653441	-0.799699794	-7.011033250
C	7.671225142	-0.411349870	-5.899158758
C	7.087265997	-0.508339839	-4.521659829
C	7.607376519	0.468378639	-3.661523240
C	8.517122511	1.429021694	-4.410643848
C	8.101558193	1.080777886	-5.909835640

d) $C_{68}Cl_{25}(OH)_3$ with three H…Cl intramolecular interactions (E=-14320.9108 a.u.)

Cl	4.373248275	0.411486595	-0.746414378
Cl	4.249778941	3.353262145	-0.875276009
Cl	1.631371772	2.196017272	-2.729050187
Cl	5.776315979	-2.353297558	-1.863039844
Cl	7.467741772	-0.012308990	-0.724332840
Cl	7.296053300	3.391741390	-0.382648799
Cl	6.234356531	6.017883725	-1.993077669
Cl	0.194529249	2.604792182	-5.400523811
Cl	0.570295149	-0.447497735	-5.161160786
Cl	5.990084637	-3.783548149	-5.750249833
Cl	8.060398720	-3.272533632	-3.544153078
Cl	9.367396510	5.482721215	-2.363769496
Cl	8.141544099	7.132349659	-4.750768552
Cl	0.187412222	0.283969476	-8.162939897
Cl	1.598202187	-2.617890395	-7.679129861
Cl	11.853383786	3.391716694	-5.104144462
Cl	10.843224249	6.138713379	-5.734187132
Cl	9.284243282	6.159051177	-8.352657460
Cl	9.493168108	3.764685911	-10.400127390
Cl	1.908320077	-1.441865283	-10.668121201
Cl	4.694241082	-3.041381520	-10.241759972
Cl	4.887323798	-0.428007036	-12.140589066
Cl	7.651804762	-1.397365783	-11.025368114

Cl	10.136325236	0.760387311	-10.074402653
Cl	7.606336857	1.644392084	-12.042785280
O	1.922059960	4.025270392	-7.064730861
H	1.344537814	4.391291957	-6.380522617
O	10.989108785	0.506529968	-6.465597017
H	11.655779727	1.001760118	-5.970034889
O	9.723858827	-1.295553255	-4.475970085
H	9.820854339	-2.183132562	-4.843244746
C	5.220759425	1.016424598	-2.192368616
C	5.257713948	2.660171889	-2.174634892
C	4.811542006	3.307553872	-3.476945408
C	3.719121984	3.048446126	-4.333872202
C	2.642023286	2.009206442	-4.175092385
C	3.421070654	0.734742464	-4.190442414
C	4.520183981	0.410593556	-3.398615327
C	5.206498678	-0.698601876	-3.825576443
C	6.356145238	-1.118275876	-3.021027498
C	6.686197185	0.239291383	-2.298624117
C	7.632580233	1.063505786	-3.119103187
C	7.676803787	2.431624246	-2.875973158
C	6.722201193	3.231369203	-2.047894451
C	6.764278613	4.579028734	-2.873280803
C	5.744028173	4.226035458	-3.913980674
C	5.881833602	4.533570189	-5.274867574
C	4.925091377	4.046716777	-6.188527468
C	3.769168944	3.473789019	-5.638832543
C	2.671424607	2.968083571	-6.517055436
C	1.838099853	1.986703857	-5.559524818
C	1.876610860	0.473615286	-5.990954687
C	3.138710134	-0.002366781	-5.335597560
C	4.010186449	-0.962611051	-5.864616098
C	5.070497281	-1.317041084	-5.040528311
C	6.312014091	-2.071455971	-5.369588879
C	7.295112784	-1.793303160	-4.114688305
C	8.418265459	-0.842079150	-4.692945812
C	8.423407732	0.554990768	-4.149642843
C	9.238156192	1.404023568	-4.890536535
C	9.338587653	2.730747798	-4.548956379
C	8.526102613	3.253889783	-3.585780795
C	8.216883225	4.699125406	-3.476795862
C	8.293890188	5.354329749	-4.900167224
C	7.150499978	4.916926387	-5.753971684
C	7.492015076	4.659938255	-7.038740381
C	6.623007554	3.980535876	-7.928262143
C	5.291115279	3.741957384	-7.541798180
C	4.492535580	2.799868467	-8.280272766
C	3.277495123	2.306447792	-7.726926731
C	2.716708769	1.169528564	-8.243569629
C	1.843942955	0.198362298	-7.509895279
C	2.567121930	-1.166825135	-7.946591730
C	3.907289230	-1.293801243	-7.263246608
C	4.954458187	-1.408027866	-8.121814673
C	6.345607571	-1.141778701	-7.782529519
C	6.933537351	-1.344386388	-6.525250411

C	8.077387908	-0.662448702	-6.163485276
C	8.690448531	0.297687099	-6.982402710
C	9.757460112	1.167252410	-6.329380015
C	9.819723025	2.647817146	-6.762063989
C	10.097936537	3.499889428	-5.549494710
C	9.565139037	4.945115691	-5.821449811
C	8.960691783	4.771851765	-7.285331820
C	9.323388254	3.361934662	-7.769095708
C	8.674820542	2.898270639	-9.037250344
C	7.201892657	3.205864787	-8.966538846
C	6.472658562	2.286470832	-9.645882096
C	5.106826791	2.085197210	-9.354108705
C	4.497598426	0.920197584	-9.834582551
C	3.293585739	0.537213830	-9.336378249
C	3.026459052	-0.923694118	-9.417521341
C	4.505821055	-1.419762974	-9.568496896
C	5.227988004	-0.266349533	-10.398323830
C	6.743733258	-0.152464610	-10.111055153
C	7.086437058	-0.354102387	-8.665252180
C	8.183910082	0.423705310	-8.270693210
C	8.617130606	1.360233750	-9.392265962
C	7.338601731	1.262353554	-10.339371682

e) $C_{68}Cl_{25}(OH)_3$ with two H…Cl and one H…O intramolecular interactions (E=-14320.9117 a.u.)

