

The Cl⁽⁻⁾ Exchange S_N2 Reaction inside Carbon Nanotubes: C-H^{··}π and Cl^{··}π Interactions Govern the Course of the Reaction

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preliminary complex (I)

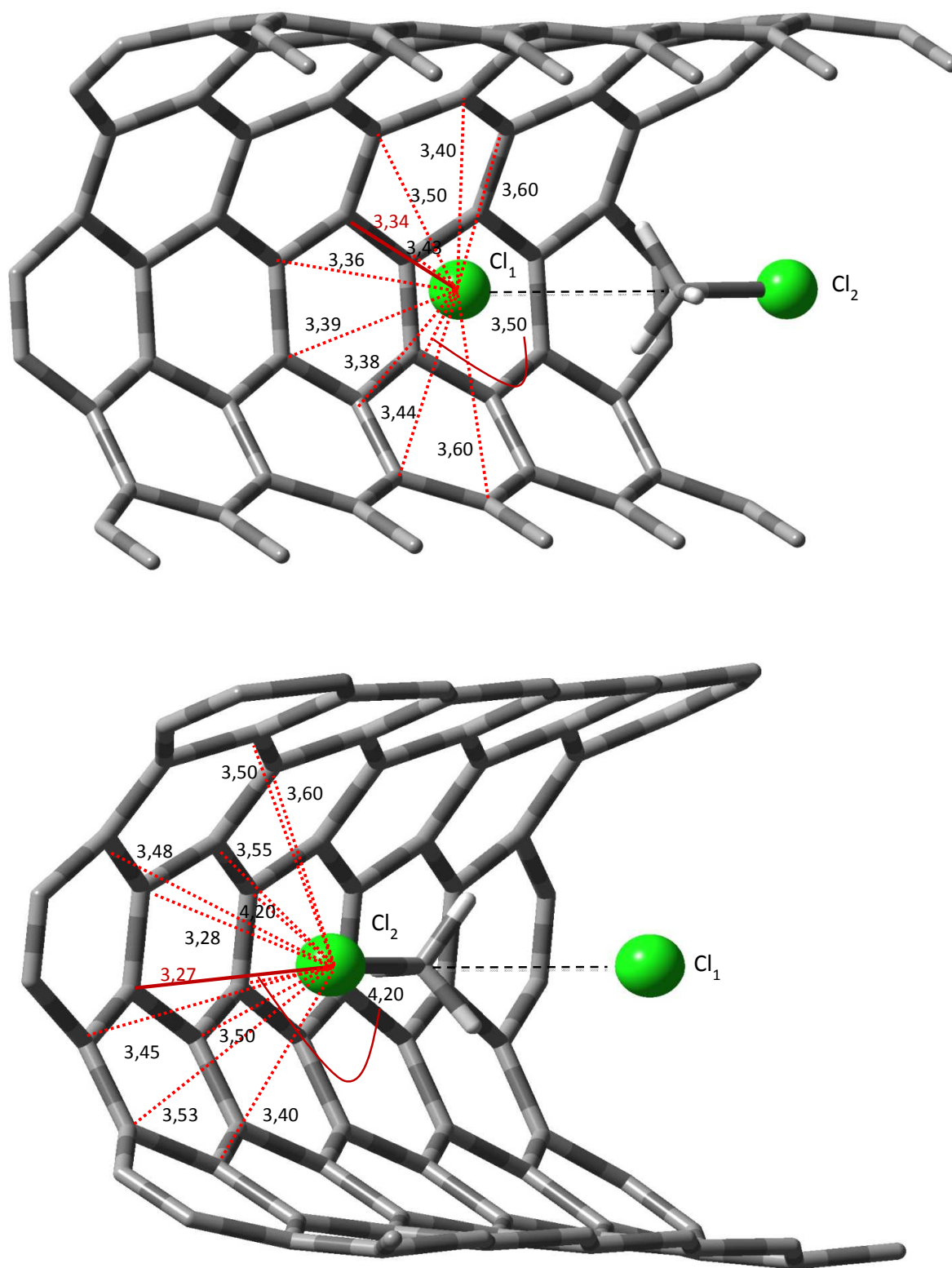


Figure S1. Cl₁...C(tube) and Cl₂...C(wall) distances (Ångstroms) computed in the preliminary complex I at the M06-2X level.

Transition State (TS)

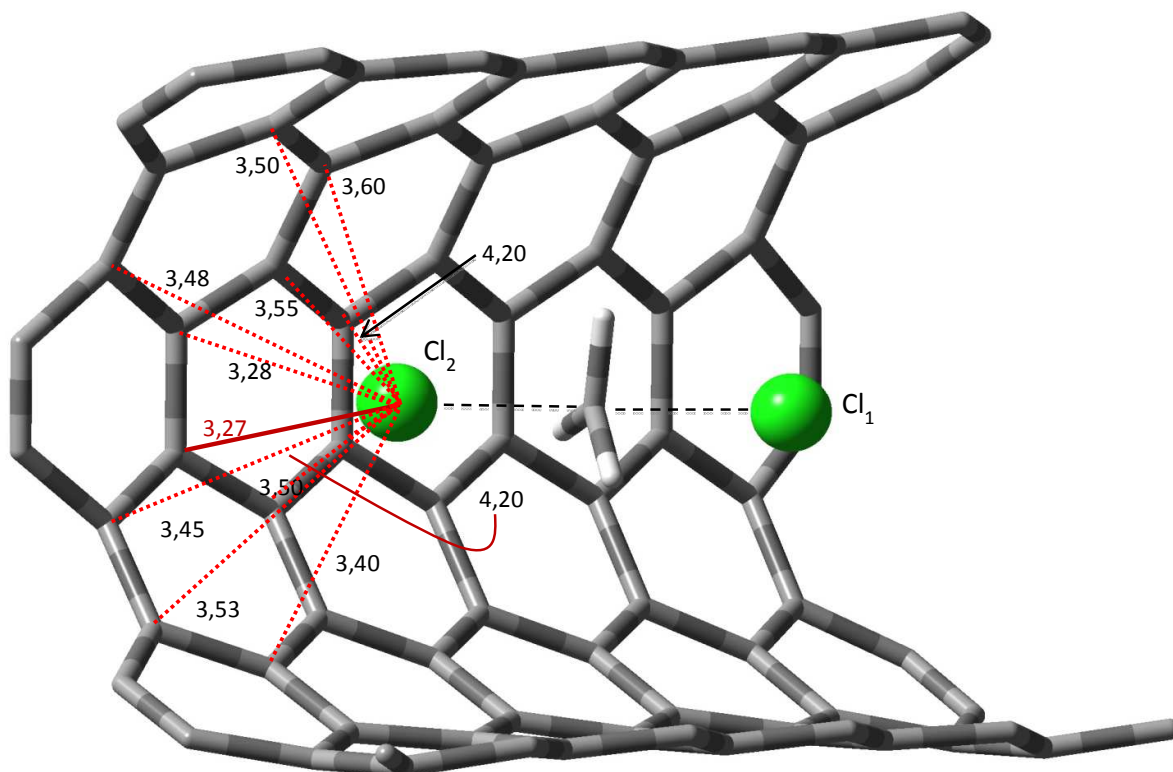
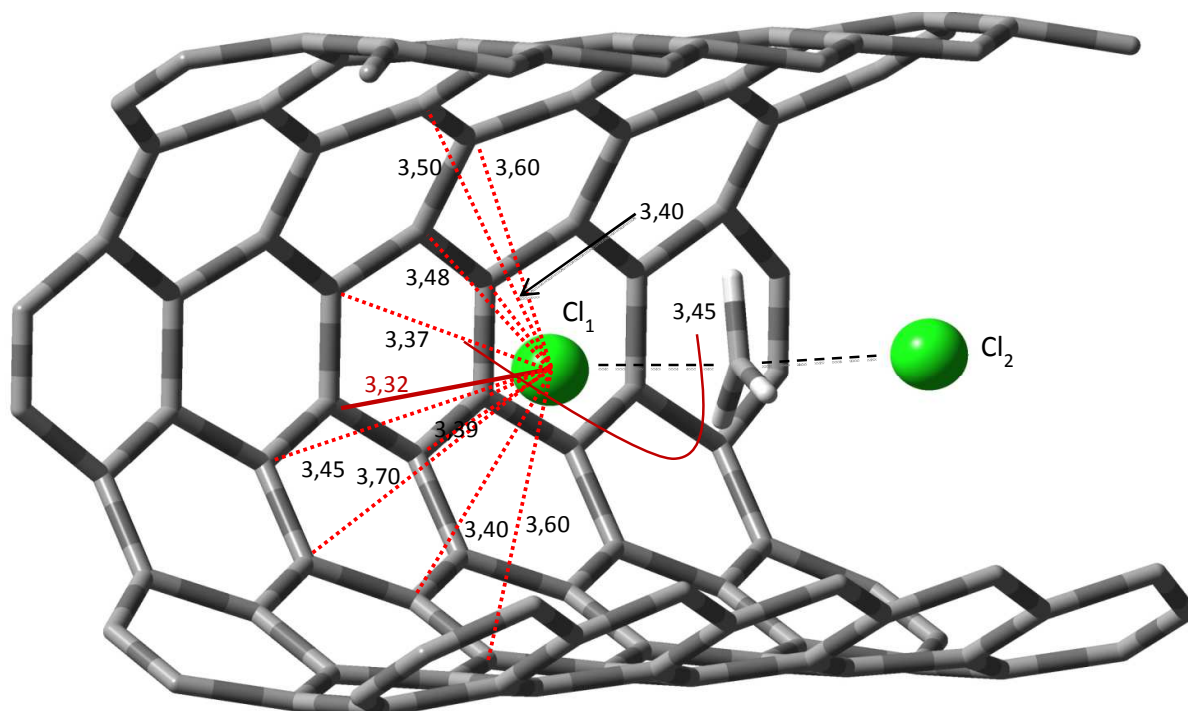


Figure S2. Cl₁⋯C(tube) and Cl₂⋯C(wall) distances (Ångstroms) computed in the transition state TS at the M06-2X level.

Table S1. Cartesian coordinates (Ångstroms) for the preliminary intermediate **I** and transition state **TS** computed at the M06-2X level for the gas-phase chloride exchange S_N2 reaction

Intermediate I

```

      6
scf done: -960.300207
C      0.123685      0.154868      0.050969
H      0.062237      0.051950      1.130072
H      1.137691     -0.030397     -0.289930
H      -0.202722      1.144269     -0.254042
Cl     -0.981277     -1.082702     -0.714167
Cl      2.024357      2.278500      1.341275

```

Transition state TS

```

      6
scf done: -960.279108
C      0.360475      0.419577      0.210617
H      0.080661      0.070009      1.188213
H      1.200097     -0.020175     -0.297292
H      -0.199047      1.208560     -0.259323
Cl     -1.042997     -1.149924     -0.749319
Cl      1.764781      1.988441      1.171282

```

Table S2. Cartesian coordinates (Ångstroms) for the preliminary intermediate **I** and transition state **TS** computed at the B3LYP level for the gas-phase chloride exchange S_N2 reaction.

Intermediate I

```

      6
scf done: -960.401446
C      0.122239      0.154351      0.048715
H      0.056212      0.046794      1.127122
H      1.132854     -0.038042     -0.298320
H      -0.213651      1.138467     -0.263759
Cl     -1.000023     -1.106785     -0.723421
Cl      2.066340      2.321704      1.373840

```

Transition state TS

```

      6
scf done: -960.387593
C      0.360521      0.419619      0.210669
H      0.081326      0.071239      1.188118
H      1.199312     -0.020109     -0.297069
H      -0.199042      1.207825     -0.258867
Cl     -1.077671     -1.189017     -0.773767
Cl      1.799525      2.026930      1.195092

```

Table S3. Cartesian coordinates (Ångstroms) for the preliminary intermediate **I** and transition state **TS** for the (6,6) CNT-confined chloride exchange S_N2 reaction computed at the M06-2X level.

Intermediate I

138			
scf done: -5959.909343			
C	-2.029859	-3.672906	12.223293
C	-2.782766	-3.195551	11.124964
C	-2.119532	-3.538794	9.891348
C	-0.741561	-3.996493	9.881377
C	0.008403	-4.138114	11.104977
C	-0.863525	-4.068135	12.217411
C	1.401834	-3.902602	11.103230
C	2.061480	-3.526390	9.877364
C	1.369847	-3.737818	8.644628
C	-0.023523	-3.968326	8.646240
C	2.202566	-3.537452	12.211323
C	3.169027	-2.774222	12.218232
C	3.711201	-2.073944	11.114831
C	3.206202	-2.631620	9.883662
C	3.596798	-2.016921	8.654570
C	4.124196	-0.707661	8.660210
C	4.247860	0.002313	9.894364
C	4.226858	-0.756531	11.121040
C	3.152279	-2.577815	7.405993
C	2.025675	-3.432182	7.401555
C	1.369444	-3.705289	6.174566
C	-0.043124	-3.939987	6.178190
C	-0.747806	-3.892536	7.406328
C	-2.093228	-3.460605	7.415338
C	-2.697117	-3.087534	8.664732
C	3.608227	-2.021168	6.183093
C	3.152563	-2.561399	4.953125
C	2.016305	-3.404237	4.949359
C	1.350114	-3.677000	3.704239
C	-0.042679	-3.910378	3.708526
C	-0.757125	-3.866405	4.956367
C	-2.106999	-3.446040	4.967356
C	-2.715130	-3.091407	6.197100
C	3.613155	-1.998599	3.711660
C	3.208361	-2.594379	2.477370
C	2.036433	-3.450557	2.472757
C	1.362405	-3.787755	1.244775
C	-0.028961	-4.024061	1.247884
C	-0.770313	-3.920576	2.479250
C	-2.157938	-3.496048	2.489284
C	-2.730109	-3.068836	3.727708
C	3.734777	-2.045010	1.256112
C	3.156459	-2.696449	0.142484
C	2.161270	-3.421056	0.137055
C	-2.844345	-3.158380	1.268021
C	-2.088388	-3.592432	0.153978
C	-0.910673	-3.951951	0.144393
C	-3.700144	-2.044429	3.737862

C	-4.096498	-1.433872	2.507397
C	-3.817531	-2.132538	1.277038
C	-3.699565	-2.048900	6.207769
C	-4.020817	-1.405294	4.986792
C	-4.282681	-0.015125	4.989777
C	-4.215146	0.701119	3.743238
C	-4.366643	-0.006958	2.510347
C	-4.361403	0.750073	1.282957
C	-4.430917	-0.126606	0.174824
C	-4.200137	-1.336295	0.172202
C	-3.671669	2.002676	3.736748
C	-3.285385	2.604885	2.499329
C	-3.816956	2.055300	1.277521
C	-4.209823	0.696347	6.213685
C	-3.659570	2.020639	6.206664
C	-3.212884	2.566941	4.977477
C	-2.079945	3.412879	4.966068
C	-1.422252	3.687888	3.716533
C	-2.117554	3.466448	2.488241
C	-1.452110	3.805138	1.255153
C	-2.265935	3.453404	0.153151
C	-3.257672	2.723847	0.163680
C	-0.027620	3.909473	3.708663
C	0.691789	3.907495	2.474926
C	-0.056440	4.015806	1.248435
C	-1.424271	3.710142	6.186297
C	-0.011115	3.941634	6.179018
C	0.694811	3.863100	4.951663
C	2.042600	3.434143	4.952115
C	2.660918	3.054273	3.710533
C	2.076771	3.475826	2.476470
C	2.757253	3.139326	1.254412
C	1.992496	3.561283	0.142477
C	0.815657	3.923370	0.139310
C	3.647383	2.044084	3.714931
C	4.049561	1.436832	2.484722
C	3.744124	2.128370	1.258516
C	2.658305	3.084537	6.180354
C	3.644722	2.043251	6.185838
C	3.977609	1.406141	4.963009
C	4.246055	0.014110	4.963966
C	4.175813	-0.703066	3.716250
C	4.325112	0.008719	2.485388
C	4.296278	-0.748238	1.260097
C	4.342057	0.124056	0.148417
C	4.106689	1.332444	0.147802
C	4.163850	-0.698259	6.188472
C	4.208397	0.011897	7.416748
C	3.945867	1.401693	7.415381
C	3.614433	2.048206	8.657383
C	2.662593	3.091053	8.651223
C	2.048477	3.462173	7.404141
C	0.702284	3.894617	7.403315
C	-0.013411	3.971152	8.648440
C	-1.405483	3.733556	8.654077
C	-2.070268	3.430923	7.415697
C	-3.194331	2.574183	7.425486
C	-3.625499	2.008399	8.674485
C	-4.155334	0.701490	8.680880

