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ELECTRONIC SUPPLEMENTARY INFORMATION

Local energy decomposition analysis and molecular properties of encapsulated methane in fullerene ($CH_4@C_{60}$)

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Table S1 DLPNO-CCSD(T) interaction energy and contributions to the correlation binding energy for the $CH_4\cdots C_6H_6$ dimer (results in kcal/mol)

PNO truncation threshold $CH_4\cdots C_6H_6/CH_4/C_6H_6$	Basis set CH_4/C_6H_6	Interaction ΔE_{int}	Contribution		
			E_{disp}	$\Delta E_{non\text{-}disp}$	ΔE_{int} C-(T) (T_0)
TightPNO/TightPNO/TightPNO	cc-pV5Z/cc-pV5Z	-1.32	-2.30	+0.12	-0.34
TightPNO/TightPNO/TightPNO	cc-pVQZ/cc-pVQZ	-1.22	-2.28	+0.19	-0.32
TightPNO/TightPNO/TightPNO	cc-pVTZ/cc-pVTZ	-0.97	-2.14	+0.27	-0.27
TightPNO/TightPNO/TightPNO	cc-pVDZ/cc-pVDZ	-0.26	-1.55	+0.29	-0.16
TightPNO/NormalPNO/LoosePNO	cc-pVQZ/cc-pVTZ	-1.34	-2.22	+0.06	-0.34
TightPNO/NormalPNO/LoosePNO	cc-pVQZ/cc-pVTZ	-1.37	-2.22	+0.06	-0.37 (T_1)

Table S2 Cartesian coordinates (Å) of the CH_4 model

C	-0.009692	0.019691	-0.015120
H	1.059776	0.260548	-0.136119
H	-0.508055	0.829714	0.543367
H	-0.112671	-0.927387	0.540625
H	-0.477817	-0.084107	-1.008345

Table S3 Cartesian coordinates (Å) of the C_{60} model

C	2.235326	0.599774	2.690663
C	3.143677	0.166118	1.641400
C	1.343573	-0.314572	3.267900
C	3.127955	-1.166308	1.207160
C	3.227162	-1.469517	-0.211681
C	3.260791	1.245184	0.673706
C	3.356501	0.952737	-0.693769
C	3.338994	-0.429529	-1.144419
C	-0.455528	1.382603	3.240338
C	0.470016	2.331117	2.641271
C	-0.026654	0.083815	3.547651
C	1.790556	1.946615	2.371404
C	2.424337	2.345702	1.124924
C	-0.266751	3.128055	1.673464
C	0.343753	3.512886	0.471946
C	1.714054	3.114198	0.192549
C	-2.151658	-0.848864	2.692884
C	-2.596793	0.498273	2.374054
C	-0.890448	-1.052516	3.269412
C	-1.764111	1.593416	2.642254
C	-1.647781	2.672721	1.674573
C	-3.343517	0.441099	1.127553
C	-3.231686	1.481087	0.194814
C	-2.367804	2.617101	0.473175
C	-0.509252	-3.010302	1.806755
C	-1.818023	-2.799234	1.209202
C	-0.053976	-2.153321	2.818216
C	-2.624304	-1.738614	1.644336
C	-3.361025	-0.941167	0.676903

C	-1.718578	-3.102628	-0.209416
C	-2.428861	-2.334132	-1.141791
C	-3.265315	-1.233613	-0.690573
C	2.202335	-2.114850	1.805477
C	1.729859	-3.004157	0.756558
C	1.326755	-1.696995	2.817149
C	0.399087	-3.443762	0.757289
C	-0.348276	-3.501316	-0.488812
C	2.363280	-2.605531	-0.490042
C	1.643258	-2.661151	-1.691439
C	0.262228	-3.116485	-1.690330
C	-2.239850	-0.588204	-2.707529
C	-1.795079	-1.935045	-2.388270
C	-0.474539	-2.319547	-2.658138
C	-1.348096	0.326142	-3.284767
C	-2.206858	2.126420	-1.822344
C	-3.132478	1.177878	-1.224026
C	-3.148201	-0.154548	-1.658266
C	-1.331278	1.708565	-2.834015
C	0.504729	3.021872	-1.823621
C	-0.403610	3.455332	-0.774156
C	-1.734382	3.015727	-0.773424
C	0.049453	2.164891	-2.835083
C	2.147134	0.860434	-2.709750
C	2.619781	1.750184	-1.661202
C	1.813499	2.810804	-1.226069
C	0.885925	1.064086	-3.286278
C	0.451005	-1.371033	-3.257204
C	1.759587	-1.581846	-2.659121
C	2.592270	-0.486703	-2.390921
C	0.022130	-0.072245	-3.564517

Table S4 Cartesian coordinates (Å) of the $CH_4@C_{60}$ model

C	-0.008384	0.019104	-0.014555
H	1.052719	0.259455	-0.135628
H	-0.504974	0.823018	0.537392
H	-0.112764	-0.920950	0.536739
H	-0.475057	-0.082168	-0.999540
C	2.236504	0.600667	2.691742
C	3.145841	0.164607	1.644032
C	1.342690	-0.311591	3.268654
C	3.126335	-1.167652	1.210787
C	3.227671	-1.473310	-0.206739
C	3.268017	1.242550	0.675458
C	3.366195	0.948141	-0.692714
C	3.346667	-0.435856	-1.142035
C	-0.453628	1.388628	3.239929
C	0.473573	2.334631	2.640318
C	-0.026389	0.088972	3.546861
C	1.793784	1.947124	2.370775
C	2.429607	2.343260	1.124538
C	-0.261838	3.133818	1.672733
C	0.350439	3.511159	0.469421
C	1.719859	3.109269	0.190882
C	-2.149869	-0.841844	2.691338
C	-2.593302	0.505449	2.371387
C	-0.890858	-1.046901	3.270316
C	-1.762841	1.601754	2.642685