Cl	4.370243037	0.415859532	-0.749829351
Cl	4.247588766	3.357800162	-0.874580534
Cl	1.635774179	2.193405613	-2.727452028
Cl	5.778564042	-2.342681090	-1.870799350
Cl	7.465607307	-0.005234412	-0.717687028
Cl	7.291894148	3.406397278	-0.376173275
Cl	6.227718273	6.028728725	-1.994309538
Cl	0.197475295	2.603833461	-5.397061899
Cl	0.576070731	-0.448132332	-5.157854795
Cl	5.998194384	-3.785272816	-5.739742734
Cl	8.076363232	-3.258172268	-3.530597446
Cl	9.362457596	5.504443636	-2.360427839
Cl	8.144554850	7.138775074	-4.760256002
Cl	0.188451069	0.287399848	-8.158521292
Cl	1.598166295	-2.615747086	-7.678937642
Cl	11.851351125	3.385328371	-5.096243543
Cl	10.849042142	6.138316629	-5.737385290
Cl	9.286529423	6.156259910	-8.354823170
Cl	9.500525225	3.763744438	-10.397747782
Cl	1.902769182	-1.435048097	-10.666906037
Cl	4.687856113	-3.037606704	-10.251211282
Cl	4.880537222	-0.420639897	-12.144382772
Cl	7.647063684	-1.392873128	-11.035546294
Cl	10.134930772	0.757661939	-10.071834768
Cl	7.605165013	1.650984521	-12.046883813
O	1.923912389	4.027047080	-7.061049234
H	1.333132876	4.379762903	-6.380972398
O	10.954216184	0.461494694	-6.365222006
H	11.640387620	1.019936330	-5.968746818

O	9.692985422	-1.398801504	-4.538311962
H	10.312236730	-0.946605130	-5.136971493
C	5.223267457	1.020911840	-2.191966830
C	5.258557471	2.666146732	-2.172017084
C	4.813265071	3.312518994	-3.474933786
C	3.721709946	3.050767724	-4.332171228
C	2.646274003	2.009421344	-4.173822380
C	3.427623081	0.736388631	-4.191867080
C	4.528620136	0.415113002	-3.401846789
C	5.218652674	-0.691577657	-3.829847528
C	6.367929914	-1.109981464	-3.024310902
C	6.688800337	0.246159475	-2.293918813
C	7.634342256	1.073501244	-3.109098660
C	7.680103744	2.442665678	-2.865983297
C	6.721690513	3.241948569	-2.041708978
C	6.762204273	4.589223660	-2.870344022
C	5.744898589	4.231802199	-3.912284804
C	5.883875202	4.536468051	-5.273835750
C	4.927522173	4.048008953	-6.187237274
C	3.771608041	3.475333461	-5.637283134
C	2.673534183	2.969117994	-6.514852240
C	1.841659651	1.986826748	-5.557347617
C	1.880972292	0.473747618	-5.988940561
C	3.145220040	-0.001167499	-5.336449602
C	4.016276050	-0.962861625	-5.865185286
C	5.079338308	-1.315453342	-5.042038126
C	6.319598080	-2.075102099	-5.370606865
C	7.316919955	-1.792759008	-4.116642420
C	8.415978299	-0.836101213	-4.706822777
C	8.410905774	0.562527077	-4.149440309
C	9.205770248	1.425026539	-4.893150155
C	9.327666313	2.745762331	-4.547884941
C	8.526858912	3.268324070	-3.575486668
C	8.216276359	4.712412824	-3.471591962
C	8.295386025	5.360499279	-4.900223184
C	7.153065439	4.918262670	-5.753117395
C	7.494492660	4.658229229	-7.037498869
C	6.624996081	3.980117992	-7.927274756
C	5.293027442	3.742558050	-7.540509849
C	4.493361720	2.801697722	-8.279556711
C	3.278747461	2.308391050	-7.725425632
C	2.717613995	1.171498124	-8.241606172
C	1.845633865	0.199821398	-7.507550239
C	2.567354422	-1.165237409	-7.945940700
C	3.908884307	-1.294560565	-7.264247334
C	4.952844245	-1.410462182	-8.126874975
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C	6.928745946	-1.346079454	-6.531073613
C	8.060864668	-0.648246070	-6.167344872
C	8.670195649	0.311547541	-6.984696842
C	9.725448028	1.178414045	-6.318111353
C	9.828525837	2.648334387	-6.762633108
C	10.096279730	3.503903777	-5.548406713
C	9.567899295	4.948385571	-5.822603769

C	8.962922426	4.771927715	-7.285852803
C	9.324925662	3.359811648	-7.769350818
C	8.675205746	2.898108560	-9.039298577
C	7.202275466	3.207676763	-8.967881586
C	6.471694069	2.289841698	-9.648501488
C	5.106094228	2.088113613	-9.355130585
C	4.495923525	0.923382298	-9.835657463
C	3.292839819	0.539997359	-9.335469518
C	3.024179100	-0.920575615	-9.417826839
C	4.502266650	-1.418145268	-9.572878790
C	5.224100177	-0.262941047	-10.402449225
C	6.740284455	-0.150150325	-10.117724685
C	7.082054816	-0.352531685	-8.671977581
C	8.174238141	0.429663834	-8.277121617
C	8.613233935	1.361867109	-9.396604239
C	7.335903171	1.265769214	-10.344733494