C	-4.254934	-0.015697	7.438452
C	-3.997095	-1.406645	7.435563
C	-3.651310	-2.048574	8.674871
C	3.985755	1.432116	9.892501
C	3.702277	2.138102	11.117678
C	2.761883	3.194850	11.110978
C	2.091885	3.542076	9.881510
C	0.713336	4.000398	9.878731
C	-0.029668	4.137510	11.107086
C	-1.422161	3.896925	11.113517
C	-2.086957	3.517774	9.891386
C	-3.229749	2.622286	9.902143
C	-3.729499	2.066978	11.135846
C	-4.247493	0.751234	11.143984
C	-4.273406	-0.006176	9.916796
C	-4.012942	-1.434480	9.913442
C	-3.724491	-2.140861	11.137173
C	4.277616	0.122584	12.229067
C	4.057347	1.334400	12.227350
C	0.850423	4.063563	12.212355
C	2.017961	3.671977	12.215789
C	-3.179805	2.767446	12.235205
C	-2.215921	3.534032	12.227741
C	-4.076405	-1.339605	12.249624
C	-4.295999	-0.127609	12.252268
Cl	-0.964703	-0.080911	6.637357
C	0.834303	0.071410	3.990689
H	1.806080	0.088221	4.482720
H	0.244911	0.940991	4.278921
H	0.285530	-0.832279	4.252782
Cl	1.072874	0.101574	2.196465

Transition state TS

138
scf done: -5959.880990

C	-2.032624	-3.691400	12.200429
C	-2.784882	-3.217696	11.100041
C	-2.122976	-3.567456	9.867509
C	-0.743162	-4.019006	9.858711
C	0.008317	-4.149362	11.082730
C	-0.864359	-4.080834	12.194499
C	1.398876	-3.897848	11.080068
C	2.053058	-3.513987	9.853563
C	1.363682	-3.735493	8.621028
C	-0.025894	-3.987962	8.623228
C	2.197584	-3.527006	12.187693
C	3.158080	-2.756271	12.192948
C	3.696899	-2.053371	11.089780
C	3.190876	-2.610571	9.858906
C	3.577635	-1.993657	8.629587
C	4.110533	-0.686149	8.635105
C	4.243064	0.021490	9.870053
C	4.217216	-0.738125	11.096235
C	3.132640	-2.555278	7.381705
C	2.014249	-3.420558	7.377909
C	1.362516	-3.703449	6.151078
C	-0.045158	-3.966876	6.155386
C	-0.751732	-3.929404	7.383340

C	-2.101303	-3.506755	7.391003
C	-2.701424	-3.121653	8.638951
C	3.582326	-1.995075	6.158388
C	3.129643	-2.535862	4.926967
C	2.002688	-3.390222	4.924646
C	1.344353	-3.679500	3.679766
C	-0.042083	-3.941611	3.683897
C	-0.758209	-3.905565	4.931778
C	-2.111154	-3.493724	4.940996
C	-2.720633	-3.136498	6.171040
C	3.588656	-1.972568	3.686054
C	3.184424	-2.568312	2.453369
C	2.027225	-3.441897	2.448996
C	1.362745	-3.797267	1.221813
C	-0.024222	-4.060970	1.224409
C	-0.768341	-3.965862	2.454451
C	-2.156975	-3.545479	2.461513
C	-2.728963	-3.113736	3.698457
C	3.703190	-2.014532	1.231735
C	3.136599	-2.678655	0.119954
C	2.155844	-3.422595	0.112494
C	-2.838932	-3.203281	1.239190
C	-2.085858	-3.643819	0.125856
C	-0.906764	-3.998851	0.121358
C	-3.680288	-2.073010	3.705369
C	-4.061490	-1.454542	2.474425
C	-3.794414	-2.159858	1.245763
C	-3.689738	-2.078054	6.178353
C	-3.987972	-1.426491	4.954391
C	-4.219808	-0.031345	4.955073
C	-4.143560	0.683758	3.707853
C	-4.303425	-0.022830	2.475703
C	-4.286590	0.733426	1.248239
C	-4.367185	-0.143227	0.141230
C	-4.160191	-1.357225	0.140030
C	-3.597770	1.983736	3.701943
C	-3.213763	2.589925	2.466082
C	-3.738985	2.037462	1.243370
C	-4.144768	0.678846	6.180129
C	-3.588945	2.000272	6.173780
C	-3.144829	2.550295	4.944121
C	-2.025573	3.414979	4.935128
C	-1.370934	3.704070	3.686629
C	-2.059945	3.469592	2.458035
C	-1.398357	3.821613	1.227533
C	-2.204828	3.455586	0.125061
C	-3.187114	2.713283	0.130339
C	0.018769	3.949745	3.681618
C	0.740835	3.960414	2.450366
C	-0.006743	4.060103	1.223582
C	-1.379302	3.725331	6.158373
C	0.030311	3.982734	6.153609
C	0.738931	3.910688	4.926134
C	2.088934	3.489064	4.928043
C	2.709996	3.112953	3.687059
C	2.127564	3.536225	2.454280
C	2.803370	3.190809	1.232851
C	2.042809	3.619946	0.121019
C	0.866034	3.981716	0.113885

C	3.674607	2.083318	3.691366
C	4.061593	1.465477	2.463138
C	3.772647	2.162924	1.237251
C	2.698015	3.133249	6.158984
C	3.665317	2.074961	6.163693
C	3.977154	1.431760	4.937377
C	4.218085	0.037012	4.937087
C	4.150048	-0.678290	3.690685
C	4.307498	0.033403	2.462677
C	4.268474	-0.720152	1.236343
C	4.336253	0.151496	0.125392
C	4.127829	1.364720	0.125591
C	4.138534	-0.673768	6.163586
C	4.198260	0.033753	7.392095
C	3.958518	1.428322	7.392043
C	3.636581	2.077658	8.635181
C	2.696381	3.131271	8.630290
C	2.088182	3.511480	7.382840
C	0.740875	3.942034	7.380326
C	0.021144	4.005769	8.624384
C	-1.367629	3.747535	8.627380
C	-2.023645	3.433317	7.386999
C	-3.135157	2.559776	7.394449
C	-3.570493	1.993237	8.641708
C	-4.107200	0.688187	8.647378
C	-4.210187	-0.030815	7.405621
C	-3.979285	-1.427552	7.404734
C	-3.645065	-2.072493	8.646230
C	3.997914	1.454342	9.869963
C	3.721989	2.162005	11.096094
C	2.790340	3.226643	11.090693
C	2.124595	3.580782	9.860904
C	0.744828	4.035889	9.856771
C	-0.002475	4.162451	11.083913
C	-1.392385	3.906346	11.086562
C	-2.049199	3.519278	9.862422
C	-3.182670	2.611392	9.869970
C	-3.685240	2.055850	11.102386
C	-4.208100	0.742370	11.110118
C	-4.237751	-0.016623	9.883728
C	-3.997216	-1.448676	9.882965
C	-3.718646	-2.155856	11.108671
C	4.276472	0.139658	12.204726
C	4.069389	1.353782	12.204765
C	0.875275	4.090850	12.191331
C	2.043225	3.700491	12.194653
C	-3.143652	2.760256	12.203112
C	-2.185807	3.534323	12.197842
C	-4.063426	-1.348503	12.218651
C	-4.268635	-0.134080	12.219477
Cl	-0.871901	-0.292216	6.950609
C	0.129830	-0.061636	4.902002
H	1.106950	-0.199849	5.341115
H	-0.285687	0.929976	4.815211
H	-0.419360	-0.912889	4.531394
Cl	1.049283	0.198751	2.792566

Table S4. Cartesian coordinates (Ångstroms) for the preliminary intermediate **I** and transition state **TS** for the (6,6) CNT-confined chloride exchange S_N2 reaction computed with different hybrid approaches.

M06-2X/Semiempirical

Intermediate **I** M06-2X/Am1

138			
C	-2.021243	-3.784246	12.267406
C	-2.749238	-3.237228	11.204297
C	-2.068619	-3.594239	9.975557
C	-0.703519	-4.091875	9.974827
C	0.048606	-4.257655	11.202630
C	-0.858539	-4.209792	12.267378
C	1.429964	-4.015707	11.202357
C	2.080463	-3.604389	9.974272
C	1.404321	-3.850008	8.747146
C	0.015361	-4.092829	8.747340
C	2.267043	-3.660205	12.266347
C	3.215772	-2.864663	12.266690
C	3.711585	-2.101935	11.202966
C	3.193740	-2.670645	9.974570
C	3.553696	-2.047295	8.747678
C	4.034251	-0.721690	8.748388
C	4.157370	-0.013813	9.976093
C	4.189782	-0.783559	11.203729
C	3.139383	-2.635571	7.500367
C	2.056079	-3.544017	7.500121
C	1.419343	-3.861656	6.273271
C	0.004246	-4.109294	6.273595
C	-0.702221	-4.026815	7.500616
C	-2.030223	-3.542123	7.501541
C	-2.620889	-3.131804	8.749044
C	3.563383	-2.063549	6.273801
C	3.140169	-2.634874	5.047455
C	2.056040	-3.544108	5.047192
C	1.403239	-3.848172	3.800478
C	0.014004	-4.091242	3.800944
C	-0.702730	-4.026948	5.047908
C	-2.031959	-3.541850	5.048705
C	-2.625151	-3.149900	6.275070
C	3.553459	-2.044553	3.801001
C	3.192213	-2.666333	2.573058
C	2.078733	-3.600320	2.572791
C	1.427180	-4.009584	1.344904
C	0.045168	-4.252415	1.345372
C	-0.706226	-4.089061	2.573618
C	-2.071920	-3.592005	2.574445
C	-2.623646	-3.130597	3.802363
C	3.708860	-2.095538	1.345444
C	3.211248	-2.855569	0.281020
C	2.262448	-3.651340	0.280821
C	-2.753793	-3.234445	1.346973
C	-2.026224	-3.778604	0.282635
C	-0.862728	-4.202593	0.281748
C	-3.531838	-2.051436	3.803391

C	-3.891718	-1.428084	2.575608
C	-3.656730	-2.160400	1.347546
C	-3.550754	-2.051328	6.275914
C	-3.836482	-1.399444	5.050292
C	-4.084793	-0.006134	5.050984
C	-4.023078	0.711230	3.804230
C	-4.145701	0.002768	2.576078
C	-4.176217	0.771765	1.348355
C	-4.283725	-0.130533	0.284138
C	-4.068517	-1.350067	0.283662
C	-3.539701	2.036344	3.804700
C	-3.178241	2.658708	2.576849
C	-3.695976	2.090147	1.348758
C	-4.041740	0.703987	6.277028
C	-3.551126	2.054285	6.277429
C	-3.126221	2.625166	5.051605
C	-2.041424	3.533950	5.051868
C	-1.389005	3.838834	3.805381
C	-2.064576	3.592274	2.577204
C	-1.414087	4.003685	1.349546
C	-2.249893	3.647170	0.285363
C	-3.198710	2.851342	0.285040
C	-0.000098	4.084756	3.805349
C	0.719388	4.084012	2.577542
C	-0.032366	4.247801	1.349692
C	-1.405590	3.852241	6.278012
C	0.009406	4.100452	6.278100
C	0.716737	4.020680	5.052253
C	2.046619	3.536770	5.051819
C	2.637115	3.125237	3.804959
C	2.085130	3.587344	2.577281
C	2.766425	3.230273	1.349256
C	2.039462	3.775971	0.285402
C	0.875301	4.198204	0.285759
C	3.544193	2.045171	3.803905
C	3.903681	1.422396	2.575916
C	3.669042	2.155958	1.348567
C	2.639297	3.142903	6.277517
C	3.562727	2.042488	6.276658
C	3.847141	1.391101	5.050145
C	4.094871	-0.002002	5.049083
C	4.034257	-0.718708	3.801889
C	4.157197	-0.008664	2.574799
C	4.188013	-0.776688	1.346355
C	4.296146	0.126417	0.282957
C	4.079667	1.345687	0.284071
C	4.053092	-0.712954	6.274604
C	4.094009	-0.003274	7.501841
C	3.846071	1.388548	7.503014
C	3.543007	2.040629	8.750569
C	2.635363	3.119688	8.751283
C	2.044493	3.532865	7.504670
C	0.716269	4.016591	7.505275
C	-0.000726	4.081364	8.752601
C	-1.389605	3.837620	8.752425
C	-2.042221	3.533157	7.504897
C	-3.125555	2.624762	7.504671
C	-3.539772	2.035327	8.752131
C	-4.021164	0.709904	8.751810

C	-4.081145	-0.007127	7.504101
C	-3.833283	-1.398783	7.503228
C	-3.527909	-2.052202	8.749781
C	3.902945	1.416726	9.977105
C	3.668062	2.148451	11.205884
C	2.765593	3.221694	11.206844
C	2.083829	3.580077	9.979068
C	0.718905	4.078059	9.979536
C	-0.032296	4.241039	11.208241
C	-1.413194	3.998837	11.208320
C	-2.064577	3.589796	9.979906
C	-3.178050	2.656395	9.979702
C	-3.694204	2.085806	11.208037
C	-4.172412	0.767982	11.207571
C	-4.142087	0.000254	9.978579
C	-3.886750	-1.430068	9.977732
C	-3.651104	-2.163570	11.205358
C	4.298971	0.118069	12.268656
C	4.080905	1.336850	12.268996
C	0.876371	4.190173	12.271899
C	2.040237	3.767814	12.272032
C	-3.197880	2.847094	12.272839
C	-2.249406	3.642895	12.273057
C	-4.064161	-1.355232	12.270791
C	-4.279531	-0.135984	12.271101
Cl	-0.530974	0.486279	7.638744
C	-0.105822	0.081379	4.498761
H	0.873025	0.199474	4.953591
H	-0.721586	0.948573	4.718063
H	-0.584678	-0.817119	4.876619
Cl	0.087157	-0.064238	2.705841

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C	-2.033339	-3.780443	12.105306
C	-2.759018	-3.233924	11.041259
C	-2.078529	-3.592882	9.813845
C	-0.714067	-4.091976	9.814204
C	0.037370	-4.255200	11.041997
C	-0.870233	-4.205349	12.105794
C	1.419234	-4.011114	11.042222
C	2.069747	-3.600258	9.814274
C	1.394729	-3.849317	8.586820
C	0.005942	-4.094836	8.586774
C	2.254681	-3.653585	12.106509
C	3.202356	-2.856499	12.106429
C	3.697268	-2.094449	11.042158
C	3.180701	-2.664112	9.814140
C	3.539856	-2.040573	8.586571
C	4.019562	-0.715310	8.586769
C	4.143304	-0.006694	9.814452
C	4.174847	-0.775550	11.042577
C	3.127102	-2.630550	7.339992
C	2.046851	-3.543475	7.339819
C	1.411447	-3.862817	6.113357
C	-0.003919	-4.113160	6.112978
C	-0.711106	-4.031127	7.339544
C	-2.039293	-3.543420	7.339388