C	-1.645195	2.681286	1.673406
C	-3.337834	0.447300	1.124258
C	-3.226143	1.485876	0.190761
C	-2.363220	2.622787	0.469354
C	-0.512373	-3.011480	1.813366
C	-1.820621	-2.798225	1.212951
C	-0.056327	-2.151134	2.823087
C	-2.622450	-1.732438	1.644076
C	-3.356101	-0.935260	0.675181
C	-1.719527	-3.101914	-0.205667
C	-2.427165	-2.332893	-1.140175
C	-3.260773	-1.230168	-0.691351
C	2.198892	-2.114165	1.809539
C	1.727408	-3.005532	0.762643
C	1.324527	-1.695111	2.821002
C	0.396726	-3.446987	0.763917
C	-0.350016	-3.502857	-0.483247
C	2.361913	-2.608036	-0.483609
C	1.641882	-2.662963	-1.684149
C	0.261237	-3.117770	-1.684141
C	-2.238606	-0.590363	-2.712137
C	-1.794595	-1.937941	-2.388665
C	-0.473338	-2.322881	-2.654911
C	-1.344503	0.323028	-3.290580
C	-2.198850	2.125722	-1.826152
C	-3.125065	1.179383	-1.227472
C	-3.144305	-0.153167	-1.661403
C	-1.324948	1.705886	-2.838502
C	0.512607	3.014249	-1.824614
C	-0.395489	3.451216	-0.776774
C	-1.727261	3.016642	-0.777732
C	0.056976	2.157554	-2.835430
C	2.153429	0.853202	-2.708325
C	2.628805	1.744512	-1.662186
C	1.820284	2.803279	-1.226717
C	0.892388	1.056830	-3.285955
C	0.454061	-1.376007	-3.254302
C	1.761107	-1.586299	-2.653323
C	2.596724	-0.493096	-2.387134
C	0.027199	-0.077748	-3.566665

Table S5 Cartesian coordinates (Å) of the Ng@C_{60} model (Ng = He, Ne, Ar, Kr)

Ng	0.000455	0.005628	-0.007976
C	2.236888	0.600443	2.691828
C	3.145152	0.164144	1.643988
C	1.343273	-0.311816	3.268916
C	3.127383	-1.168612	1.211381
C	3.227261	-1.473866	-0.206430
C	3.263958	1.241366	0.675028
C	3.360646	0.946987	-0.691679
C	3.342166	-0.435634	-1.140529
C	-0.453199	1.386849	3.236633
C	0.473697	2.333309	2.637930
C	-0.026334	0.088597	3.546970
C	1.793976	1.947151	2.370251
C	2.428723	2.343373	1.123873
C	-0.261150	3.130082	1.669187
C	0.350646	3.511960	0.467704

C	1.720269	3.111381	0.190105
C	-2.151884	-0.842318	2.692357
C	-2.594267	0.504594	2.370565
C	-0.891174	-1.046431	3.269273
C	-1.761138	1.599044	2.638605
C	-1.642208	2.676125	1.669341
C	-3.341114	0.446987	1.124720
C	-3.226239	1.485231	0.190635
C	-2.361504	2.620411	0.467964
C	-0.511761	-3.006499	1.810424
C	-1.819507	-2.794633	1.211796
C	-0.056150	-2.148589	2.820453
C	-2.624467	-1.732368	1.644633
C	-3.359638	-0.935634	0.675888
C	-1.719225	-3.100014	-0.205909
C	-2.427707	-2.332032	-1.139680
C	-3.262895	-1.230004	-0.690813
C	2.200403	-2.114995	1.810174
C	1.727985	-3.005466	0.762628
C	1.324856	-1.694495	2.820231
C	0.396680	-3.443166	0.762781
C	-0.349613	-3.500589	-0.483511
C	2.362551	-2.609065	-0.483765
C	1.643228	-2.664745	-1.685123
C	0.262190	-3.118728	-1.684994
C	-2.235849	-0.589089	-2.707620
C	-1.792936	-1.935796	-2.386051
C	-0.472663	-2.321959	-2.653750
C	-1.342233	0.323169	-3.284725
C	-2.199353	2.126333	-1.825962
C	-3.126339	1.179966	-1.227179
C	-3.144127	-0.152794	-1.659781
C	-1.323813	1.705863	-2.836038
C	0.512804	3.017900	-1.826245
C	-0.395640	3.454507	-0.778584
C	-1.726952	3.016836	-0.778427
C	0.057190	2.159926	-2.836213
C	2.152896	0.853660	-2.708129
C	2.625518	1.743740	-1.660439
C	1.820527	2.805974	-1.227585
C	0.892216	1.057804	-3.285106
C	0.454236	-1.375512	-3.252465
C	1.762177	-1.587705	-2.654410
C	2.595285	-0.493241	-2.386360
C	0.027374	-0.077247	-3.562749

Table S6 Cartesian coordinates (Å) of the $He_2@C_{60}$ model

He	0.102260	-0.369146	0.883112
He	-0.099949	0.378753	-0.895472
C	2.235372	0.601624	2.697538
C	3.143048	0.164997	1.648840
C	1.344195	-0.310694	3.281873
C	3.124922	-1.167877	1.218304
C	3.225703	-1.473888	-0.200076
C	3.261917	1.240602	0.676695
C	3.358562	0.945559	-0.690166
C	3.339789	-0.437178	-1.136581
C	-0.453566	1.388782	3.240123

C	0.472762	2.334162	2.637696
C	-0.027031	0.090626	3.557808
C	1.792683	1.947813	2.371390
C	2.426770	2.342796	1.123330
C	-0.260931	3.129519	1.665760
C	0.350297	3.510586	0.463394
C	1.719638	3.109793	0.187030
C	-2.151362	-0.840481	2.698748
C	-2.593290	0.506041	2.372394
C	-0.892852	-1.046397	3.283339
C	-1.760119	1.600403	2.638183
C	-1.641557	2.675906	1.666221
C	-3.338535	0.447766	1.124747
C	-3.224459	1.484480	0.188245
C	-2.360396	2.619976	0.464128
C	-0.511825	-3.005757	1.821616
C	-1.818613	-2.793243	1.219577
C	-0.056645	-2.151084	2.836867
C	-2.623780	-1.730754	1.650378
C	-3.357305	-0.934971	0.678330
C	-1.718385	-3.099206	-0.198865
C	-2.425520	-2.332210	-1.135166
C	-3.260655	-1.230010	-0.688530
C	2.199218	-2.114043	1.820669
C	1.727160	-3.004169	0.772086
C	1.326037	-1.696046	2.835899
C	0.396273	-3.441887	0.772579
C	-0.349045	-3.499995	-0.475229
C	2.361644	-2.609385	-0.475961
C	1.642808	-2.665320	-1.678058
C	0.262181	-3.118926	-1.677596
C	-2.234119	-0.591038	-2.709375
C	-1.791435	-1.937230	-2.383228
C	-0.471510	-2.323570	-2.649530
C	-1.342938	0.321276	-3.293709
C	-2.197965	2.124628	-1.832495
C	-3.123671	1.178466	-1.230133
C	-3.141788	-0.154407	-1.660672
C	-1.324775	1.706619	-2.847713
C	0.513079	3.016343	-1.833447
C	-0.395021	3.452471	-0.784412
C	-1.725908	3.014757	-0.783918
C	0.057902	2.161657	-2.848688
C	2.152613	0.851065	-2.710583
C	2.625032	1.741340	-1.662213
C	1.819867	2.803830	-1.231409
C	0.894112	1.056986	-3.295197
C	0.454820	-1.378197	-3.251969
C	1.761374	-1.589820	-2.650021
C	2.594545	-0.495457	-2.384229
C	0.028288	-0.080041	-3.569668