C	-2.629415	-3.130018	8.586154
C	3.547781	-2.057257	6.114099
C	3.126899	-2.629939	4.887473
C	2.047171	-3.542681	4.886902
C	1.396065	-3.849114	3.639466
C	0.007075	-4.094078	3.638771
C	-0.710422	-4.029873	4.885732
C	-2.038032	-3.541807	4.885600
C	-2.630686	-3.148279	6.112627
C	3.540855	-2.040300	3.641075
C	3.182652	-2.663918	2.413713
C	2.071580	-3.600158	2.412842
C	1.421043	-4.010243	1.184257
C	0.039767	-4.253293	1.183890
C	-0.712317	-4.090299	2.411444
C	-2.076652	-3.590385	2.411412
C	-2.627835	-3.128069	3.638741
C	3.698902	-2.092860	1.185598
C	3.204324	-2.855418	0.120888
C	2.257268	-3.652963	0.120200
C	-2.756473	-3.230298	1.183719
C	-2.030377	-3.777082	0.120045
C	-0.867710	-4.202579	0.120105
C	-3.532310	-2.046267	3.639258
C	-3.890990	-1.422200	2.412400
C	-3.656440	-2.154866	1.183634
C	-3.551753	-2.045635	6.112817
C	-3.834449	-1.392594	4.886363
C	-4.082224	-0.000227	4.886974
C	-4.023270	0.717589	3.640452
C	-4.145002	0.008724	2.412956
C	-4.176697	0.777782	1.184413
C	-4.284179	-0.124747	0.119367
C	-4.067924	-1.344037	0.118985
C	-3.544409	2.043312	3.640908
C	-3.184125	2.666453	2.413831
C	-3.700037	2.096466	1.185072
C	-4.041687	0.709346	6.113770
C	-3.553954	2.060032	6.114232
C	-3.131274	2.632300	4.887954
C	-2.048974	3.542204	4.888125
C	-1.396983	3.849325	3.641267
C	-2.072316	3.601829	2.414148
C	-1.421275	4.012571	1.186076
C	-2.257089	3.655817	0.121494
C	-3.204670	2.858920	0.120985
C	-0.007985	4.094136	3.641100
C	0.711756	4.092171	2.413948
C	-0.040080	4.255744	1.186292
C	-1.412703	3.859562	6.114918
C	0.002467	4.109273	6.115078
C	0.709474	4.028721	4.888016
C	2.038465	3.544220	4.887905
C	2.628673	3.131658	3.640773
C	2.076581	3.593495	2.413765
C	2.756578	3.233785	1.185915
C	2.030294	3.780716	0.122207
C	0.867531	4.206037	0.122400
C	3.533616	2.049924	3.640913

C	3.891423	1.425602	2.414066
C	3.656843	2.158440	1.185814
C	2.631993	3.151365	6.114944
C	3.553820	2.049016	6.114807
C	3.835475	1.395979	4.888002
C	4.079339	0.003192	4.888041
C	4.020107	-0.714350	3.641365
C	4.143998	-0.005267	2.414284
C	4.175711	-0.773934	1.185938
C	4.284781	0.128782	0.121617
C	4.068843	1.347962	0.121573
C	4.036127	-0.706760	6.114381
C	4.079988	0.002557	7.340529
C	3.835997	1.395854	7.340901
C	3.533409	2.048951	8.588029
C	2.628546	3.130193	8.588603
C	2.038840	3.543850	7.341727
C	0.709374	4.028356	7.341773
C	-0.008121	4.091785	8.588632
C	-1.396756	3.846731	8.588112
C	-2.049077	3.541591	7.341070
C	-3.131594	2.631336	7.340598
C	-3.543999	2.040875	8.586989
C	-4.023208	0.715660	8.586527
C	-4.083166	-0.001088	7.339594
C	-3.835874	-1.393928	7.339300
C	-3.533751	-2.048248	8.586004
C	3.891291	1.424288	9.815103
C	3.657198	2.156799	11.043570
C	2.756705	3.232533	11.043598
C	2.076514	3.591641	9.816287
C	0.711571	4.089557	9.816320
C	-0.039997	4.252818	11.043780
C	-1.421628	4.008770	11.043907
C	-2.072051	3.598266	9.815486
C	-3.183874	2.663080	9.814918
C	-3.700111	2.092554	11.043055
C	-4.177762	0.773883	11.042384
C	-4.145917	0.006013	9.813802
C	-3.892835	-1.424747	9.813458
C	-3.659342	-2.158064	11.041391
C	4.283412	0.126484	12.107588
C	4.068009	1.346054	12.108096
C	0.867274	4.202779	12.107415
C	2.030534	3.778404	12.107399
C	-3.204623	2.853796	12.108091
C	-2.256906	3.650937	12.108610
C	-4.070800	-1.348087	12.106072
C	-4.286522	-0.128659	12.106485
Cl	-0.062780	-0.044237	8.273282
C	0.012258	0.021623	5.976723
H	1.027885	-0.333783	5.994316
H	-0.187225	1.078281	6.000395
H	-0.803098	-0.678129	5.931489
Cl	0.067739	0.086762	3.678573

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C	-2.022526	-3.759510	12.279468
C	-2.746340	-3.223118	11.201146
C	-2.076626	-3.582208	9.981806
C	-0.710419	-4.079114	9.981598
C	0.033912	-4.234397	11.200671
C	-0.864923	-4.180704	12.279376
C	1.417736	-3.990174	11.200724
C	2.064003	-3.589637	9.981651
C	1.390284	-3.835461	8.754255
C	0.006759	-4.079351	8.754200
C	2.243852	-3.631685	12.279349
C	3.187352	-2.839683	12.279517
C	3.683647	-2.087980	11.201073
C	3.177420	-2.654902	9.981822
C	3.536376	-2.033717	8.754585
C	4.016228	-0.713354	8.754843
C	4.140092	-0.007199	9.982378
C	4.163898	-0.767383	11.201322
C	3.123102	-2.624432	7.507884
C	2.043870	-3.530540	7.507720
C	1.408426	-3.849528	6.283927
C	-0.005112	-4.098084	6.283937
C	-0.711593	-4.016010	7.507607
C	-2.035884	-3.534240	7.507831
C	-2.626767	-3.121479	8.754647
C	3.547450	-2.053580	6.284265
C	3.124433	-2.624445	5.061337
C	2.044150	-3.531554	5.061167
C	1.390818	-3.835364	3.814752
C	0.006790	-4.078387	3.814764
C	-0.710966	-4.015535	5.061151
C	-2.036495	-3.533109	5.061374
C	-2.630197	-3.142965	6.284334
C	3.536942	-2.033297	3.815104
C	3.178716	-2.654678	2.587076
C	2.065030	-3.589791	2.586898
C	1.418320	-3.989865	1.368111
C	0.033363	-4.233813	1.368213
C	-0.710965	-4.078396	2.587034
C	-2.077549	-3.581160	2.587257
C	-2.627110	-3.119960	3.815164
C	3.684978	-2.086788	1.368497
C	3.187577	-2.837453	0.290232
C	2.243968	-3.629669	0.290088
C	-2.748106	-3.221917	1.368658
C	-2.023648	-3.757026	0.290520
C	-0.865840	-4.178309	0.290292
C	-3.531548	-2.044514	3.815569
C	-3.890865	-1.423194	2.587824
C	-3.652653	-2.145164	1.368913
C	-3.553868	-2.044462	6.284723
C	-3.836975	-1.392218	5.062123
C	-4.082399	-0.003087	5.062541
C	-4.019040	0.715001	3.816352
C	-4.143806	0.008818	2.588235
C	-4.167354	0.769319	1.369713

C	-4.268649	-0.125417	0.291404
C	-4.054432	-1.338728	0.291045
C	-3.537492	2.035119	3.816665
C	-3.178982	2.657093	2.589010
C	-3.686138	2.090689	1.370132
C	-4.039648	0.706026	6.285536
C	-3.548082	2.054460	6.285859
C	-3.123949	2.624878	5.063153
C	-2.043374	3.531631	5.063326
C	-1.390581	3.836873	3.817029
C	-2.065095	3.591963	2.589198
C	-1.419131	3.993564	1.370542
C	-2.245115	3.634212	0.292504
C	-3.188791	2.842076	0.292347
C	-0.007023	4.082582	3.817018
C	0.710348	4.083580	2.589055
C	-0.034381	4.238659	1.370435
C	-1.408354	3.850363	6.286195
C	0.004844	4.100942	6.286186
C	0.710946	4.020503	5.063343
C	2.036723	3.538587	5.063109
C	2.626593	3.125101	3.816594
C	2.077002	3.586674	2.588819
C	2.747004	3.227212	1.369958
C	2.022501	3.762705	0.292044
C	0.864582	4.183703	0.292287
C	3.529082	2.048015	3.816174
C	3.888133	1.426939	2.588229
C	3.650757	2.149781	1.369694
C	2.629771	3.146558	6.285786
C	3.551641	2.046530	6.285384
C	3.833274	1.394461	5.062335
C	4.078245	0.005319	5.061914
C	4.015972	-0.712259	3.815395
C	4.140794	-0.005184	2.587821
C	4.165131	-0.765013	1.368903
C	4.266526	0.130377	0.291146
C	4.052354	1.343691	0.291500
C	4.037010	-0.704425	6.284575
C	4.078455	0.005336	7.508393
C	3.833580	1.393075	7.508816
C	3.529199	2.046292	8.755692
C	2.626216	3.122516	8.756107
C	2.035575	3.536811	7.509677
C	0.711245	4.018386	7.509907
C	-0.007185	4.080323	8.756554
C	-1.390594	3.835669	8.756496
C	-2.044006	3.530850	7.509790
C	-3.123384	2.624864	7.509628
C	-3.536979	2.033944	8.756177
C	-4.017539	0.713817	8.755911
C	-4.080794	-0.004254	7.509113
C	-3.835722	-1.391968	7.508687
C	-3.530271	-2.045674	8.755059
C	3.887404	1.424438	9.982804
C	3.649555	2.146052	11.202215
C	2.746116	3.222325	11.202673
C	2.076283	3.582382	9.983686
C	0.710089	4.079305	9.983897

C	-0.034125	4.233519	11.203151
C	-1.417877	3.989092	11.203098
C	-2.064166	3.589094	9.983846
C	-3.177626	2.654404	9.983678
C	-3.683717	2.086964	11.202753
C	-4.164118	0.766466	11.202499
C	-4.140943	0.006995	9.983117
C	-3.888166	-1.424616	9.982689
C	-3.649821	-2.146887	11.201600
C	4.266521	0.127014	12.280170
C	4.052272	1.340086	12.280472
C	0.864905	4.178912	12.281661
C	2.022603	3.757978	12.281568
C	-3.187285	2.838113	12.281521
C	-2.243842	3.630170	12.281691
C	-4.052226	-1.341697	12.280559
C	-4.266287	-0.128590	12.280857
Cl	-0.047133	0.034009	7.478474
C	0.010944	0.006429	4.292165
H	1.034357	0.118089	4.642486
H	-0.592981	0.840243	4.640923
H	-0.405498	-0.929645	4.655835
Cl	0.007037	-0.009022	2.480641

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C	-2.025095	-3.759840	12.105191
C	-2.748564	-3.224018	11.026465
C	-2.078762	-3.583933	9.807531
C	-0.712694	-4.081769	9.807762
C	0.031487	-4.236054	11.026984
C	-0.867467	-4.181238	12.105471
C	1.415732	-3.991765	11.027400
C	2.062915	-3.591983	9.808675
C	1.389179	-3.838449	8.581142
C	0.005501	-4.082620	8.580684
C	2.240996	-3.632821	12.106338
C	3.184425	-2.840648	12.106770
C	3.681290	-2.089364	11.028537
C	3.176082	-2.656715	9.809264
C	3.535524	-2.034747	8.582352
C	4.015732	-0.714365	8.583101
C	4.139462	-0.007984	9.810729
C	4.161710	-0.768537	11.029282
C	3.121774	-2.624903	7.335696
C	2.042720	-3.532490	7.334979
C	1.407591	-3.850345	6.111202
C	-0.006154	-4.099708	6.110725
C	-0.712492	-4.018594	7.334067
C	-2.037031	-3.535115	7.333973
C	-2.628647	-3.122466	8.580308
C	3.544384	-2.052874	6.112579
C	3.122232	-2.623593	4.888749
C	2.043149	-3.531300	4.888061
C	1.390298	-3.836217	3.641293
C	0.006726	-4.080335	3.640809
C	-0.711786	-4.017260	4.887143
C	-2.036359	-3.533645	4.887023

C	-2.629123	-3.142014	6.110517
C	3.536735	-2.032436	3.642838
C	3.177914	-2.653409	2.415163
C	2.064674	-3.588570	2.414329
C	1.418063	-3.987207	1.194981
C	0.033765	-4.231522	1.194505
C	-0.710977	-4.078390	2.413391
C	-2.077094	-3.580767	2.413401
C	-2.627489	-3.120108	3.640771
C	3.683632	-2.084853	1.196700
C	3.187119	-2.834915	0.117435
C	2.243620	-3.627062	0.116697
C	-2.746089	-3.219462	1.194551
C	-2.022156	-3.754142	0.115697
C	-0.864527	-4.175576	0.115648
C	-3.530553	-2.043852	3.641065
C	-3.888858	-1.421423	2.413974
C	-3.649586	-2.142657	1.194846
C	-3.551867	-2.042437	6.110815
C	-3.834917	-1.390300	4.887582
C	-4.080861	-0.001801	4.888171
C	-4.018408	0.717110	3.642034
C	-4.141689	0.010355	2.414450
C	-4.163229	0.770715	1.195762
C	-4.264688	-0.123343	0.116686
C	-4.050869	-1.336602	0.116355
C	-3.537688	2.037300	3.642733
C	-3.177398	2.659061	2.415841
C	-3.682329	2.091632	1.196458
C	-4.038981	0.707069	6.111961
C	-3.547739	2.055970	6.112665
C	-3.123679	2.626915	4.889550
C	-2.042843	3.532518	4.890172
C	-1.389304	3.838862	3.644120
C	-2.063406	3.593326	2.416584
C	-1.416180	3.993204	1.198063
C	-2.241292	3.634628	0.118971
C	-3.184974	2.842700	0.118264
C	-0.005823	4.083367	3.644554
C	0.712307	4.083502	2.417440
C	-0.031997	4.237597	1.198498
C	-1.407384	3.849290	6.113938
C	0.006132	4.099359	6.114400
C	0.712422	4.019558	4.891038
C	2.037999	3.538555	4.891209
C	2.629310	3.125919	3.644713
C	2.078777	3.586903	2.417492
C	2.748080	3.226456	1.198555
C	2.024404	3.762005	0.119958
C	0.866650	4.183051	0.119974
C	3.532095	2.049382	3.644507
C	3.890158	1.427372	2.417122
C	3.651517	2.149502	1.198382
C	2.631005	3.146884	6.114709
C	3.553292	2.046733	6.114483
C	3.835493	1.394893	4.890811
C	4.078670	0.005920	4.890238
C	4.017053	-0.712161	3.643587
C	4.141815	-0.004582	2.416676

C	4.164372	-0.763978	1.197478
C	4.266763	0.130830	0.119166
C	4.053165	1.344118	0.119498
C	4.034879	-0.703830	6.113352
C	4.078224	0.004892	7.337180
C	3.834928	1.393759	7.337751
C	3.530648	2.047122	8.584425
C	2.627915	3.123806	8.584663
C	2.037353	3.537712	7.338229
C	0.711930	4.018872	7.338086
C	-0.007039	4.081570	8.584197
C	-1.390622	3.837125	8.583733
C	-2.043684	3.531811	7.337159
C	-3.124349	2.626120	7.336504
C	-3.538740	2.035247	8.582615
C	-4.019278	0.714929	8.581935
C	-4.081440	-0.002932	7.335145
C	-3.835600	-1.391361	7.334563
C	-3.531619	-2.046037	8.580606
C	3.887819	1.424010	9.811442
C	3.648590	2.145107	11.030770
C	2.745472	3.222213	11.030987
C	2.076812	3.583712	9.811933
C	0.710378	4.080467	9.811663
C	-0.034483	4.233961	11.030393
C	-1.418513	3.989336	11.029975
C	-2.065066	3.590259	9.810737
C	-3.178881	2.655746	9.810185
C	-3.684347	2.087207	11.028890
C	-4.165154	0.766424	11.028169
C	-4.142776	0.007152	9.808823
C	-3.890084	-1.424645	9.808110
C	-3.651876	-2.147185	11.026703
C	4.263299	0.125347	12.108474
C	4.049594	1.338594	12.109134
C	0.863747	4.178624	12.109290
C	2.021380	3.757286	12.109600
C	-3.187506	2.837384	12.107988
C	-2.244032	3.629506	12.108397
C	-4.053500	-1.341925	12.105669
C	-4.267136	-0.128674	12.106319
Cl	-0.004882	0.008749	8.305274
C	0.000181	0.004680	6.004096
H	1.040481	-0.273895	6.005699
H	-0.279320	1.044818	6.000266
H	-0.761022	-0.757080	6.003168
Cl	0.004031	-0.001149	3.700704

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C	-2.025517	-3.799408	12.239048
C	-2.770503	-3.248778	11.185956
C	-2.080910	-3.599315	9.958415
C	-0.699497	-4.091556	9.956799
C	0.058593	-4.260181	11.182550
C	-0.859789	-4.224461	12.241618
C	1.446661	-4.017516	11.180288
C	2.097917	-3.599301	9.953280

C	1.412478	-3.835578	8.722855
C	0.022682	-4.077169	8.724307
C	2.301084	-3.659478	12.233403
C	3.258688	-2.870517	12.235458
C	3.758048	-2.096970	11.177626
C	3.227006	-2.663033	9.951749
C	3.582390	-2.034012	8.719458
C	4.072036	-0.711306	8.718544
C	4.209838	-0.000922	9.950023
C	4.246855	-0.774999	11.176530
C	3.159773	-2.624735	7.462375
C	2.067802	-3.528111	7.464574
C	1.430680	-3.848576	6.235813
C	0.004857	-4.098261	6.237348
C	-0.701600	-4.015258	7.467071
C	-2.035990	-3.538649	7.468627
C	-2.636659	-3.134611	8.727582
C	3.588444	-2.058032	6.232464
C	3.156517	-2.625721	5.003408
C	2.066135	-3.529272	5.005363
C	1.409204	-3.840112	3.748585
C	0.018637	-4.084121	3.750558
C	-0.702804	-4.017812	5.008183
C	-2.036284	-3.540133	5.009369
C	-2.637022	-3.156197	6.238027
C	3.576617	-2.036420	3.744961
C	3.218548	-2.665622	2.514885
C	2.090993	-3.604619	2.517021
C	1.437809	-4.025945	1.291034
C	0.051503	-4.270097	1.292488
C	-0.704562	-4.098537	2.519624
C	-2.085193	-3.602346	2.519899
C	-2.635135	-3.133068	3.750625
C	3.745102	-2.098585	1.286469
C	3.242976	-2.875966	0.231807
C	2.289239	-3.668954	0.234495
C	-2.777155	-3.252380	1.292553
C	-2.038358	-3.809176	0.237639
C	-0.872196	-4.231779	0.236971
C	-3.548252	-2.056587	3.750384
C	-3.917934	-1.436691	2.518357
C	-3.685195	-2.176842	1.291590
C	-3.578291	-2.055930	6.238066
C	-3.856804	-1.399910	5.007636
C	-4.103119	-0.006271	5.007732
C	-4.038252	0.716521	3.750512
C	-4.173041	0.007578	2.518430
C	-4.207941	0.782781	1.291726
C	-4.324277	-0.133912	0.235683
C	-4.108647	-1.355460	0.235606
C	-3.549207	2.040684	3.750920
C	-3.193249	2.670107	2.520260
C	-3.723267	2.104292	1.292836
C	-4.066335	0.705326	6.238211
C	-3.558948	2.061452	6.238327
C	-3.126216	2.628213	5.009729
C	-2.037017	3.533801	5.008691
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C	-2.066305	3.609443	2.520170

C	-1.414884	4.030056	1.293112
C	-2.269380	3.677404	0.237510
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C	0.007906	4.091394	3.749235
C	0.729153	4.104293	2.517684
C	-0.028935	4.276134	1.291721
C	-1.399840	3.851786	6.237888
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C	2.065739	3.549665	5.003989
C	2.662529	3.140483	3.745447
C	2.110361	3.608939	2.515463
C	2.799335	3.256918	1.286962
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C	0.893283	4.233079	0.235162
C	3.575542	2.063578	3.743903
C	3.942806	1.442596	2.512488
C	3.708329	2.182206	1.285382
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C	3.602937	2.060194	6.231725
C	3.882142	1.405520	5.001333
C	4.128263	0.011075	5.001186
C	4.065457	-0.711926	3.743618
C	4.197863	-0.002505	2.512342
C	4.230918	-0.777495	1.285105
C	4.345447	0.139055	0.228836
C	4.129830	1.360487	0.228970
C	4.090388	-0.699920	6.231394
C	4.132734	0.010834	7.460505
C	3.886208	1.406615	7.460684
C	3.581692	2.063968	8.718853
C	2.668430	3.138817	8.719979
C	2.068977	3.549179	7.462966
C	0.733484	4.023415	7.465211
C	0.012413	4.087333	8.723488
C	-1.376005	3.837953	8.724871
C	-2.035090	3.531501	7.467566
C	-3.125421	2.626612	7.469010
C	-3.551277	2.041060	8.727916
C	-4.035534	0.716058	8.728368
C	-4.108216	-0.005697	7.466396
C	-3.861499	-1.402588	7.466305
C	-3.545582	-2.055734	8.728167
C	3.954595	1.443585	9.950187
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C	2.811771	3.257612	11.178164
C	2.118895	3.607616	9.952341
C	0.737294	4.100195	9.953919
C	-0.017918	4.269616	11.180939
C	-1.405077	4.021968	11.183113
C	-2.059419	3.603814	9.957287
C	-3.188531	2.668022	9.958796
C	-3.716204	2.102190	11.186276
C	-4.204697	0.780915	11.187308
C	-4.176317	0.006321	9.961568
C	-3.921155	-1.437409	9.961484
C	-3.682229	-2.174893	11.187117
C	4.364687	0.141044	12.232115
C	4.148785	1.362848	12.232251

C	0.907473	4.225984	12.234062
C	2.077443	3.812912	12.236086
C	-3.205130	2.874775	12.239436
C	-2.255617	3.673517	12.242144
C	-4.103978	-1.355378	12.245117
C	-4.319895	-0.133643	12.245215
Cl	-1.333412	-0.233976	8.389714
C	-0.208668	-0.005229	5.413140
H	0.635905	-0.018391	6.095789
H	-0.836364	0.858845	5.608664
H	-0.784376	-0.920590	5.509124
Cl	0.418191	0.107979	3.715511

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C	-2.036368	-3.785148	12.127574
C	-2.793897	-3.246197	11.083472
C	-2.098338	-3.590553	9.847397
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C	0.037022	-4.245005	11.075335
C	-0.879475	-4.238466	12.133127
C	1.426817	-4.011698	11.071349
C	2.072458	-3.580301	9.837490
C	1.394534	-3.834128	8.607617
C	-0.005402	-4.071193	8.609442
C	2.276468	-3.635755	12.116169
C	3.256398	-2.870602	12.123061
C	3.729890	-2.083258	11.067441
C	3.200830	-2.652987	9.836786
C	3.557227	-2.026063	8.601483
C	4.062413	-0.700297	8.601788
C	4.186030	0.010236	9.833186
C	4.231789	-0.766937	11.064757
C	3.139854	-2.614079	7.354684
C	2.037228	-3.511947	7.356759
C	1.398237	-3.832517	6.125155
C	-0.018768	-4.075818	6.128910
C	-0.726374	-4.024224	7.363271
C	-2.058698	-3.526532	7.366220
C	-2.668754	-3.145531	8.618722
C	3.552997	-2.034040	6.119724
C	3.135946	-2.614638	4.887569
C	2.033263	-3.509256	4.890531
C	1.383264	-3.831671	3.642897
C	-0.014670	-4.071759	3.647264
C	-0.731249	-4.017643	4.896021
C	-2.067616	-3.535389	4.900638
C	-2.670646	-3.155036	6.132104
C	3.546560	-2.022046	3.637009
C	3.185630	-2.653053	2.405027
C	2.056701	-3.576854	2.409920
C	1.404784	-4.012186	1.179360
C	0.017986	-4.248480	1.181541
C	-0.739864	-4.087702	2.414978
C	-2.113026	-3.594350	2.418523
C	-2.672457	-3.140523	3.650290
C	3.704680	-2.079697	1.170965
C	3.227096	-2.871626	0.118369

C	2.248638	-3.636957	0.128128
C	-2.816910	-3.255975	1.187629
C	-2.065440	-3.795471	0.138384
C	-0.907330	-4.245237	0.129904
C	-3.583516	-2.054083	3.652320
C	-3.951637	-1.433212	2.417716
C	-3.715958	-2.173187	1.186538
C	-3.591453	-2.050764	6.135098
C	-3.892644	-1.404083	4.899662
C	-4.121355	-0.001984	4.900862
C	-4.069204	0.717196	3.649562
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C	-4.239155	0.782247	1.186342
C	-4.340720	-0.139292	0.139668
C	-4.166239	-1.369587	0.132856
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C	-3.206599	2.668408	2.413471
C	-3.734755	2.097659	1.183006
C	-4.078488	0.711234	6.132506
C	-3.559525	2.050911	6.131094
C	-3.147002	2.631531	4.895957
C	-2.045814	3.531046	4.893255
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C	-2.079132	3.596111	2.412210
C	-1.433940	4.027488	1.179869
C	-2.281649	3.649837	0.135248
C	-3.261330	2.884786	0.128106
C	-0.002551	4.090333	3.640944
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C	-0.044154	4.262516	1.175212
C	-1.406490	3.853376	6.125324
C	0.010006	4.098050	6.122111
C	0.718263	4.041254	4.888217
C	2.055236	3.554349	4.885108
C	2.660951	3.168100	3.636277
C	2.090348	3.610564	2.405110
C	2.788056	3.269926	1.171213
C	2.028980	3.803113	0.126820
C	0.871849	4.257764	0.118696
C	3.559843	2.068235	3.635267
C	3.935566	1.450976	2.400110
C	3.685988	2.184402	1.169269
C	2.658911	3.171402	6.119887
C	3.581589	2.068141	6.117369
C	3.888092	1.425214	4.885610
C	4.108116	0.020918	4.883839
C	4.065178	-0.701993	3.635212
C	4.171052	0.011115	2.402491
C	4.212424	-0.768290	1.169390
C	4.304724	0.152233	0.121247
C	4.133342	1.382906	0.112488
C	4.068738	-0.692700	6.119482
C	4.113005	0.019367	7.351160
C	3.882482	1.421288	7.353201
C	3.572845	2.070421	8.600454
C	2.661709	3.158573	8.603027
C	2.057981	3.554800	7.352400
C	0.722358	4.039862	7.356172
C	0.005276	4.095609	8.604961

C	-1.392798	3.854139	8.609102
C	-2.042058	3.529991	7.360320
C	-3.143107	2.634136	7.364070
C	-3.554058	2.042969	8.614217
C	-4.066297	0.721118	8.617763
C	-4.114700	-0.003409	7.367829
C	-3.901801	-1.407486	7.368614
C	-3.573163	-2.051008	8.618232
C	3.940644	1.448767	9.835083
C	3.702354	2.186532	11.066888
C	2.802734	3.269774	11.066363
C	2.102160	3.612760	9.834875
C	0.729179	4.108537	9.838043
C	-0.029097	4.270842	11.070763
C	-1.415799	4.035730	11.071814
C	-2.066728	3.601313	9.841393
C	-3.193206	2.673424	9.846102
C	-3.717039	2.103992	11.079278
C	-4.219695	0.792121	11.081740
C	-4.178227	0.011143	9.850033
C	-3.939838	-1.428448	9.853790
C	-3.692033	-2.162465	11.085722
C	4.332624	0.153900	12.111128
C	4.154156	1.383318	12.119743
C	0.894625	4.263466	12.122959
C	2.051636	3.811045	12.114757
C	-3.238690	2.895550	12.130635
C	-2.261674	3.662229	12.121596
C	-4.137870	-1.356088	12.141240
C	-4.314934	-0.126702	12.131507
Cl	-1.016286	-0.727709	7.660271
C	0.083868	-0.178706	5.709459
H	0.917126	-0.787346	6.013951
H	0.050514	0.862580	5.979572
H	-0.714986	-0.610827	5.131833
Cl	1.203861	0.354853	3.761440

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C	-2.593509	-3.585573	12.469858
C	-3.161916	-3.191101	11.361286
C	-2.330676	-3.574675	10.204069
C	-0.960004	-4.071151	10.453176
C	-0.485625	-4.160485	11.847592
C	-1.485044	-3.986794	12.671317
C	0.878062	-3.916604	12.096065
C	1.741405	-3.586520	10.945558
C	1.320104	-3.861411	9.629259
C	-0.047647	-4.107418	9.380048

C	1.413592	-3.467085	13.199906
C	2.317644	-2.702024	13.365772
C	3.059924	-2.068656	12.496584
C	2.859952	-2.640539	11.150856
C	3.461371	-2.048447	10.022291
C	3.938969	-0.722569	10.111802
C	3.798966	-0.022684	11.326899
C	3.534474	-0.746531	12.585601
C	3.253502	-2.630801	8.728417
C	2.183388	-3.535354	8.531942
C	1.762950	-3.820872	7.213761
C	0.374884	-4.074543	6.960422
C	-0.539927	-4.027731	8.035736
C	-1.851017	-3.552764	7.797765
C	-2.672795	-3.155080	8.903160
C	3.864767	-2.041332	7.599496
C	3.689372	-2.625382	6.325404
C	2.619321	-3.529869	6.128965
C	2.198339	-3.853038	4.797326
C	0.831203	-4.102903	4.547301
C	-0.104207	-4.029957	5.631939
C	-1.416725	-3.557425	5.393655
C	-2.201127	-3.141029	6.492833
C	4.339808	-2.039088	5.190384
C	4.175013	-2.627353	3.920717
C	3.057141	-3.573904	3.715694
C	2.656998	-3.901639	2.334173
C	1.294062	-4.146689	2.084589
C	0.356468	-4.062519	3.221168
C	-1.013694	-3.564140	2.971009
C	-1.795778	-3.155302	4.069895
C	4.836254	-2.051678	2.733977
C	4.449871	-2.682709	1.657081
C	3.546877	-3.448874	1.491378
C	-1.376021	-3.166848	1.596053
C	-0.453530	-3.559556	0.758554
C	0.652637	-3.965515	0.961067
C	-2.687944	-2.072873	3.912815
C	-2.786639	-1.433457	2.643783
C	-2.267934	-2.091187	1.431175
C	-3.113411	-2.047221	6.328261
C	-3.200681	-1.407379	5.072291
C	-3.458798	-0.017306	5.026095
C	-3.201627	0.714420	3.819185
C	-3.063935	0.017866	2.601515
C	-2.800081	0.744157	1.343793
C	-2.576880	-0.104017	0.374934
C	-2.354822	-1.278504	0.411753
C	-2.729866	2.042509	3.909545
C	-2.129183	2.636610	2.781706
C	-2.329345	2.067259	1.435163
C	-3.612677	0.685760	6.241678
C	-3.133600	2.033849	6.332574
C	-2.525007	2.626451	5.203609
C	-1.455223	3.531605	5.400906
C	-0.589466	3.855549	4.304597
C	-1.010484	3.581845	2.988139
C	-0.146601	3.911956	1.838339
C	-0.682725	3.465748	0.733631