Table S7 Cartesian coordinates (Å) of the open cage C_{60} model

C	2.753183	-0.456860	2.713832
C	3.340030	-0.653370	1.396278
C	1.785516	-1.366109	3.169896
C	3.168850	-1.893454	0.740791
C	3.161878	-2.016218	-0.702177

C	3.559430	0.528313	0.568071
C	3.499220	0.402955	-0.824402
C	3.326623	-0.873306	-1.481409
C	-1.276241	2.765814	4.122426
C	-0.222365	3.812128	3.544051
C	0.515242	-1.052785	3.995939
C	3.278556	1.827305	1.129365
C	-0.354278	3.740701	2.041572
C	0.482014	3.855078	0.928426
C	2.581320	2.768518	0.393510
C	-1.825267	-1.390645	2.916514
C	-2.671576	1.069229	2.668627
C	-0.567535	-1.878714	3.289442
C	-2.042416	2.288318	2.945856
C	-1.643734	3.117464	1.855271
C	-3.052941	0.721825	1.310528
C	-2.990995	1.771866	0.352560
C	-2.190980	2.936866	0.610207
C	-0.554114	-3.402859	1.360067
C	-1.801156	-2.813288	0.923325
C	0.086098	-2.823962	2.449892
C	-2.367501	-1.701718	1.600001
C	-3.042337	-0.661877	0.809157
C	-1.862255	-2.963952	-0.507622
C	-2.520898	-1.998601	-1.259523
C	-3.135253	-0.863992	-0.600351
C	2.230319	-2.859123	1.252203
C	1.589588	-3.532342	0.135766
C	1.501387	-2.529646	2.393277
C	0.208569	-3.792368	0.188797
C	-0.614403	-3.546070	-0.975402
C	2.177679	-3.015225	-1.082703
C	1.384801	-2.815396	-2.228524
C	-0.040539	-3.090662	-2.172047
C	-2.272877	-0.171395	-2.695748
C	-1.964911	-1.575133	-2.534787
C	-0.729628	-2.084615	-2.963936
C	-1.309963	0.702503	-3.237247
C	-1.942704	2.443195	-1.626072
C	-2.927538	1.535729	-1.060966
C	-3.045416	0.240926	-1.541265
C	-1.113196	2.013190	-2.651907
C	0.866075	2.933570	-1.416993
C	-0.027234	3.498344	-0.399298
C	-1.408653	3.238158	-0.554558
C	0.310429	2.283268	-2.554548
C	2.218494	0.740769	-2.742102
C	2.805602	1.402691	-1.605158
C	2.175012	2.481610	-0.959247
C	0.981145	1.174837	-3.209562
C	0.270233	-1.182257	-3.513096
C	1.572222	-1.628599	-3.044287
C	2.530146	-0.674365	-2.671316
C	-0.009557	0.189748	-3.617168
S	-2.598813	-0.169191	3.947132
O	-1.386703	2.478736	5.299492
O	0.353188	-0.219647	4.863689
O	0.434237	4.543455	4.261161

C	3.634692	2.006378	2.579026
C	3.054561	0.815174	3.438840
C	2.007082	4.036907	1.013547
C	2.504277	4.243554	2.421122
C	3.184413	3.330122	3.128121
O	2.916100	0.937560	4.644339
H	2.223827	5.192122	2.886398
H	3.447040	3.531496	4.172171
N	5.604206	0.575008	2.515482
N	1.397456	5.876353	-0.489288
C	2.411502	5.220493	0.136668
C	1.672428	6.918263	-1.325614
C	3.004880	7.330751	-1.540720
C	4.051877	6.659987	-0.883384
C	3.760242	5.580911	-0.028945
C	0.486078	7.576372	-2.025265
C	-0.846293	6.983480	-1.501703
C	0.603346	7.301142	-3.557453
C	0.506651	9.112807	-1.768885
H	0.588857	6.209894	-3.751997
H	1.542453	7.722758	-3.968884
H	-0.253090	7.768082	-4.085261
H	0.451662	9.323275	-0.681844
H	-0.367451	9.581978	-2.264491
H	1.425374	9.580698	-2.174854
H	-0.889968	5.893841	-1.677966
H	-0.947353	7.149341	-0.412046
H	-1.692741	7.473665	-2.024213
H	3.224590	8.165038	-2.216300
H	5.091672	6.972518	-1.042786
H	4.551071	5.025565	0.490214
C	6.937622	0.291487	2.549368
C	7.876731	1.321159	2.763778
C	5.160414	1.848716	2.678306
C	7.420706	2.642891	2.926889
C	6.042517	2.925151	2.881455
H	5.664894	3.946599	3.000384
H	8.140999	3.454758	3.089681
H	8.947602	1.099757	2.802259
C	7.286072	-1.174348	2.304623
C	8.783740	-1.471375	2.564829
C	6.940648	-1.495247	0.816413
C	6.403334	-2.061621	3.231348
H	9.437217	-0.908499	1.867496
H	8.974263	-2.551976	2.408237
H	9.065601	-1.219659	3.607833
H	7.551060	-0.872698	0.131035
H	5.871953	-1.293984	0.627208
H	7.148260	-2.564353	0.607595
H	6.620942	-1.848380	4.297534
H	6.614565	-3.131408	3.031025
H	5.334971	-1.857512	3.041387