C	-1.587552	2.702047	0.566686
C	0.779572	4.094931	4.554141
C	1.692085	4.058378	3.481114
C	1.217723	4.150578	2.087076
C	-1.033156	3.812321	6.719594
C	0.356748	4.056080	6.972838
C	1.271857	4.010016	5.897889
C	2.582898	3.533991	6.135147
C	3.405723	3.139707	5.029431
C	3.062230	3.559708	3.729055
C	3.892082	3.175829	2.571129
C	3.323582	3.571069	1.463069
C	2.215927	3.974617	1.262568
C	4.313627	2.070609	5.192234
C	4.850372	1.444740	4.049512
C	4.794873	2.108559	2.732771
C	2.934699	3.121231	7.439435
C	3.856913	2.036245	7.605190
C	4.389170	1.403817	6.459521
C	4.642530	0.012367	6.503255
C	4.819045	-0.713846	5.279406
C	5.115224	-0.009840	4.095202
C	5.310092	-0.729466	2.821655
C	5.448667	0.124333	1.842467
C	5.234910	1.300186	1.805539
C	4.352165	-0.696161	7.690525
C	4.204008	0.007915	8.906314
C	3.951499	1.399479	8.862764
C	3.435831	2.062667	10.025155
C	2.529320	3.132944	9.861989
C	2.147249	3.530755	8.538354
C	0.835600	4.004939	8.300866
C	-0.097863	4.082302	9.386106
C	-1.465966	3.838590	9.136948
C	-1.889670	3.521193	7.804505
C	-2.960221	2.617482	7.607317
C	-3.607954	2.028095	8.742851
C	-4.083425	0.701631	8.652782
C	-3.904160	-0.023713	7.428427
C	-3.648750	-1.414908	7.472534
C	-3.576549	-2.082734	8.739586
C	3.535886	1.432351	11.281570
C	3.022433	2.092794	12.497455
C	2.120275	3.160833	12.335005
C	1.749971	3.548381	10.960092
C	0.378486	4.043446	10.711649
C	-0.556826	4.128544	11.849882
C	-1.920375	3.883791	11.601593
C	-2.322963	3.558641	10.219629
C	-3.441895	2.613832	10.013745
C	-4.102877	2.037084	11.200331
C	-4.577693	0.715241	11.110547
C	-4.378976	-0.003139	9.836762
C	-4.114244	-1.457399	9.882034
C	-4.063941	-2.123145	11.198251
C	3.321977	0.104598	13.554037
C	3.109617	1.280864	13.517515
C	0.088504	3.952629	12.972389
C	1.197308	3.552105	13.173267

C	-3.714545	2.665942	12.278009
C	-2.810144	3.430507	12.444322
C	-4.508038	-1.315796	12.124633
C	-4.721189	-0.139693	12.088252
Cl	-0.521160	0.025785	8.436735
C	0.672932	0.010595	5.617549
H	1.503766	0.089353	6.319624
H	-0.000257	0.855316	5.720797
H	0.124884	-0.912382	5.778387
Cl	1.384835	-0.000666	3.933908

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C	-2.980431	-3.887371	11.515442
C	-3.572853	-3.455033	10.433932
C	-2.765444	-3.794957	9.246500
C	-1.387105	-4.292589	9.449499
C	-0.883849	-4.430602	10.829842
C	-1.866717	-4.290993	11.679464
C	0.483711	-4.190300	11.059998
C	1.323288	-3.814829	9.905854
C	0.875673	-4.040027	8.588838
C	-0.496047	-4.282857	8.358009
C	1.040207	-3.780902	12.169048
C	1.946730	-3.021213	12.345761
C	2.671864	-2.355107	11.486680
C	2.445740	-2.876241	10.124634
C	3.026115	-2.242277	9.007789
C	3.509182	-0.921823	9.138164
C	3.392962	-0.267436	10.380827
C	3.149410	-1.037418	11.616156
C	2.791773	-2.774359	7.697043
C	1.716114	-3.669280	7.487821
C	1.269692	-3.904266	6.168467
C	-0.122165	-4.154010	5.934226
C	-1.015917	-4.154719	7.027993
C	-2.335448	-3.682897	6.833347
C	-3.136852	-3.330630	7.968848
C	3.383860	-2.144638	6.579498
C	3.181277	-2.678869	5.287544
C	2.104579	-3.572771	5.078426
C	1.656379	-3.845889	3.744361
C	0.285751	-4.094652	3.513389
C	-0.627837	-4.065129	4.618254
C	-1.948467	-3.595702	4.423246
C	-2.715149	-3.227085	5.551340
C	3.810609	-2.050673	4.162577
C	3.615231	-2.587104	2.874380
C	2.491006	-3.522763	2.656195
C	2.062804	-3.799079	1.271740
C	0.696988	-4.047015	1.041349
C	-0.216590	-4.012320	2.199541
C	-1.596752	-3.521577	1.995342
C	-2.357087	-3.150988	3.122508
C	4.255560	-1.969495	1.697481
C	3.843291	-2.556113	0.605036
C	2.934739	-3.313375	0.428543
C	-1.995385	-3.086123	0.642881

C	-1.086591	-3.439919	-0.226769
C	0.029104	-3.837214	-0.061756
C	-3.264404	-2.074124	3.016760
C	-3.386703	-1.397210	1.786878
C	-2.900900	-2.014000	0.537430
C	-3.638441	-2.135304	5.443672
C	-3.753317	-1.451862	4.212700
C	-3.996779	-0.058133	4.225876
C	-3.752886	0.715043	3.043194
C	-3.641498	0.059676	1.800765
C	-3.399296	0.827875	0.564372
C	-3.212567	0.012431	-0.439286
C	-3.006236	-1.165339	-0.450466
C	-3.270096	2.035807	3.171046
C	-2.688953	2.666478	2.052926
C	-2.915944	2.143389	0.691894
C	-4.118651	0.601274	5.469163
C	-3.627030	1.941818	5.599080
C	-3.038229	2.572590	4.480337
C	-1.965969	3.472449	4.687835
C	-1.122144	3.836809	3.586869
C	-1.566546	3.604735	2.270020
C	-0.725118	3.974801	1.115835
C	-1.280280	3.563056	0.007097
C	-2.188200	2.804904	-0.168409
C	0.250011	4.076610	3.818861
C	1.142574	4.081501	2.728557
C	0.641758	4.215827	1.347355
C	-1.520224	3.709924	6.007138
C	-0.127311	3.954065	6.242421
C	0.768009	3.950799	5.149774
C	2.086051	3.475158	5.346366
C	2.891454	3.124826	4.212940
C	2.521389	3.587526	2.934507
C	3.332969	3.251070	1.749179
C	2.741058	3.679717	0.665961
C	1.626125	4.078614	0.499263
C	3.805887	2.054001	4.320912
C	4.323342	1.471399	3.146607
C	4.244021	2.183815	1.856448
C	2.461993	3.016637	6.628430
C	3.388074	1.927976	6.737936
C	3.901519	1.339304	5.560729
C	4.151607	-0.053523	5.547556
C	4.301777	-0.733143	4.293568
C	4.581245	0.014504	3.132008
C	4.745502	-0.656710	1.827900
C	4.873658	0.232969	0.879818
C	4.665960	1.410353	0.891749
C	3.879180	-0.805671	6.712302
C	3.754309	-0.147442	7.956146
C	3.504007	1.245079	7.969168
C	3.010233	1.865417	9.164301
C	2.100919	2.940460	9.056806
C	1.693696	3.384172	7.755482
C	0.376204	3.860910	7.558967
C	-0.537376	3.897842	8.663456
C	-1.909000	3.655677	8.431592
C	-2.355262	3.379134	7.097413

C	-3.427500	2.479766	6.889841
C	-4.055989	1.852886	8.015870
C	-4.539779	0.532335	7.888080
C	-4.390973	-0.149370	6.634841
C	-4.146085	-1.543221	6.621965
C	-4.046669	-2.255858	7.862823
C	3.132018	1.188795	10.394432
C	2.640788	1.804026	11.642787
C	1.736832	2.877619	11.536001
C	1.341213	3.314865	10.183151
C	-0.035973	3.814857	9.977765
C	-0.950345	3.856109	11.135388
C	-2.317580	3.614993	10.904152
C	-2.745471	3.336335	9.519612
C	-3.866288	2.395434	9.302579
C	-4.504138	1.777055	10.480835
C	-4.982895	0.459589	10.354292
C	-4.815054	-0.213546	9.051593
C	-4.556887	-1.670100	9.038562
C	-4.477695	-2.382067	10.328963
C	2.954899	-0.222705	12.619039
C	2.744089	0.954348	12.630071
C	-0.284000	3.641473	12.238677
C	0.828957	3.236565	12.404584
C	-4.095711	2.368864	11.571932
C	-3.189942	3.129775	11.747290
C	-4.897136	-1.606698	11.293381
C	-5.106432	-0.429408	11.303865
Cl	-0.824076	-0.305086	6.965872
C	0.111494	-0.054614	4.888993
H	1.076934	-0.192182	5.336927
H	-0.305298	0.930876	4.805798
H	-0.436785	-0.899556	4.517996
Cl	1.086847	0.182699	2.817311

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C	-2.498359	-3.367844	12.757494
C	-3.009173	-3.036765	11.486169
C	-2.275604	-3.507267	10.283349
C	-0.902449	-4.005929	10.497724
C	-0.398309	-3.990606	11.894875
C	-1.322579	-3.797620	12.941502
C	0.974677	-3.756790	12.101806
C	1.834371	-3.536258	10.910269
C	1.359301	-3.821164	9.618935
C	-0.011339	-4.056667	9.412471
C	1.444962	-3.327761	13.359167
C	2.414174	-2.526828	13.499435
C	3.126036	-1.978801	12.413192
C	2.966872	-2.602798	11.074303
C	3.545807	-2.017422	9.935393
C	4.038399	-0.701918	9.997762
C	3.946260	0.023460	11.198001
C	3.617269	-0.660628	12.475301
C	3.305891	-2.632565	8.603893
C	2.223401	-3.523068	8.447141
C	1.781295	-3.858896	7.152124

C	0.327694	-4.110858	6.933129
C	-0.551335	-4.003107	8.029143
C	-1.864803	-3.531762	7.824849
C	-2.665283	-3.095674	8.997950
C	3.930366	-2.089834	7.463147
C	3.672162	-2.654789	6.198480
C	2.588942	-3.543953	6.041638
C	2.111645	-3.864004	4.671385
C	0.741386	-4.099411	4.464238
C	-0.184957	-4.026160	5.623511
C	-1.498391	-3.557528	5.419817
C	-2.282775	-3.177159	6.527407
C	4.302217	-2.065951	4.988433
C	4.086306	-2.673231	3.739926
C	2.950608	-3.601829	3.575590
C	2.484318	-3.845484	2.186578
C	1.112050	-4.080645	1.979405
C	0.214168	-4.068613	3.161615
C	-1.160834	-3.574560	2.945862
C	-1.915439	-3.152548	4.053183
C	4.643308	-2.077210	2.498630
C	4.282617	-2.644069	1.259498
C	3.309871	-3.440482	1.118866
C	-1.508426	-3.146913	1.561163
C	-0.635750	-3.504230	0.512796
C	0.543000	-3.923164	0.700425
C	-2.854148	-2.123482	3.908687
C	-3.007122	-1.465503	2.599795
C	-2.428050	-2.091395	1.388099
C	-3.248985	-2.050500	6.367679
C	-3.341073	-1.415604	5.114423
C	-3.544332	-0.019122	5.053509
C	-3.259153	0.708435	3.782450
C	-3.179801	-0.004374	2.572091
C	-2.840065	0.681364	1.299235
C	-2.633228	-0.103739	0.146097
C	-2.445266	-1.354684	0.186187
C	-2.761235	2.022210	3.847776
C	-2.182904	2.612156	2.709922
C	-2.340125	1.994337	1.368400
C	-3.691863	0.709457	6.253084
C	-3.159395	2.101789	6.317786
C	-2.529513	2.640499	5.178461
C	-1.454439	3.539727	5.336382
C	-0.588625	3.842156	4.167584
C	-1.057623	3.553109	2.875872
C	-0.196622	3.779911	1.686740
C	-0.660776	3.348824	0.428060
C	-1.626570	2.544660	0.284686
C	0.779613	4.086391	4.377841
C	1.674062	4.039927	3.295626
C	1.173791	4.023337	1.897313
C	-1.019315	3.882613	6.631160
C	0.432652	4.140820	6.854516
C	1.315372	4.033768	5.762191
C	2.626957	3.559910	5.970824
C	3.431074	3.126304	4.799298
C	3.047177	3.543345	3.513741
C	3.784593	3.076267	2.312014

C	3.277819	3.410376	1.039926
C	2.101629	3.836941	0.853074
C	4.328199	2.054544	4.949403
C	4.835140	1.402466	3.812727
C	4.682525	2.002460	2.462077
C	3.037308	3.198869	7.269299
C	3.990017	2.062323	7.428968
C	4.440638	1.391663	6.274629
C	4.675515	0.002101	6.325344
C	4.800374	-0.752967	5.051573
C	5.079270	-0.052927	3.865457
C	5.144157	-0.763159	2.562108
C	5.291145	0.000514	1.386861
C	5.083163	1.247281	1.341783
C	4.456721	-0.695620	7.529922
C	4.303580	0.027067	8.729941
C	4.067666	1.416591	8.678984
C	3.560251	2.105602	9.894338
C	2.662411	3.177051	9.743585
C	2.253284	3.584762	8.374539
C	0.941401	4.058141	8.165362
C	0.010388	4.137273	9.320177
C	-1.358629	3.896643	9.109463
C	-1.829943	3.568243	7.739194
C	-2.909740	2.674532	7.581449
C	-3.544613	2.091624	8.792180
C	-4.043273	0.778509	8.733415
C	-3.920145	0.018239	7.461343
C	-3.690117	-1.372038	7.519349
C	-3.567119	-2.027559	8.847125
C	3.697217	1.478299	11.144308
C	3.142427	2.103950	12.372630
C	2.242336	3.176308	12.221376
C	1.906620	3.617609	10.843307
C	0.533567	4.114889	10.623806
C	-0.368139	4.127051	11.804108
C	-1.740094	3.890735	11.592853
C	-2.200844	3.638206	10.203227
C	-3.333349	2.705266	10.039058
C	-3.893138	2.114540	11.281800
C	-4.387208	0.797570	11.224020
C	-4.319563	0.082548	9.923276
C	-4.070084	-1.371616	9.982531
C	-3.910697	-1.965623	11.335066
C	3.400004	0.127615	13.623475
C	3.185801	1.373554	13.577206
C	0.197632	3.961831	13.084419
C	1.373353	3.533565	13.272332
C	-3.539669	2.690327	12.519108
C	-2.569643	3.490280	12.659319
C	-4.312938	-1.207998	12.453107
C	-4.528112	0.037607	12.402898
Cl	-0.576433	0.039452	8.402034
C	0.693566	0.005556	5.630115
H	1.541360	0.083780	6.304109
H	0.026392	0.850647	5.758270
H	0.159173	-0.923030	5.800050
Cl	1.320942	0.011595	3.912421