Table S8 Cartesian coordinates (Å) of the transition state model

C	0.451337	1.523183	3.738517
H	0.702803	0.932497	2.845404
H	-0.553694	1.259579	4.075973
H	0.552761	2.573169	3.474252

H	1.131034	1.324586	4.571472
S	-2.653613	0.017440	3.853642
O	-2.096170	3.173645	5.124565
O	0.412614	-0.835002	5.341642
O	-0.097184	5.082212	3.999571
O	3.373132	0.661943	4.786330
C	-1.796133	3.250332	3.948136
C	-0.681931	4.240012	3.343047
C	0.497398	-1.286917	4.222073
C	3.193347	0.624195	3.581389
C	2.285744	4.075776	2.515919
C	2.994392	3.182598	3.228828
H	1.958312	5.006728	2.989238
H	3.236235	3.392127	4.277595
C	2.745670	-0.623056	2.870370
C	3.279998	-0.807324	1.528284
C	1.756847	-1.512960	3.326351
C	3.108445	-2.047120	0.872880
C	3.111432	-2.174380	-0.568897
C	3.462013	0.379104	0.698237
C	3.433993	0.245986	-0.693301
C	3.290873	-1.034628	-1.349288
C	3.129737	1.674411	1.245749
C	-0.628545	3.932335	1.869104
C	0.326164	3.855797	0.847815
C	2.430333	2.603426	0.491702
C	-1.849175	-1.265486	2.899839
C	-2.814487	1.219431	2.533897
C	-0.638053	-1.831788	3.326725
C	-2.343465	2.522636	2.771328
C	-1.898823	3.282406	1.644544
C	-3.128393	0.783356	1.181399
C	-3.094337	1.783746	0.167781
C	-2.340550	2.982496	0.387182
C	-0.656505	-3.407695	1.432556
C	-1.869503	-2.784804	0.960983
C	-0.018285	-2.830369	2.518354
C	-2.395541	-1.623909	1.588518
C	-3.067662	-0.621003	0.746582
C	-1.921042	-2.998677	-0.463106
C	-2.550476	-2.055296	-1.261132
C	-3.159144	-0.890765	-0.654531
C	2.145945	-2.991989	1.377912
C	1.501242	-3.652261	0.256719
C	1.415078	-2.631473	2.506960
C	0.112247	-3.865999	0.289973
C	-0.683378	-3.629946	-0.893213
C	2.121128	-3.164420	-0.957506
C	1.354369	-2.970018	-2.121909
C	-0.076160	-3.221451	-2.091684
C	-2.262703	-0.293104	-2.764367
C	-1.969669	-1.690982	-2.544028
C	-0.730957	-2.227568	-2.926448
C	-1.275982	0.555395	-3.304174
C	-1.964685	2.363954	-1.792774
C	-2.972857	1.481334	-1.228017
C	-3.063585	0.166250	-1.647696
C	-1.090230	1.882861	-2.754235

C	0.832370	2.794883	-1.426902
C	-0.100851	3.426693	-0.489498
C	-1.479445	3.207278	-0.735646
C	0.329380	2.134180	-2.585898
C	2.224104	0.569363	-2.657154
C	2.758113	1.237019	-1.497335
C	2.096323	2.316024	-0.881926
C	1.014547	1.005601	-3.186680
C	0.294717	-1.350740	-3.470591
C	1.577141	-1.799685	-2.952711
C	2.529633	-0.845466	-2.563134
C	0.032743	0.020580	-3.617059
C	3.533653	1.890735	2.677602
C	1.862157	3.897909	1.073328
N	1.464755	5.834163	-0.357639
N	5.608602	0.664827	2.451992
C	2.407841	5.058038	0.240796
C	1.842385	6.875929	-1.152810
C	3.209725	7.163170	-1.352391
C	4.183716	6.366068	-0.723913
C	3.786016	5.287405	0.087597
C	0.726452	7.672034	-1.823579
C	-0.657843	7.173234	-1.336464
C	0.833453	7.467488	-3.367544
C	0.881449	9.185217	-1.486749
H	0.728033	6.393129	-3.619524
H	1.808461	7.828282	-3.752411
H	0.024856	8.032688	-3.874242
H	0.829992	9.343202	-0.390743
H	0.060040	9.756072	-1.965484
H	1.844607	9.587994	-1.858514
H	-0.789797	6.098175	-1.556519
H	-0.757701	7.304354	-0.242010
H	-1.453555	7.753673	-1.846018
H	3.512391	7.997692	-1.994847
H	5.249658	6.579802	-0.873600
H	4.518056	4.635555	0.579377
C	6.958599	0.497415	2.376243
C	7.819001	1.605666	2.524769
C	5.071775	1.894685	2.663085
C	7.264989	2.881023	2.742725
C	5.867233	3.043440	2.811017
H	5.413116	4.025499	2.982058
H	7.923399	3.750897	2.861993
H	8.904613	1.478697	2.473808
C	7.407402	-0.934335	2.097661
C	8.943251	-1.098566	2.209002
C	6.944875	-1.299767	0.652324
C	6.699534	-1.883828	3.109618
H	9.473307	-0.482827	1.453950
H	9.211486	-2.158925	2.029780
H	9.302023	-0.819022	3.220790
H	7.434491	-0.640680	-0.093263
H	5.850351	-1.184222	0.565677
H	7.215838	-2.351725	0.429765
H	7.003893	-1.643188	4.148380
H	6.979508	-2.933925	2.890001
H	5.603641	-1.771490	3.027890

Table S9 Cartesian coordinates (Å) of the CH_4@Open cage C_{60} model

C	0.144702	-0.139137	-0.029401
H	1.182745	0.147513	-0.223007
H	-0.265606	-0.652275	-0.906981
H	-0.445895	0.762962	0.181846
H	0.113490	-0.805721	0.840827
C	2.732625	-0.424832	2.698781
C	3.338561	-0.652003	1.395011
C	1.753639	-1.318935	3.161913
C	3.163386	-1.902380	0.763210
C	3.168950	-2.052541	-0.676564
C	3.584522	0.510820	0.545603
C	3.535694	0.361473	-0.846171
C	3.351127	-0.927324	-1.477198
C	-1.274581	2.794761	4.036198
C	-0.201120	3.817742	3.449426
C	0.476208	-0.987000	3.968996
C	3.307144	1.821566	1.079790
C	-0.325525	3.729949	1.947233
C	0.514081	3.837529	0.835935
C	2.618993	2.752189	0.322438
C	-1.860959	-1.362527	2.890245
C	-2.681276	1.091666	2.596789
C	-0.601479	-1.834473	3.277578
C	-2.034010	2.303708	2.860109
C	-1.615796	3.110387	1.760845
C	-3.055162	0.726485	1.241155
C	-2.970875	1.761535	0.269034
C	-2.160828	2.922407	0.516351
C	-0.573159	-3.394635	1.378357
C	-1.818808	-2.816408	0.921212
C	0.059592	-2.794731	2.461573
C	-2.393755	-1.696091	1.575298
C	-3.053780	-0.664721	0.761121
C	-1.863581	-2.987125	-0.508256
C	-2.513229	-2.033461	-1.282858
C	-3.128118	-0.885975	-0.646567
C	2.214996	-2.852634	1.283971
C	1.581703	-3.544147	0.175887
C	1.475770	-2.499774	2.410530
C	0.200519	-3.802675	0.221139
C	-0.610936	-3.575061	-0.954146
C	2.183025	-3.053125	-1.045910
C	1.401538	-2.873558	-2.201623
C	-0.024831	-3.145129	-2.153922
C	-2.239502	-0.228827	-2.743341
C	-1.942029	-1.632316	-2.559839
C	-0.703662	-2.151980	-2.969965
C	-1.266370	0.631600	-3.288010
C	-1.901354	2.397631	-1.709182
C	-2.896476	1.504588	-1.139617
C	-3.020039	0.204173	-1.602005
C	-1.066260	1.949327	-2.721305
C	0.911509	2.889784	-1.496088
C	0.012051	3.464796	-0.489479
C	-1.369636	3.205177	-0.647120
C	0.356796	2.217093	-2.620755

C	2.260847	0.668014	-2.774159
C	2.851898	1.351984	-1.651411
C	2.220972	2.445379	-1.028312
C	1.026395	1.096394	-3.253603
C	0.305738	-1.262174	-3.524751
C	1.601364	-1.703604	-3.036549
C	2.561334	-0.747096	-2.673662
C	0.033928	0.108816	-3.651260
S	-2.644503	-0.126541	3.895445
O	-1.405283	2.536395	5.217514
O	0.306200	-0.130174	4.811651
O	0.462417	4.547587	4.161431
C	3.647824	2.023080	2.530260
C	3.035409	0.857890	3.403193
C	2.038515	4.026803	0.919890
C	2.532614	4.262988	2.323831
C	3.208611	3.362102	3.050220
O	2.876112	1.007176	4.603067
H	2.252426	5.221941	2.767364
H	3.468963	3.583204	4.090726
N	5.597763	0.562628	2.512509
N	1.389815	5.912021	-0.495150
C	2.426041	5.203673	0.029656
C	1.635750	6.963687	-1.328021
C	2.961442	7.330484	-1.644487
C	4.031957	6.606226	-1.089478
C	3.769694	5.518508	-0.236186
C	0.421954	7.684555	-1.908462
C	-0.885037	7.109307	-1.306327
C	0.412812	7.471964	-3.454803
C	0.512966	9.207403	-1.592230
H	0.353265	6.390734	-3.692000
H	1.328181	7.887949	-3.921483
H	-0.468535	7.981701	-3.894659
H	0.538880	9.372433	-0.496310
H	-0.375922	9.724766	-2.006958
H	1.418525	9.662338	-2.040620
H	-0.972844	6.027415	-1.513583
H	-0.900037	7.240262	-0.207429
H	-1.753077	7.639933	-1.747610
H	3.157498	8.171055	-2.319640
H	5.066507	6.883974	-1.327840
H	4.577910	4.922729	0.205770
C	6.926013	0.260112	2.572081
C	7.876158	1.278535	2.791218
C	5.169422	1.844058	2.654102
C	7.436620	2.608416	2.931575
C	6.063640	2.910020	2.859814
H	5.699584	3.938235	2.960785
H	8.165761	3.411779	3.097095
H	8.942917	1.042339	2.850417
C	7.257090	-1.213328	2.350024
C	8.746106	-1.528340	2.637067
C	6.930621	-1.547585	0.860503
C	6.347369	-2.076686	3.273270
H	9.418001	-0.982080	1.944061
H	8.923724	-2.613111	2.494901
H	9.015349	-1.269336	3.681614

H	7.562365	-0.944011	0.177497
H	5.868715	-1.331515	0.650744
H	7.123947	-2.622522	0.668692
H	6.550138	-1.852461	4.340125
H	6.547535	-3.151678	3.090238
H	5.285165	-1.861272	3.062756

Table S10 Cartesian coordinates (Å) of the C_{60} in 1,2-dichlorobenzene model

C	2.043700	0.955409	2.205716
C	2.848321	0.635438	1.039383
C	1.175755	-0.002433	2.747136
C	2.735698	-0.632858	0.454063
C	2.683749	-0.767103	-0.987450
C	2.897078	1.814860	0.195302
C	2.853585	1.685419	-1.197611
C	2.748433	0.368370	-1.798938
C	-0.561962	1.712298	3.095694
C	0.330115	2.710481	2.531901
C	-0.144078	0.381418	3.206113
C	1.607343	2.336112	2.090922
C	2.126072	2.859108	0.842490
C	-0.472187	3.627998	1.741016
C	0.031923	4.117713	0.532210
C	1.355663	3.745403	0.082350
C	-2.357852	-0.403730	2.458514
C	-2.793309	0.977578	2.341824
C	-1.059512	-0.700410	2.889124
C	-1.913073	2.019622	2.662120
C	-1.857171	3.203561	1.822742
C	-3.668269	1.082534	1.187314
C	-3.600665	2.219538	0.372433
C	-2.685685	3.300125	0.696467
C	-0.874308	-2.469202	1.181101
C	-2.224408	-2.170660	0.740384
C	-0.303506	-1.758716	2.243363
C	-2.951651	-1.149625	1.365132
C	-3.760480	-0.235581	0.581155
C	-2.263384	-2.302261	-0.702897
C	-3.035124	-1.419354	-1.464979
C	-3.787356	-0.365247	-0.811717
C	1.837642	-1.620966	1.019865
C	1.248900	-2.371649	-0.071921
C	1.079318	-1.324202	2.156327
C	-0.082277	-2.791001	0.006713
C	-0.938946	-2.686653	-1.155839
C	1.775727	-1.848526	-1.314481
C	0.950142	-1.755968	-2.439407
C	-0.433069	-2.189506	-2.362082
C	-2.942859	0.491598	-2.826352
C	-2.510344	-0.889284	-2.710533
C	-1.235494	-1.265691	-3.147289
C	-2.085295	1.452369	-3.374463
C	-2.750947	3.077834	-1.641479
C	-3.646397	2.087463	-1.073371
C	-3.726344	0.817348	-1.650469
C	-1.987552	2.768515	-2.773287
C	-0.031424	3.925530	-1.804461
C	-0.824663	4.240694	-0.628422