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C	-2.831234	-3.739137	11.841493
C	-3.360298	-3.356817	10.592129
C	-2.639315	-3.770142	9.360821
C	-1.259279	-4.265830	9.537195
C	-0.736911	-4.303042	10.927413
C	-1.649617	-4.165335	11.992504
C	0.635598	-4.059536	11.127021
C	1.477389	-3.780427	9.935137
C	0.988997	-4.018363	8.639326
C	-0.381528	-4.261607	8.440113
C	1.116233	-3.674620	12.394805
C	2.078204	-2.868723	12.555635
C	2.771416	-2.270219	11.484124
C	2.601386	-2.840929	10.123063
C	3.159768	-2.203531	9.002000
C	3.642070	-0.887300	9.112112
C	3.561537	-0.213021	10.342451
C	3.253765	-0.951815	11.594285
C	2.908698	-2.766090	7.649656
C	1.834259	-3.661932	7.470290
C	1.379677	-3.950515	6.168519
C	-0.073733	-4.210389	5.957411
C	-0.939672	-4.155314	7.067143
C	-2.258229	-3.684215	6.898393
C	-3.046742	-3.304117	8.099193
C	3.512906	-2.170805	6.524343
C	3.244747	-2.686868	5.241082
C	2.169835	-3.582087	5.061994
C	1.679433	-3.854434	3.686302
C	0.309848	-4.101534	3.487124
C	-0.603835	-4.079737	4.658784
C	-1.922728	-3.609500	4.489609
C	-2.691442	-3.273726	5.622005
C	3.852284	-2.041730	4.048190
C	3.625690	-2.599574	2.778873
C	2.500581	-3.536781	2.591607
C	2.020688	-3.732773	1.199851
C	0.649437	-3.980718	1.000226
C	-0.233734	-4.029311	2.193704
C	-1.614357	-3.537250	2.016297
C	-2.355679	-3.148305	3.144935
C	4.159893	-1.947599	1.556004
C	3.790294	-2.468920	0.299606
C	2.826729	-3.272887	0.139168
C	-1.975037	-3.042174	0.662915
C	-1.120771	-3.349099	-0.415440
C	0.061830	-3.771839	-0.263472
C	-3.259900	-2.075788	3.052691
C	-3.418374	-1.397470	1.832305
C	-2.881530	-1.969052	0.570463
C	-3.652710	-2.137055	5.523743
C	-3.750764	-1.440118	4.303073
C	-3.992620	-0.050938	4.313374
C	-3.750221	0.731326	3.073405
C	-3.672304	0.057124	1.843133

C	-3.365650	0.795219	0.590783
C	-3.163757	0.056867	-0.592553
C	-2.945558	-1.189082	-0.601708
C	-3.267352	2.047113	3.182508
C	-2.709210	2.683142	2.060824
C	-2.880693	2.112331	0.700174
C	-4.133929	0.620490	5.543833
C	-3.619836	2.016029	5.659903
C	-3.017230	2.611673	4.534015
C	-1.944958	3.510461	4.712227
C	-1.098398	3.863561	3.543065
C	-1.585385	3.622144	2.247542
C	-0.743115	3.898389	1.055592
C	-1.224013	3.513539	-0.211954
C	-2.187151	2.709050	-0.372044
C	0.272159	4.105425	3.742450
C	1.150256	4.105643	2.645727
C	0.629061	4.140903	1.255394
C	-1.490713	3.800932	6.013820
C	-0.036953	4.059175	6.225229
C	0.829474	4.001348	5.115796
C	2.146909	3.527527	5.285509
C	2.936737	3.147192	4.085558
C	2.530067	3.611509	2.823493
C	3.253435	3.199832	1.593249
C	2.724518	3.579671	0.343091
C	1.542271	4.003412	0.190855
C	3.845223	2.078208	4.179213
C	4.342403	1.477706	3.009845
C	4.164427	2.130528	1.686941
C	2.578600	3.116771	6.562163
C	3.539897	1.980586	6.661266
C	3.979670	1.361751	5.474168
C	4.225323	-0.026937	5.464208
C	4.340159	-0.727770	4.158900
C	4.598328	0.022998	2.999195
C	4.650290	-0.632613	1.666767
C	4.774958	0.179813	0.522064
C	4.555981	1.425511	0.531182
C	4.027246	-0.775545	6.641563
C	3.884363	-0.104434	7.872269
C	3.638929	1.284293	7.882192
C	3.146429	1.919674	9.132233
C	2.241964	2.992327	9.039167
C	1.809688	3.453199	7.694076
C	0.492308	3.927341	7.524265
C	-0.421461	3.953341	8.695908
C	-1.791637	3.708484	8.496353
C	-2.280756	3.432812	7.120651
C	-3.353087	2.534305	6.942453
C	-3.960064	1.889958	8.135922
C	-4.444713	0.574405	8.026840
C	-4.333061	-0.127542	6.721469
C	-4.090896	-1.517341	6.711389
C	-3.953158	-2.232971	8.006881
C	3.304835	1.241582	10.352883
C	2.765852	1.812837	11.614131
C	1.860485	2.887394	11.521074
C	1.501352	3.383676	10.167560

C	0.122010	3.880923	9.989668
C	-0.761806	3.835156	11.182994
C	-2.133991	3.590172	10.983055
C	-2.613867	3.392740	9.591097
C	-3.736624	2.451528	9.404523
C	-4.268856	1.798966	10.628274
C	-4.752846	0.481128	10.519367
C	-4.699806	-0.175537	9.187530
C	-4.445013	-1.630338	9.177266
C	-4.266983	-2.283407	10.499978
C	3.047990	-0.213545	12.777143
C	2.828148	1.032260	12.786089
C	-0.174869	3.623167	12.446693
C	1.006329	3.196298	12.598977
C	-3.901591	2.323538	11.884018
C	-2.940088	3.130205	12.043809
C	-4.655124	-1.576886	11.656129
C	-4.874109	-0.330976	11.664867
Cl	-0.837145	-0.303546	6.964643
C	0.116836	-0.055349	4.889166
H	1.085570	-0.193371	5.333969
H	-0.301579	0.931330	4.808475
H	-0.434220	-0.902515	4.523357
Cl	1.079654	0.185587	2.813288

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C	-2.736505	-3.503339	12.438034
C	-3.108743	-3.115848	11.136979
C	-2.306478	-3.508542	10.041512
C	-0.995955	-3.987569	10.282157
C	-0.521639	-4.061570	11.611772
C	-1.438772	-3.977529	12.676258
C	0.847399	-3.821694	11.863089
C	1.698409	-3.514793	10.776741
C	1.285864	-3.803667	9.457902
C	-0.083370	-4.043494	9.206690
C	1.257922	-3.503825	13.171396
C	2.320425	-2.610259	13.366604
C	2.964539	-2.040546	12.252152
C	2.771960	-2.612701	10.973891
C	3.390340	-2.033872	9.844294
C	3.871170	-0.708471	9.932919
C	3.715808	-0.006451	11.147977
C	3.444659	-0.715291	12.340708
C	3.206088	-2.606593	8.567505
C	2.135666	-3.506117	8.371081
C	1.725243	-3.799724	7.053133
C	0.357206	-4.041158	6.802276
C	-0.554177	-3.979279	7.877818
C	-1.860952	-3.501696	7.637931
C	-2.654622	-3.103434	8.734701
C	3.827078	-2.030707	7.438597
C	3.645131	-2.604990	6.162472
C	2.575507	-3.505164	5.966324
C	2.166650	-3.803296	4.648946
C	0.798113	-4.046563	4.397984
C	-0.113566	-3.982067	5.473293

C	-1.420355	-3.504556	5.233331
C	-2.211219	-3.102024	6.330730
C	4.268894	-2.031211	5.034278
C	4.091478	-2.609345	3.758817
C	3.019573	-3.512927	3.562374
C	2.610631	-3.820962	2.244935
C	1.242587	-4.064527	1.994035
C	0.326937	-3.992051	3.068470
C	-0.983466	-3.513270	2.827670
C	-1.772231	-3.107032	3.925752
C	4.724343	-2.036479	2.632286
C	4.518101	-2.605349	1.361612
C	3.457441	-3.500908	1.167260
C	-1.342860	-3.118754	1.518753
C	-0.533208	-3.506380	0.434662
C	0.764053	-3.980889	0.673114
C	-2.671869	-2.030833	3.760028
C	-2.750944	-1.395177	2.502079
C	-2.241182	-2.041972	1.353221
C	-3.113087	-2.028635	6.164805
C	-3.188032	-1.391933	4.907768
C	-3.433960	-0.002587	4.862565
C	-3.153256	0.700475	3.671515
C	-2.996293	-0.001620	2.456951
C	-2.724046	0.706828	1.264470
C	-2.542013	-0.006237	0.064713
C	-2.299771	-1.386142	0.109257
C	-2.673820	2.025990	3.760415
C	-2.055095	2.605073	2.631380
C	-2.245550	2.032345	1.353182
C	-3.597004	0.699365	6.075904
C	-3.115069	2.023347	6.165144
C	-2.491869	2.598952	5.037205
C	-1.422245	3.499063	5.234485
C	-0.572122	3.797915	4.148267
C	-0.983435	3.508799	2.829205
C	-0.132618	3.816919	1.743257
C	-0.541148	3.497907	0.434741
C	-1.601420	2.602176	0.239000
C	0.796685	4.039121	4.399935
C	1.709466	3.984742	3.324515
C	1.235595	4.058715	1.994927
C	-1.012527	3.791078	6.552845
C	0.355491	4.032374	6.804184
C	1.267153	3.973503	5.728800
C	2.574108	3.496454	5.968301
C	3.367338	3.099163	4.870980
C	3.019780	3.505515	3.564621
C	3.821180	3.112044	2.468808
C	3.449555	3.500003	1.167983
C	2.152353	3.975018	0.930263
C	4.268610	2.024315	5.035570
C	4.789871	1.389414	3.887743
C	4.720987	2.036433	2.632993
C	2.924871	3.095398	7.274996
C	3.826636	2.021881	7.439865
C	4.344216	1.385450	6.291639
C	4.590024	-0.004045	6.336143
C	4.750274	-0.706456	5.122711

C	5.035575	-0.003933	3.932159
C	5.204499	-0.711668	2.720404
C	5.461352	0.001838	1.534788
C	5.218636	1.381605	1.490933
C	4.308825	-0.706724	7.527241
C	4.149975	-0.004952	8.741372
C	3.904080	1.384721	8.696774
C	3.388600	2.023103	9.845315
C	2.486693	3.097794	9.680200
C	2.133733	3.495640	8.372868
C	0.826123	3.971182	8.133153
C	-0.085719	4.033665	9.208392
C	-1.454427	3.791335	8.956878
C	-1.863713	3.495637	7.639020
C	-2.935533	2.597904	7.441557
C	-3.561830	2.024447	8.568987
C	-4.045636	0.700034	8.479607
C	-3.883600	-0.003111	7.266162
C	-3.635066	-1.392677	7.311716
C	-3.558542	-2.030614	8.568616
C	3.469365	1.387235	11.103234
C	2.959171	2.033437	12.252489
C	2.057878	3.108233	12.087362
C	1.697157	3.502157	10.778532
C	0.385680	3.978832	10.537924
C	-0.530153	4.050745	11.612332
C	-1.898726	3.808632	11.360812
C	-2.308074	3.501585	10.042980
C	-3.382671	2.601121	9.845180
C	-4.017539	2.029546	10.971323
C	-4.499367	0.705131	10.882528
C	-4.329577	-0.002702	9.670675
C	-4.080881	-1.395755	9.716085
C	-4.011141	-2.042202	10.971442
C	3.264381	-0.002070	13.540771
C	3.020530	1.377702	13.496485
C	-0.050920	3.967270	12.933196
C	1.247338	3.494526	13.171457
C	-3.810624	2.598203	12.242280
C	-2.747402	3.490810	12.437790
C	-4.512049	-1.388133	12.112660
C	-4.757149	-0.008662	12.067999
Cl	-0.548595	0.025315	8.391362
C	0.689726	0.010011	5.636247
H	1.525610	0.085606	6.321499
H	0.029270	0.862358	5.743860
H	0.150841	-0.915950	5.799810
Cl	1.318149	0.000661	3.914223

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C	-3.030336	-3.809231	11.639614
C	-3.437014	-3.376792	10.363311
C	-2.661510	-3.726423	9.234319
C	-1.341785	-4.203316	9.424689
C	-0.833743	-4.320922	10.738649
C	-1.724423	-4.283145	11.827884
C	0.539009	-4.077647	10.965044

C	1.360862	-3.724409	9.870380
C	0.917463	-3.967040	8.552150
C	-0.455582	-4.210591	8.325797
C	0.979011	-3.804115	12.273786
C	2.040860	-2.911369	12.476117
C	2.656192	-2.298456	11.368394
C	2.434596	-2.824018	10.074873
C	3.024168	-2.201479	8.953181
C	3.506657	-0.879796	9.079720
C	3.380124	-0.223294	10.323204
C	3.136489	-0.976201	11.494649
C	2.809884	-2.726246	7.660619
C	1.737917	-3.622123	7.456754
C	1.297070	-3.868473	6.139111
C	-0.074615	-4.113260	5.913095
C	-0.959661	-4.101532	7.012119
C	-2.276370	-3.628917	6.821961
C	-3.044453	-3.276145	7.952188
C	3.403699	-2.107824	6.539561
C	3.191967	-2.633822	5.247357
C	2.119138	-3.528640	5.043629
C	1.679489	-3.779689	3.726397
C	0.307238	-4.026657	3.500160
C	-0.578375	-4.011481	4.598941
C	-1.895493	-3.540094	4.408539
C	-2.661380	-3.184091	5.539254
C	3.789814	-2.017694	4.127093
C	3.579752	-2.546169	2.835172
C	2.503780	-3.443239	2.630975
C	2.064057	-3.704446	1.313401
C	0.692422	-3.951845	1.087060
C	-0.197049	-3.928781	2.185383
C	-1.517936	-3.456700	1.994151
C	-2.282630	-3.098128	3.125375
C	4.187012	-1.932129	1.716307
C	3.948254	-2.452081	0.430289
C	2.883101	-3.340805	0.228113
C	-1.913096	-3.018720	0.709625
C	-1.127446	-3.359625	-0.407387
C	0.180406	-3.827258	-0.218000
C	-3.190572	-2.021170	3.021857
C	-3.302264	-1.339597	1.790659
C	-2.821375	-1.942547	0.606044
C	-3.569924	-2.108590	5.435720
C	-3.676987	-1.425733	4.205400
C	-3.920199	-0.035225	4.218303
C	-3.669770	0.711443	3.047115
C	-3.546747	0.054775	1.803573
C	-3.304347	0.806719	0.631403
C	-3.156534	0.138499	-0.598451
C	-2.914049	-1.242034	-0.611190
C	-3.185787	2.032461	3.172202
C	-2.595923	2.652576	2.049505
C	-2.819813	2.127117	0.756546
C	-4.048170	0.621251	5.460856
C	-3.563409	1.941132	5.585852
C	-2.971187	2.559145	4.463774
C	-1.900237	3.456682	4.665898
C	-1.078333	3.796979	3.570160

C	-1.520645	3.550777	2.252469
C	-0.697923	3.899664	1.157330
C	-1.138431	3.626061	-0.151121
C	-2.203659	2.737258	-0.352181
C	0.294856	4.038760	3.796533
C	1.181545	4.026926	2.698197
C	0.674741	4.141159	1.383750
C	-1.459704	3.705751	5.983157
C	-0.087739	3.948966	6.209375
C	0.797926	3.933313	5.110799
C	2.113801	3.459111	5.302474
C	2.884091	3.106236	4.173733
C	2.501725	3.553249	2.890564
C	3.280143	3.205369	1.763247
C	2.873260	3.633558	0.485651
C	1.565963	4.102424	0.295106
C	3.796219	2.032833	4.279353
C	4.294938	1.442367	3.097873
C	4.193468	2.133591	1.868931
C	2.497065	3.015131	6.585915
C	3.405718	1.940148	6.691081
C	3.899549	1.348068	5.509071
C	4.145702	-0.041972	5.496470
C	4.278817	-0.698604	4.254348
C	4.540774	0.047964	3.085022
C	4.677766	-0.614209	1.843623
C	4.910568	0.142583	0.680073
C	4.667467	1.522887	0.692840
C	3.888769	-0.788326	6.666390
C	3.758065	-0.132439	7.909088
C	3.512110	1.257662	7.921685
C	3.023477	1.852940	9.104498
C	2.116302	2.930780	8.999650
C	1.730564	3.372364	7.715785
C	0.414987	3.847503	7.524068
C	-0.470854	3.867976	8.622657
C	-1.843650	3.623319	8.396085
C	-2.281958	3.367870	7.079117
C	-3.352548	2.469997	6.877005
C	-3.948911	1.854852	7.998483
C	-4.433206	0.533606	7.873666
C	-4.303800	-0.124425	6.631620
C	-4.060427	-1.515335	6.618822
C	-3.953176	-2.199422	7.848855
C	3.133695	1.171145	10.335868
C	2.650432	1.774176	11.519632
C	1.744958	2.853146	11.415093
C	1.352059	3.292834	10.130229
C	0.032960	3.770814	9.937948
C	-0.857149	3.798591	11.035887
C	-2.229677	3.554195	10.809246
C	-2.668984	3.289852	9.491841
C	-3.742018	2.388225	9.289200
C	-4.346402	1.773453	10.409469
C	-4.827939	0.451538	10.285281
C	-4.690007	-0.212029	9.044631
C	-4.444905	-1.606586	9.032021
C	-4.343513	-2.298618	10.260574
C	2.984087	-0.307923	12.724062

C	2.740177	1.072585	12.736601
C	-0.345827	3.671805	12.341129
C	0.959583	3.197317	12.531374
C	-4.110515	2.297855	11.694266
C	-3.048830	3.191223	11.894801
C	-4.812372	-1.685679	11.437707
C	-5.055648	-0.305126	11.450088
Cl	-0.840508	-0.303475	6.965096
C	0.118166	-0.055317	4.888640
H	1.087175	-0.193558	5.332915
H	-0.300410	0.931444	4.808971
H	-0.433251	-0.903077	4.524730
Cl	1.077942	0.186119	2.812545

Table S5. Cartesian coordinates (Ångstroms) for the preliminary intermediate **I** and transition state **TS** computed at the M06-2X/UFF level for the chloride exchange S_N2 reaction occurring inside various (6,6) CNTs of different lengths.

CNT 12,4 Å Intermediate **I**

138			
C	-2.498359	-3.367844	12.757494
C	-3.009173	-3.036765	11.486169
C	-2.275604	-3.507267	10.283349
C	-0.902449	-4.005929	10.497724
C	-0.398309	-3.990606	11.894875
C	-1.322579	-3.797620	12.941502
C	0.974677	-3.756790	12.101806
C	1.834371	-3.536258	10.910269
C	1.359301	-3.821164	9.618935
C	-0.011339	-4.056667	9.412471
C	1.444962	-3.327761	13.359167
C	2.414174	-2.526828	13.499435
C	3.126036	-1.978801	12.413192
C	2.966872	-2.602798	11.074303
C	3.545807	-2.017422	9.935393
C	4.038399	-0.701918	9.997762
C	3.946260	0.023460	11.198001
C	3.617269	-0.660628	12.475301
C	3.305891	-2.632565	8.603893
C	2.223401	-3.523068	8.447141
C	1.781295	-3.858896	7.152124
C	0.327694	-4.110858	6.933129
C	-0.551335	-4.003107	8.029143
C	-1.864803	-3.531762	7.824849
C	-2.665283	-3.095674	8.997950
C	3.930366	-2.089834	7.463147
C	3.672162	-2.654789	6.198480
C	2.588942	-3.543953	6.041638
C	2.111645	-3.864004	4.671385
C	0.741386	-4.099411	4.464238
C	-0.184957	-4.026160	5.623511
C	-1.498391	-3.557528	5.419817
C	-2.282775	-3.177159	6.527407

C	4.302217	-2.065951	4.988433
C	4.086306	-2.673231	3.739926
C	2.950608	-3.601829	3.575590
C	2.484318	-3.845484	2.186578
C	1.112050	-4.080645	1.979405
C	0.214168	-4.068613	3.161615
C	-1.160834	-3.574560	2.945862
C	-1.915439	-3.152548	4.053183
C	4.643308	-2.077210	2.498630
C	4.282617	-2.644069	1.259498
C	3.309871	-3.440482	1.118866
C	-1.508426	-3.146913	1.561163
C	-0.635750	-3.504230	0.512796
C	0.543000	-3.923164	0.700425
C	-2.854148	-2.123482	3.908687
C	-3.007122	-1.465503	2.599795
C	-2.428050	-2.091395	1.388099
C	-3.248985	-2.050500	6.367679
C	-3.341073	-1.415604	5.114423
C	-3.544332	-0.019122	5.053509
C	-3.259153	0.708435	3.782450
C	-3.179801	-0.004374	2.572091
C	-2.840065	0.681364	1.299235
C	-2.633228	-0.103739	0.146097
C	-2.445266	-1.354684	0.186187
C	-2.761235	2.022210	3.847776
C	-2.182904	2.612156	2.709922
C	-2.340125	1.994337	1.368400
C	-3.691863	0.709457	6.253084
C	-3.159395	2.101789	6.317786
C	-2.529513	2.640499	5.178461
C	-1.454439	3.539727	5.336382
C	-0.588625	3.842156	4.167584
C	-1.057623	3.553109	2.875872
C	-0.196622	3.779911	1.686740
C	-0.660776	3.348824	0.428060
C	-1.626570	2.544660	0.284686
C	0.779613	4.086391	4.377841
C	1.674062	4.039927	3.295626
C	1.173791	4.023337	1.897313
C	-1.019315	3.882613	6.631160
C	0.432652	4.140820	6.854516
C	1.315372	4.033768	5.762191
C	2.626957	3.559910	5.970824
C	3.431074	3.126304	4.799298
C	3.047177	3.543345	3.513741
C	3.784593	3.076267	2.312014
C	3.277819	3.410376	1.039926
C	2.101629	3.836941	0.853074
C	4.328199	2.054544	4.949403
C	4.835140	1.402466	3.812727
C	4.682525	2.002460	2.462077
C	3.037308	3.198869	7.269299
C	3.990017	2.062323	7.428968
C	4.440638	1.391663	6.274629
C	4.675515	0.002101	6.325344
C	4.800374	-0.752967	5.051573
C	5.079270	-0.052927	3.865457
C	5.144157	-0.763159	2.562108

C	5.291145	0.000514	1.386861
C	5.083163	1.247281	1.341783
C	4.456721	-0.695620	7.529922
C	4.303580	0.027067	8.729941
C	4.067666	1.416591	8.678984
C	3.560251	2.105602	9.894338
C	2.662411	3.177051	9.743585
C	2.253284	3.584762	8.374539
C	0.941401	4.058141	8.165362
C	0.010388	4.137273	9.320177
C	-1.358629	3.896643	9.109463
C	-1.829943	3.568243	7.739194
C	-2.909740	2.674532	7.581449
C	-3.544613	2.091624	8.792180
C	-4.043273	0.778509	8.733415
C	-3.920145	0.018239	7.461343
C	-3.690117	-1.372038	7.519349
C	-3.567119	-2.027559	8.847125
C	3.697217	1.478299	11.144308
C	3.142427	2.103950	12.372630
C	2.242336	3.176308	12.221376
C	1.906620	3.617609	10.843307
C	0.533567	4.114889	10.623806
C	-0.368139	4.127051	11.804108
C	-1.740094	3.890735	11.592853
C	-2.200844	3.638206	10.203227
C	-3.333349	2.705266	10.039058
C	-3.893138	2.114540	11.281800
C	-4.387208	0.797570	11.224020
C	-4.319563	0.082548	9.923276
C	-4.070084	-1.371616	9.982531
C	-3.910697	-1.965623	11.335066
C	3.400004	0.127615	13.623475
C	3.185801	1.373554	13.577206
C	0.197632	3.961831	13.084419
C	1.373353	3.533565	13.272332
C	-3.539669	2.690327	12.519108
C	-2.569643	3.490280	12.659319
C	-4.312938	-1.207998	12.453107
C	-4.528112	0.037607	12.402898
Cl	-0.576433	0.039452	8.402034
C	0.693566	0.005556	5.630115
H	1.541360	0.083780	6.304109
H	0.026392	0.850647	5.758270
H	0.159173	-0.923030	5.800050
Cl	1.320942	0.011595	3.912421

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C	-2.831234	-3.739137	11.841493
C	-3.360298	-3.356817	10.592129
C	-2.639315	-3.770142	9.360821
C	-1.259279	-4.265830	9.537195
C	-0.736911	-4.303042	10.927413
C	-1.649617	-4.165335	11.992504
C	0.635598	-4.059536	11.127021
C	1.477389	-3.780427	9.935137
C	0.988997	-4.018363	8.639326

C	-0.381528	-4.261607	8.440113
C	1.116233	-3.674620	12.394805
C	2.078204	-2.868723	12.555635
C	2.771416	-2.270219	11.484124
C	2.601386	-2.840929	10.123063
C	3.159768	-2.203531	9.002000
C	3.642070	-0.887300	9.112112
C	3.561537	-0.213021	10.342451
C	3.253765	-0.951815	11.594285
C	2.908698	-2.766090	7.649656
C	1.834259	-3.661932	7.470290
C	1.379677	-3.950515	6.168519
C	-0.073733	-4.210389	5.957411
C	-0.939672	-4.155314	7.067143
C	-2.258229	-3.684215	6.898393
C	-3.046742	-3.304117	8.099193
C	3.512906	-2.170805	6.524343
C	3.244747	-2.686868	5.241082
C	2.169835	-3.582087	5.061994
C	1.679433	-3.854434	3.686302
C	0.309848	-4.101534	3.487124
C	-0.603835	-4.079737	4.658784
C	-1.922728	-3.609500	4.489609
C	-2.691442	-3.273726	5.622005
C	3.852284	-2.041730	4.048190
C	3.625690	-2.599574	2.778873
C	2.500581	-3.536781	2.591607
C	2.020688	-3.732773	1.199851
C	0.649437	-3.980718	1.000226
C	-0.233734	-4.029311	2.193704
C	-1.614357	-3.537250	2.016297
C	-2.355679	-3.148305	3.144935
C	4.159893	-1.947599	1.556004
C	3.790294	-2.468920	0.299606
C	2.826729	-3.272887	0.139168
C	-1.975037	-3.042174	0.662915
C	-1.120771	-3.349099	-0.415440
C	0.061830	-3.771839	-0.263472
C	-3.259900	-2.075788	3.052691
C	-3.418374	-1.397470	1.832305
C	-2.881530	-1.969052	0.570463
C	-3.652710	-2.137055	5.523743
C	-3.750764	-1.440118	4.303073
C	-3.992620	-0.050938	4.313374
C	-3.750221	0.731326	3.073405
C	-3.672304	0.057124	1.843133
C	-3.365650	0.795219	0.590783
C	-3.163757	0.056867	-0.592553
C	-2.945558	-1.189082	-0.601708
C	-3.267352	2.047113	3.182508
C	-2.709210	2.683142	2.060824
C	-2.880693	2.112331	0.700174
C	-4.133929	0.620490	5.543833
C	-3.619836	2.016029	5.659903
C	-3.017230	2.611673	4.534015
C	-1.944958	3.510461	4.712227
C	-1.098398	3.863561	3.543065
C	-1.585385	3.622144	2.247542
C	-0.743115	3.898389	1.055592

C	-1.224013	3.513539	-0.211954
C	-2.187151	2.709050	-0.372044
C	0.272159	4.105425	3.742450
C	1.150256	4.105643	2.645727
C	0.629061	4.140903	1.255394
C	-1.490713	3.800932	6.013820
C	-0.036953	4.059175	6.225229
C	0.829474	4.001348	5.115796
C	2.146909	3.527527	5.285509
C	2.936737	3.147192	4.085558
C	2.530067	3.611509	2.823493
C	3.253435	3.199832	1.593249
C	2.724518	3.579671	0.343091
C	1.542271	4.003412	0.190855
C	3.845223	2.078208	4.179213
C	4.342403	1.477706	3.009845
C	4.164427	2.130528	1.686941
C	2.578600	3.116771	6.562163
C	3.539897	1.980586	6.661266
C	3.979670	1.361751	5.474168
C	4.225323	-0.026937	5.464208
C	4.340159	-0.727770	4.158900
C	4.598328	0.022998	2.999195
C	4.650290	-0.632613	1.666767
C	4.774958	0.179813	0.522064
C	4.555981	1.425511	0.531182
C	4.027246	-0.775545	6.641563
C	3.884363	-0.104434	7.872269
C	3.638929	1.284293	7.882192
C	3.146429	1.919674	9.132233
C	2.241964	2.992327	9.039167
C	1.809688	3.453199	7.694076
C	0.492308	3.927341	7.524265
C	-0.421461	3.953341	8.695908
C	-1.791637	3.708484	8.496353
C	-2.280756	3.432812	7.120651
C	-3.353087	2.534305	6.942453
C	-3.960064	1.889958	8.135922
C	-4.444713	0.574405	8.026840
C	-4.333061	-0.127542	6.721469
C	-4.090896	-1.517341	6.711389
C	-3.953158	-2.232971	8.006881
C	3.304835	1.241582	10.352883
C	2.765852	1.812837	11.614131
C	1.860485	2.887394	11.521074
C	1.501352	3.383676	10.167560
C	0.122010	3.880923	9.989668
C	-0.761806	3.835156	11.182994
C	-2.133991	3.590172	10.983055
C	-2.613867	3.392740	9.591097
C	-3.736624	2.451528	9.404523
C	-4.268856	1.798966	10.628274
C	-4.752846	0.481128	10.519367
C	-4.699806	-0.175537	9.187530
C	-4.445013	-1.630338	9.177266
C	-4.266983	-2.283407	10.499978
C	3.047990	-0.213545	12.777143
C	2.828148	1.032260	12.786089
C	-0.174869	3.623167	12.446693

C	1.006329	3.196298	12.598977
C	-3.901591	2.323538	11.884018
C	-2.940088	3.130205	12.043809
C	-4.655124	-1.576886	11.656129
C	-4.874109	-0.330976	11.664867
Cl	-0.837145	-0.303546	6.964643
C	0.116836	-0.055349	4.889166
H	1.085570	-0.193371	5.333969
H	-0.301579	0.931330	4.808475
H	-0.434220	-0.902515	4.523357
Cl	1.079654	0.185587	2.813288

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C	0.830534	6.152071	2.074378
C	0.437940	7.136231	2.979752
C	0.405905	6.859565	4.356073
C	-0.592259	7.449321	5.170666
C	-1.544328	8.308203	4.598080
C	-2.851266	8.330981	5.081792
C	-3.227169	7.495121	6.145720
C	-4.532901	6.946190	6.183995
C	-5.445109	7.240760	5.157832
C	-6.363978	6.280748	4.737705
C	-6.385188	5.011027	5.337142
C	-6.694896	3.868781	4.557988
C	-6.977840	4.012171	3.190019
C	-6.585065	3.028149	2.284515
C	-5.903304	1.885295	2.732804
C	-4.904664	1.295425	1.918871
C	-4.602346	1.855485	0.667133
C	-3.295244	1.832092	0.183952
C	-2.269397	1.248431	0.944808
C	-0.963530	1.796965	0.906533
C	-0.701405	2.922108	0.108306
C	0.217125	3.882592	0.528039
C	0.888025	3.732998	1.752575
C	1.197138	4.875760	2.531103
C	1.481943	4.706156	3.908916
C	1.082079	5.708091	4.830667
C	1.051254	5.397555	6.208040
C	0.055432	5.985571	7.020355
C	-0.877848	6.866211	6.430212
C	-2.208575	6.888980	6.922432
C	-2.559355	6.029844	7.987052
C	-3.861520	5.481854	8.024831
C	-4.772598	5.810415	6.996912
C	-5.708617	4.833292	6.569577
C	-5.700531	3.562195	7.185409
C	-6.010758	2.423043	6.408814
C	-6.317523	2.590868	5.040445
C	-5.917387	1.589162	4.118560
C	-5.225109	0.455381	4.598026
C	-4.228273	-0.132033	3.786633
C	-3.956213	0.431228	2.520340
C	-2.625332	0.407734	2.028626
C	-1.613094	-0.177806	2.820608
C	-0.310487	0.369003	2.782146