C	-2.161134	3.831136	-0.550379
C	-0.604098	3.200953	-2.857565
C	1.455190	1.851119	-3.080410
C	2.044930	2.598882	-1.985159
C	1.316931	3.618313	-1.362676
C	0.154741	2.148006	-3.511748
C	-0.343165	-0.264333	-3.704611
C	1.006534	-0.570199	-3.275419
C	1.887337	0.470024	-2.962532
C	-0.761481	1.067024	-3.826956
Cl	5.774083	2.206310	6.590966
Cl	7.410617	-0.249251	5.152119
C	4.357043	-2.180147	7.117151
C	5.476960	-1.907151	6.307050
C	3.695308	-1.131939	7.786221
C	5.912886	-0.585259	6.171731
C	4.136459	0.196906	7.630762
C	5.238418	0.455111	6.810715
H	4.001204	-3.211312	7.214406
H	6.007594	-2.709423	5.783584
H	2.827470	-1.338181	8.421163
H	3.638218	1.024628	8.144754
Cl	-7.356360	3.012665	2.307158
Cl	-9.544405	2.804238	-0.115516
C	-6.379261	4.749319	-1.880176
C	-7.618740	4.116553	-1.661589
C	-5.456936	4.874345	-0.825525
C	-7.910024	3.609074	-0.391377
C	-5.766794	4.369575	0.451918
C	-6.990200	3.720259	0.652520
H	-6.137730	5.148273	-2.869957
H	-8.353963	4.013131	-2.467189
H	-4.495391	5.365888	-0.992669
H	-5.072737	4.493552	1.287567
Cl	-3.849720	2.362890	9.052380
Cl	-4.596923	5.426065	8.119828
C	-1.591595	4.357681	5.535657
C	-2.614328	5.069576	6.189786
C	-1.253081	3.061380	5.958088
C	-3.287706	4.469900	7.259229
C	-1.946101	2.463838	7.024609
C	-2.962441	3.177261	7.665033
H	-1.068100	4.820663	4.693983
H	-2.893271	6.079204	5.871487
H	-0.448380	2.515528	5.461663
H	-1.704807	1.455733	7.365767
Cl	-9.456238	-2.225710	1.774137
Cl	-6.877422	-0.645123	3.020433
C	-5.245246	-4.156367	1.638251
C	-5.419041	-2.898051	2.243651
C	-6.354175	-4.840958	1.106276
C	-6.690990	-2.320542	2.285941
C	-7.637259	-4.260214	1.172431
C	-7.791551	-2.995397	1.755472
H	-4.242512	-4.587988	1.587219
H	-4.565240	-2.374759	2.676073
H	-6.227874	-5.823041	0.639620
H	-8.511964	-4.773094	0.756862

Cl	-2.497689	6.595995	2.879227
Cl	-2.809271	7.348020	-0.261984
C	1.252315	7.018359	0.190034
C	-0.031275	7.184757	-0.362967
C	1.398472	6.758953	1.566881
C	-1.149696	7.080462	0.468596
C	0.262964	6.638144	2.390140
C	-1.006297	6.793245	1.823085
H	2.130558	7.115673	-0.454051
H	-0.167896	7.399628	-1.426275
H	2.398055	6.655519	2.001862
H	0.359690	6.425781	3.460334
Cl	0.242025	0.241834	9.083342
Cl	0.879015	-0.778404	6.038528
C	2.317051	3.065219	6.053386
C	1.983926	1.755976	5.662194
C	1.993363	3.525344	7.343516
C	1.324178	0.919508	6.567074
C	1.350211	2.665743	8.254665
C	1.028543	1.365883	7.852328
H	2.835769	3.720745	5.347623
H	2.249192	1.383135	4.669697
H	2.245733	4.546758	7.650606
H	1.100028	2.998543	9.268105
Cl	-2.242539	-3.354350	-5.976801
Cl	-5.167262	-3.575031	-7.434816
C	-4.663276	0.477856	-6.937498
C	-5.189306	-0.779535	-7.299339
C	-3.397611	0.560266	-6.329788
C	-4.449336	-1.934465	-7.017477
C	-2.657162	-0.606115	-6.079591
C	-3.202097	-1.848156	-6.402101
H	-5.248714	1.385430	-7.123293
H	-6.172236	-0.867736	-7.775428
H	-2.980263	1.526287	-6.039465
H	-1.663325	-0.550309	-5.634381
Cl	2.252572	-3.744860	4.763517
Cl	4.563561	-5.910046	4.006105
C	6.102233	-2.377536	2.592154
C	5.951089	-3.729487	2.955399
C	5.089925	-1.446862	2.900377
C	4.780105	-4.135307	3.605541
C	3.936530	-1.864156	3.586364
C	3.784332	-3.213627	3.915294
H	7.018628	-2.049759	2.089692
H	6.725457	-4.468291	2.721718
H	5.201791	-0.394053	2.628907
H	3.166153	-1.149141	3.883083
Cl	2.742070	3.671799	-7.542354
Cl	3.039003	6.848709	-6.734656
C	6.574513	5.210585	-5.437540
C	5.528801	6.113413	-5.711901
C	6.477021	3.866469	-5.846097
C	4.388659	5.651152	-6.375223
C	5.322947	3.414117	-6.513464
C	4.279726	4.313051	-6.754515
H	7.463645	5.560827	-4.899939
H	5.591003	7.162780	-5.401391

H	7.289264	3.157629	-5.648503
H	5.232688	2.374167	-6.838213
Cl	-7.856766	5.153500	6.260317
Cl	-5.673756	6.077494	4.018105
C	-4.422659	2.304314	5.035808
C	-4.524256	3.562869	4.423242
C	-5.351033	1.909862	6.014782
C	-5.558753	4.418635	4.806947
C	-6.394539	2.776426	6.383739
C	-6.487647	4.028598	5.767015
H	-3.601436	1.646662	4.753754
H	-3.810537	3.871804	3.655176
H	-5.255323	0.936000	6.503457
H	-7.123295	2.493498	7.151152
Cl	7.919056	5.907104	0.524491
Cl	5.182267	7.486561	1.288510
C	6.049568	5.415336	4.734835
C	5.452491	6.290973	3.806195
C	7.182477	4.663770	4.368791
C	6.009908	6.408913	2.530129
C	7.738203	4.799113	3.081758
C	7.149356	5.687038	2.178906
H	5.618360	5.318146	5.738125
H	4.560221	6.871878	4.067475
H	7.638535	3.963852	5.077178
H	8.621191	4.223315	2.784193
Cl	-0.165047	-3.838223	7.250335
Cl	1.369459	-6.721470	7.025331
C	-2.609818	-7.763708	6.981400
C	-1.201324	-7.820721	6.956976
C	-3.264474	-6.523751	7.083822
C	-0.467552	-6.633739	7.043246
C	-2.513295	-5.335841	7.146970
C	-1.119044	-5.403580	7.133188
H	-3.186603	-8.692966	6.916939
H	-0.676058	-8.778591	6.870507
H	-4.357662	-6.468627	7.113706
H	-2.999719	-4.362963	7.201799
Cl	-2.324733	5.894929	-3.270460
Cl	-4.378439	3.833512	-4.819100
C	-1.399731	4.463515	-7.573011
C	-2.575268	4.019943	-6.935983
C	-0.491720	5.288644	-6.881647
C	-2.832347	4.417237	-5.619470
C	-0.771572	5.686509	-5.561745
C	-1.949150	5.254861	-4.945255
H	-1.206286	4.164517	-8.609213
H	-3.285768	3.382150	-7.470866
H	0.426686	5.634528	-7.365960
H	-0.096022	6.353925	-5.021159
Cl	0.842287	-4.916399	-5.256800
Cl	1.765463	-5.103587	-2.124490
C	-1.098178	-8.034459	-2.424935
C	-0.092264	-7.180138	-1.935274
C	-1.506902	-7.946661	-3.769988
C	0.485781	-6.240269	-2.795052
C	-0.909173	-7.004290	-4.629431
C	0.085270	-6.157518	-4.127699

H	-1.563221	-8.761654	-1.749651
H	0.239960	-7.239136	-0.896942
H	-2.295609	-8.603985	-4.154390
H	-1.219164	-6.915751	-5.676896
Cl	8.044052	0.849789	1.586166
Cl	7.441992	2.727513	-1.006691
C	4.603975	3.945905	1.711814
C	5.359388	3.801283	0.533787
C	4.860007	3.130206	2.823430
C	6.386453	2.858975	0.500821
C	5.890544	2.175380	2.775391
C	6.650636	2.056518	1.610035
H	3.821617	4.708208	1.747901
H	5.155490	4.426973	-0.337476
H	4.289666	3.251426	3.747198
H	6.136766	1.571108	3.651993
Cl	-3.244386	-2.654372	9.418610
Cl	-5.953967	-3.551297	7.791721
C	-4.066493	-1.019694	5.166159
C	-5.011092	-1.867225	5.772115
C	-2.862375	-0.714941	5.823695
C	-4.744213	-2.384316	7.042554
C	-2.616554	-1.222030	7.112006
C	-3.573462	-2.039576	7.718451
H	-4.283437	-0.601955	4.180274
H	-5.948475	-2.117056	5.266025
H	-2.102934	-0.094495	5.341020
H	-1.687818	-1.003549	7.642948
Cl	-7.141481	0.262522	-0.443181
Cl	-6.392458	1.267867	-3.459429
C	-5.231089	-2.668075	-3.468669
C	-5.466466	-1.332643	-3.845092
C	-5.606077	-3.112330	-2.186142
C	-6.073192	-0.461418	-2.939045
C	-6.199633	-2.218746	-1.278809
C	-6.421958	-0.893193	-1.661539
H	-4.749816	-3.348677	-4.176926
H	-5.192989	-0.966914	-4.834222
H	-5.426682	-4.146072	-1.877562
H	-6.476173	-2.535250	-0.274401
Cl	-2.169305	9.601714	-3.510999
Cl	-5.143733	8.396894	-2.803971
C	-4.407603	6.933238	-6.571076
C	-5.017873	7.237190	-5.337812
C	-3.143895	7.463348	-6.881266
C	-4.351389	8.065818	-4.430671
C	-2.480622	8.293809	-5.957173
C	-3.093022	8.584668	-4.734437
H	-4.920622	6.266354	-7.273111
H	-5.994885	6.819786	-5.072442
H	-2.648794	7.205073	-7.823287
H	-1.485757	8.698032	-6.173705
Cl	4.394089	0.274311	-5.081908
Cl	3.623407	-2.866564	-4.575311
C	5.427598	-1.771988	-1.068195
C	4.758353	-2.502654	-2.069309
C	5.818493	-0.444817	-1.304645
C	4.478402	-1.887587	-3.290349

C	5.520067	0.165581	-2.535390
C	4.840129	-0.564304	-3.512681
H	5.648572	-2.245584	-0.106425
H	4.449755	-3.539286	-1.904612
H	6.357629	0.118423	-0.540384
H	5.808536	1.200195	-2.732979
Cl	5.500466	-7.434535	-0.827012
Cl	2.675221	-8.774143	0.165100
C	2.343890	-4.868964	1.393668
C	2.089963	-6.231792	1.161957
C	3.547650	-4.292024	0.954266
C	3.043128	-6.999221	0.488292
C	4.508596	-5.078996	0.296178
C	4.241553	-6.431022	0.062038
H	1.601132	-4.272858	1.929300
H	1.159153	-6.693177	1.503708
H	3.753049	-3.233550	1.138400
H	5.470587	-4.659116	-0.015842
Cl	-1.777025	-5.509696	0.479620
Cl	-2.677449	-4.943795	-2.628717
C	-5.326850	-7.823194	-1.396521
C	-4.637776	-6.866805	-2.168389
C	-4.933907	-8.073113	-0.065586
C	-3.562821	-6.171261	-1.600889
C	-3.851355	-7.366927	0.495433
C	-3.179263	-6.421083	-0.284435
H	-6.168353	-8.369361	-1.838928
H	-4.924287	-6.663452	-3.206431
H	-5.465629	-8.814822	0.542430
H	-3.539414	-7.544264	1.528838
Cl	-1.716155	-1.951400	-9.454796
Cl	-2.015303	1.295183	-9.359441
C	0.885776	0.542115	-6.546200
C	-0.039457	1.194820	-7.381323
C	1.021355	-0.857685	-6.595828
C	-0.811258	0.435120	-8.266062
C	0.232660	-1.610807	-7.486558
C	-0.680561	-0.951797	-8.316930
H	1.500665	1.133213	-5.860720
H	-0.165922	2.280289	-7.340462
H	1.738965	-1.365654	-5.944532
H	0.319362	-2.700224	-7.535438
Cl	1.503623	7.695468	-3.557622
Cl	4.181035	8.493756	-1.929863
C	4.889578	4.586648	-2.982867
C	5.013749	5.871026	-2.416201
C	3.740700	4.240132	-3.711269
C	3.981709	6.792586	-2.603745
C	2.695765	5.169013	-3.872001
C	2.833548	6.442238	-3.316949
H	5.703931	3.869462	-2.850919
H	5.908353	6.166022	-1.856951
H	3.655290	3.247758	-4.162906
H	1.795796	4.904145	-4.434874
Cl	-2.439228	-3.700356	4.192025
Cl	-0.210446	-6.025746	3.821968
C	-3.729090	-8.141173	3.965055
C	-2.362989	-7.805361	3.877130

C	-4.695344	-7.131084	4.132705
C	-1.985269	-6.461959	3.942723
C	-4.299369	-5.781941	4.211389
C	-2.942662	-5.464420	4.104184
H	-4.029530	-9.194081	3.908705
H	-1.596516	-8.578969	3.757937
H	-5.758969	-7.385356	4.210537
H	-5.035101	-4.987302	4.366473
Cl	7.554432	0.568365	-7.057341
Cl	6.249642	-2.416560	-7.208618
C	7.719097	-2.243271	-3.375015
C	7.105738	-2.685299	-4.562268
C	8.245593	-0.941313	-3.295325
C	7.045231	-1.825933	-5.663356
C	8.180634	-0.082199	-4.410792
C	7.586930	-0.542836	-5.589155
H	7.772025	-2.916895	-2.513261
H	6.676592	-3.689924	-4.637638
H	8.705344	-0.583377	-2.367067
H	8.590632	0.933334	-4.366516

Table S11 Cartesian coordinates (Å) of the $CH_4@C_{60}$ in 1,2-dichlorobenzene model

C	-0.521356	0.746817	-0.272441
H	0.555596	0.870116	-0.421784
H	-0.704658	0.153668	0.628180
H	-0.951859	0.235748	-1.139053
H	-0.993334	1.727971	-0.164152
C	2.005838	0.924276	2.239102
C	2.804916	0.630612	1.062415
C	1.142482	-0.046273	2.765568
C	2.690335	-0.625208	0.451437
C	2.629608	-0.728862	-0.992292
C	2.846980	1.828484	0.242281
C	2.797999	1.728366	-1.153339
C	2.692669	0.422861	-1.782281
C	-0.595881	1.656614	3.159641
C	0.290361	2.667432	2.610543
C	-0.174609	0.324760	3.243929
C	1.566153	2.306613	2.154825
C	2.076036	2.857368	0.915438
C	-0.517704	3.599325	1.844406
C	-0.022225	4.119918	0.644437
C	1.300203	3.759293	0.179004
C	-2.393085	-0.450439	2.494099
C	-2.829764	0.933013	2.406168
C	-1.090077	-0.753607	2.911588
C	-1.949616	1.969833	2.741632
C	-1.901207	3.170730	1.925825
C	-3.708633	1.059969	1.257849
C	-3.652108	2.214933	0.467011
C	-2.738819	3.292095	0.807936
C	-0.911197	-2.484542	1.161557
C	-2.265183	-2.179755	0.734973
C	-0.334997	-1.796666	2.237124
C	-2.990547	-1.174263	1.386206
C	-3.804110	-0.245278	0.625656
C	-2.312264	-2.280390	-0.710912
C	-3.091161	-1.384986	-1.450968

C	-3.836274	-0.344371	-0.769947
C	1.798095	-1.626618	1.001913
C	1.203522	-2.355009	-0.102312
C	1.046745	-1.355904	2.149550
C	-0.126037	-2.778929	-0.024438
C	-0.989860	-2.652594	-1.179566
C	1.722147	-1.805513	-1.336364
C	0.890301	-1.691948	-2.454477
C	-0.491481	-2.130426	-2.378423
C	-3.010642	0.555615	-2.772460
C	-2.575645	-0.827731	-2.689597
C	-1.300663	-1.192115	-3.139790
C	-2.157666	1.529572	-3.303809
C	-2.819708	3.120434	-1.534465
C	-3.705516	2.113551	-0.980892
C	-3.783315	0.854728	-1.583010
C	-2.059043	2.832843	-2.673982
C	-0.098915	3.974896	-1.694237
C	-0.887419	4.265977	-0.508686
C	-2.226116	3.855326	-0.431393
C	-0.676543	3.267231	-2.755251
C	1.381024	1.926681	-3.017232
C	1.980679	2.657348	-1.915471
C	1.254709	3.663588	-1.267685
C	0.079882	2.230020	-3.435909
C	-0.413410	-0.176954	-3.680466
C	0.939188	-0.488511	-3.264301
C	1.822545	0.546820	-2.937918
C	-0.835847	1.155501	-3.771515
Cl	5.871532	2.090562	6.491080
Cl	7.454478	-0.388963	5.038937
C	4.385905	-2.270777	7.031168
C	5.501142	-2.016083	6.208581
C	3.751769	-1.212307	7.711146
C	5.958520	-0.701779	6.069594
C	4.214662	0.108762	7.552775
C	5.309774	0.348876	6.717829
H	4.012005	-3.295392	7.131006
H	6.012195	-2.826954	5.679315
H	2.888766	-1.404554	8.357006
H	3.739212	0.943761	8.076341
Cl	-7.113479	2.996082	1.960975
Cl	-9.465875	2.934771	-0.326769
C	-6.475288	5.111599	-2.117117
C	-7.679549	4.423503	-1.874184
C	-5.487708	5.179097	-1.116478
C	-7.870937	3.798922	-0.636285
C	-5.698465	4.558524	0.128923
C	-6.885759	3.852449	0.349783
H	-6.307497	5.602167	-3.080583
H	-8.465204	4.366649	-2.635979
H	-4.556082	5.716819	-1.302084
H	-4.956844	4.638571	0.928639
Cl	-3.940726	2.308907	9.011400
Cl	-4.724797	5.332561	7.981746
C	-1.621881	4.269779	5.511752
C	-2.681241	4.971553	6.117875
C	-1.257643	2.998451	5.987536

C	-3.369550	4.385119	7.185019
C	-1.967227	2.413407	7.050538
C	-3.026051	3.112142	7.635648
H	-1.088807	4.721358	4.669383
H	-2.977840	5.963420	5.762545
H	-0.421536	2.455284	5.542786
H	-1.692208	1.428729	7.432362
Cl	-9.484796	-2.377133	2.018182
Cl	-6.929023	-0.740691	3.245784
C	-5.213464	-4.148736	1.710509
C	-5.414181	-2.911932	2.350801
C	-6.312951	-4.863694	1.199467
C	-6.704117	-2.383878	2.446956
C	-7.613092	-4.330653	1.314977
C	-7.794802	-3.084870	1.930578
H	-4.197399	-4.540095	1.616644
H	-4.565361	-2.367060	2.764636
H	-6.164924	-5.834577	0.715606
H	-8.481484	-4.867033	0.916105
Cl	-2.525140	6.576056	2.872880
Cl	-2.773449	7.434979	-0.238069
C	1.277009	7.024086	0.265957
C	0.005800	7.222571	-0.306318
C	1.395382	6.735584	1.640199
C	-1.127265	7.120785	0.505718
C	0.243822	6.613128	2.440295
C	-1.012209	6.798012	1.854459
H	2.169133	7.119660	-0.360880
H	-0.107292	7.459933	-1.367634
H	2.385021	6.608239	2.090164
H	0.317420	6.372212	3.506544
Cl	0.339712	0.261304	9.111236
Cl	0.897684	-0.789304	6.061693
C	2.389841	3.032951	6.014516
C	2.036241	1.722952	5.644004
C	2.093295	3.510033	7.305223
C	1.380434	0.904860	6.567947
C	1.457800	2.666501	8.237618
C	1.114204	1.366167	7.854544
H	2.902293	3.677691	5.293931
H	2.280235	1.332778	4.653259
H	2.361563	4.531858	7.597637
H	1.230252	3.012652	9.251928
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