C	-0.060973	1.485146	1.953640
C	0.874638	2.462738	2.380624
C	1.527703	2.289381	3.620929
C	1.836442	3.429149	4.397326
C	2.143844	3.264300	5.766516
C	1.745114	4.262916	6.685186
C	1.713582	3.954153	8.063533
C	0.716896	4.542568	8.876277
C	-0.218263	5.422306	8.286705
C	-1.544682	5.444147	8.776643
C	-1.897181	4.585042	9.841252
C	-3.199910	4.035868	9.878412
C	-4.112073	4.363000	8.850539
C	-5.045528	3.389550	8.425241
C	-5.039493	2.117507	9.040593
C	-5.352156	0.977538	8.264264
C	-5.657999	1.144124	6.895009
C	-5.258891	0.146088	5.976303
C	-4.566056	-0.988497	6.454395
C	-3.567326	-1.574836	5.642990
C	-3.293212	-1.011488	4.376642
C	-1.966852	-1.034566	3.886770
C	-0.953167	-1.620115	4.677522
C	0.350632	-1.073650	4.638470
C	0.601715	0.043483	3.810873
C	1.534928	1.017404	4.235994
C	2.189484	0.845391	5.476375
C	2.498734	1.986138	6.253403
C	2.805241	1.820850	7.622741
C	2.407102	2.819807	8.541272
C	2.375133	2.511278	9.919597
C	1.378946	3.100316	10.732465
C	0.443759	3.979882	10.142896
C	-0.883022	4.000910	10.632175
C	-1.235825	3.141947	11.696545
C	-2.538442	2.591930	11.732974
C	-3.450486	2.917887	10.704857
C	-4.384922	1.944596	10.280326
C	-4.380120	0.672913	10.896084
C	-4.695304	-0.467785	10.120519
C	-5.002060	-0.301888	8.751242
C	-4.601794	-1.299832	7.832076
C	-3.908185	-2.434615	8.309275
C	-2.908166	-3.019802	7.497835
C	-2.633078	-2.454806	6.232742
C	-1.306623	-2.477520	5.743052
C	-0.293048	-3.063747	6.532923
C	1.010836	-2.517270	6.494138
C	1.262559	-1.400152	5.666744
C	2.195805	-0.426311	6.092076
C	2.848556	-0.597983	7.333136
C	3.157970	0.542506	8.109948
C	3.465393	0.377329	9.478980
C	3.068292	1.376698	10.397435
C	3.036706	1.068361	11.775855
C	2.040389	1.657394	12.588568
C	1.105420	2.537284	11.998838
C	-0.221507	2.558052	12.487657
C	-0.574116	1.698861	13.551735

C	-1.876098	1.148310	13.587390
C	-2.788565	1.474053	12.559197
C	-3.722732	0.500359	12.134740
C	-3.714905	-0.771263	12.749778
C	-4.028911	-1.911651	11.974660
C	-4.340845	-1.746769	10.606476
C	-3.942027	-2.745388	9.686998
C	-3.246424	-3.879562	10.164030
C	-2.247977	-4.465909	9.351721
C	-1.973559	-3.900538	8.086672
C	-0.646608	-3.922294	7.597458
C	0.367274	-4.508475	8.387497
C	1.670816	-3.960998	8.349806
C	1.922383	-2.843686	7.522718
C	2.855186	-1.869668	7.948542
C	3.508586	-2.041569	9.189338
C	3.818627	-0.901029	9.966093
C	4.126376	-1.066193	11.335208
C	3.729669	-0.066479	12.253801
C	3.697417	-0.375299	13.632353
C	2.701303	0.214195	14.445167
C	1.766847	1.094631	13.855222
C	0.439915	1.115719	14.343937
C	0.087035	0.256931	15.408823
C	-1.215077	-0.293537	15.444391
C	-2.125774	0.030873	14.414038
C	-3.057836	-0.943387	13.988614
C	-3.050453	-2.214348	14.604859
C	-3.362291	-3.354612	13.829321
C	-3.672972	-3.189526	12.460912
C	-3.276743	-4.188562	11.542152
C	-2.582563	-5.322988	12.019735
C	-1.586030	-5.910922	11.206768
C	-1.312733	-5.346445	9.940771
C	0.014121	-5.367974	9.451494
C	1.028172	-5.953889	10.242117
C	2.331355	-5.405371	10.205331
C	2.582523	-4.287582	9.378432
C	3.515261	-3.313418	9.804619
C	4.168158	-3.485469	11.045837
C	4.478446	-2.344932	11.822668
C	4.786074	-2.509699	13.191943
C	4.390078	-1.510545	14.109861
C	4.358982	-1.820441	15.487586
C	3.359965	-1.228509	16.303266
C	2.427191	-0.347916	15.712304
C	1.101234	-0.325993	16.201178
C	0.749816	-1.184484	17.266295
C	-0.557068	-1.736397	17.302453
C	-1.466496	-1.410555	16.272100
C	-2.397294	-2.384952	15.846162
C	-2.389181	-3.655247	16.463258
C	-2.700824	-4.799762	15.684407
C	-3.010010	-4.633177	14.316309
C	-2.614447	-5.631940	13.398186
C	-1.922023	-6.765955	13.877170
C	-0.922835	-7.356793	13.061036
C	-0.651155	-6.792290	11.795111
C	0.674632	-6.814044	11.305845

C	1.687091	-7.400275	12.097259
C	2.994296	-6.849174	12.060916
C	3.243367	-5.731563	11.234044
C	4.174790	-4.757734	11.660534
C	4.826958	-4.931495	12.901234
C	5.138113	-3.787239	13.680741
C	5.469689	-3.947533	15.049224
C	5.073049	-2.945692	15.969464
C	5.012130	-3.241372	17.340937
C	4.031187	-2.659732	18.142183
C	3.095619	-1.773309	17.584579
C	1.766393	-1.750803	18.075053
C	1.391069	-2.614441	19.116838
C	0.107448	-3.156399	19.152451
C	-0.821396	-2.843398	18.146822
C	-1.754282	-3.820655	17.719404
C	-1.745140	-5.097932	18.302867
C	-2.050588	-6.222113	17.537610
C	-2.370162	-6.086716	16.176860
C	-1.973477	-7.088255	15.256296
C	-1.262663	-8.211410	15.709264
C	-0.281759	-8.792292	14.907459
C	0.003955	-8.259054	13.640141
C	1.332966	-8.281295	13.149263
C	2.357839	-8.837171	13.931995
C	3.641592	-8.295636	13.896485
C	3.921040	-7.189655	13.077548
C	4.854121	-6.212965	13.505691
C	5.494255	-6.355074	14.747478
C	5.799621	-5.231238	15.513189
C	-0.930269	0.272531	8.742099
H	-0.253652	-0.554215	8.561385
H	-0.534861	0.935924	9.508538
H	-1.897414	-0.113392	9.035104
Cl	-1.020859	1.339438	7.254897
Cl	-0.770309	-1.493306	11.136237

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C	5.141650	0.994224	0.186072
C	4.912471	2.355376	0.378959
C	4.487629	2.831375	1.629868
C	3.592834	3.927661	1.700373
C	3.134479	4.532779	0.518959
C	1.837740	5.038448	0.446047
C	0.979022	4.946813	1.553362
C	-0.408589	4.740411	1.354292
C	-0.918545	4.628536	0.050628
C	-1.985408	3.771998	-0.215446
C	-2.559316	3.013957	0.817969
C	-3.050495	1.712353	0.548793
C	-2.960901	1.186244	-0.750128
C	-2.731217	-0.174975	-0.942571
C	-2.587301	-1.031632	0.160838
C	-1.691809	-2.127524	0.090787
C	-0.952926	-2.352305	-1.082005
C	0.343690	-2.858300	-1.009309
C	0.921862	-3.147563	0.237311

C	2.309579	-2.941613	0.435760
C	3.099984	-2.448256	-0.614860
C	4.166449	-1.591240	-0.348987
C	4.459180	-1.214139	0.971635
C	4.949569	0.087520	1.241027
C	4.848464	0.595565	2.560051
C	4.615479	1.981167	2.756410
C	4.180403	2.428993	4.023093
C	3.288698	3.522592	4.093501
C	2.858786	4.133519	2.894845
C	1.538681	4.648095	2.820627
C	0.695487	4.533039	3.947602
C	-0.688354	4.327238	3.749071
C	-1.185770	4.243044	2.429793
C	-2.272161	3.371379	2.158910
C	-2.823086	2.615373	3.216928
C	-3.313319	1.317430	2.948465
C	-3.236865	0.815916	1.630395
C	-3.002593	-0.569829	1.434573
C	-2.852502	-1.404808	2.563759
C	-1.958580	-2.497139	2.494142
C	-1.243557	-2.721153	1.297065
C	0.076353	-3.236581	1.371036
C	0.634527	-3.509861	2.639450
C	2.018594	-3.305782	2.837145
C	2.800866	-2.833129	1.760566
C	3.886169	-1.960437	2.031250
C	4.150200	-1.591595	3.368726
C	4.637864	-0.293164	3.637345
C	4.560283	0.210121	4.955109
C	4.329278	1.591034	5.150858
C	3.896925	2.041903	6.417862
C	3.004809	3.136986	6.488480
C	2.571592	3.746957	5.289670
C	1.255691	4.258784	5.215555
C	0.411204	4.144395	6.341952
C	-0.973693	3.938323	6.143188
C	-1.472687	3.853092	4.824059
C	-2.555980	2.985235	4.554131
C	-3.108746	2.228639	5.611327
C	-3.599726	0.929982	5.342690
C	-3.522700	0.426602	4.024843
C	-3.288374	-0.954236	3.829839
C	-3.137459	-1.790649	4.958372
C	-2.241910	-2.882935	4.888962
C	-1.525209	-3.107362	3.692618
C	-0.209947	-3.621361	3.766370
C	0.350202	-3.896484	5.034287
C	1.736153	-3.695561	5.231742
C	2.518654	-3.220407	4.155953
C	3.599717	-2.350325	4.425720
C	3.866807	-1.981537	5.763167
C	4.352182	-0.680592	6.031921
C	4.277801	-0.177551	7.349971
C	4.048485	1.204984	7.546240
C	3.616045	1.657029	8.813323
C	2.722939	2.752958	8.884025
C	2.289161	3.362949	7.685179
C	0.971369	3.872089	7.610286

C	0.125792	3.757052	8.735965
C	-1.259379	3.551088	8.537103
C	-1.758317	3.465666	7.218305
C	-2.842336	2.598479	6.948483
C	-3.395457	1.841976	8.005443
C	-3.886560	0.543237	7.736843
C	-3.809763	0.039675	6.419150
C	-3.574551	-1.341096	6.224181
C	-3.423116	-2.177439	7.352404
C	-2.527010	-3.269407	7.282972
C	-1.809406	-3.493596	6.087210
C	-0.494129	-4.008555	6.160961
C	0.065506	-4.285024	7.428383
C	1.452577	-4.086778	7.626138
C	2.238442	-3.614786	6.550330
C	3.321025	-2.743857	6.820372
C	3.586006	-2.371764	8.157965
C	4.070024	-1.068986	8.426392
C	3.991990	-0.564933	9.744077
C	3.761461	0.817157	9.940344
C	3.324437	1.266586	11.206514
C	2.431829	2.361205	11.277078
C	2.002122	2.974189	10.079232
C	0.684878	3.484396	10.004132
C	-0.161363	3.370547	11.130009
C	-1.546601	3.165321	10.931231
C	-2.044899	3.079229	9.612255
C	-3.129060	2.211932	9.342549
C	-3.682274	1.455367	10.399637
C	-4.172997	0.156313	10.131040
C	-4.096104	-0.347215	8.813279
C	-3.860690	-1.728048	8.618156
C	-3.709976	-2.564751	9.746219
C	-2.814280	-3.657140	9.676557
C	-2.095558	-3.880640	8.480894
C	-0.780293	-4.395681	8.554875
C	-0.221988	-4.671064	9.822664
C	1.163704	-4.469227	10.021205
C	1.950710	-3.999358	8.945464
C	3.033122	-3.129067	9.215364
C	3.295668	-2.756011	10.552641
C	3.782378	-1.455449	10.820758
C	3.705866	-0.951982	12.138711
C	3.473170	0.429115	12.334421
C	3.037464	0.879121	13.601029
C	2.144040	1.973199	13.671339
C	1.713326	2.585037	12.472962
C	0.397343	3.097826	12.398449
C	-0.448543	2.984274	13.524709
C	-1.833853	2.779188	13.325922
C	-2.332375	2.693620	12.006637
C	-3.416182	1.825581	11.736882
C	-3.968532	1.068271	12.794220
C	-4.458961	-0.230998	12.525565
C	-4.382679	-0.734321	11.207492
C	-4.147799	-2.115444	11.012142
C	-3.997225	-2.952282	12.140474
C	-3.102192	-4.045340	12.070653
C	-2.383685	-4.269118	10.874583

C	-1.068179	-4.783415	10.948883
C	-0.509843	-5.057874	12.217243
C	0.875469	-4.854058	12.416104
C	1.661321	-4.382518	11.340433
C	2.743509	-3.513046	11.610202
C	3.008146	-3.141887	12.947599
C	3.496968	-1.842265	13.215853
C	3.421311	-1.338274	14.533823
C	3.188106	0.041927	14.729159
C	2.752739	0.490256	15.995857
C	1.855727	1.587604	16.066167
C	1.425979	2.198141	14.867318
C	0.111016	2.711041	14.793015
C	-0.732888	2.597284	15.919911
C	-2.122763	2.391568	15.720478
C	-2.619719	2.306811	14.401108
C	-3.702301	1.438929	14.131458
C	-4.253542	0.682879	15.189520
C	-4.745462	-0.620680	14.919933
C	-4.668853	-1.122133	13.601773
C	-4.434848	-2.502363	13.406443
C	-4.285517	-3.337838	14.535326
C	-3.387986	-4.434855	14.465229
C	-2.671113	-4.657675	13.268713
C	-1.356333	-5.171080	13.343139
C	-0.799444	-5.444947	14.611810
C	0.590418	-5.239695	14.811413
C	1.374286	-4.768157	13.735173
C	2.456232	-3.899769	14.004805
C	2.720582	-3.530637	15.342216
C	3.211996	-2.226958	15.611504
C	3.159553	-1.723865	16.935332
C	2.925618	-0.340161	17.131065
C	2.468404	0.122035	18.375792
C	1.587215	1.199651	18.444755
C	1.149275	1.832292	17.270071
C	-0.169004	2.346527	17.195619
C	-1.031274	2.220954	18.296849
C	-2.396318	2.018917	18.100978
C	-2.920756	1.939212	16.800753
C	-4.005858	1.068954	16.530368
C	-4.551416	0.290324	17.563875
C	-5.034559	-0.989932	17.299077
C	-4.979836	-1.511875	15.996547
C	-4.745737	-2.895631	15.800659
C	-4.570034	-3.738536	16.909964
C	-3.688683	-4.816051	16.841105
C	-2.968922	-5.067818	15.661857
C	-1.650673	-5.582070	15.736563
C	-1.070150	-5.836996	16.989527
C	0.294871	-5.635066	17.185585
C	1.101016	-5.175122	16.131738
C	2.185980	-4.304782	16.402074
C	2.449980	-3.906616	17.722548
C	2.932997	-2.626331	17.987077
C	0.482727	-0.264009	7.703473
H	0.962186	-1.203396	7.506732
H	1.062692	0.593080	7.991056
H	-0.584962	-0.185833	7.601492

C1	0.788394	0.316134	5.425260
C1	0.266919	-0.863368	9.983819

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270			
C	9.158233	-0.063658	-8.291133
C	8.844402	1.272256	-8.534347
C	8.012409	1.976442	-7.649041
C	7.117456	2.954104	-8.149980
C	7.066877	3.213385	-9.529168
C	5.857184	3.541785	-10.138447
C	4.678983	3.616474	-9.378134
C	3.444798	3.218466	-9.949265
C	3.405828	2.750892	-11.272768
C	2.511494	1.745908	-11.636946
C	1.641855	1.192197	-10.683470
C	1.299951	-0.180998	-10.754451
C	1.831783	-0.981215	-11.778477
C	2.145497	-2.317082	-11.535003
C	1.932487	-2.873857	-10.263595
C	2.827824	-3.851561	-9.763468
C	3.923878	-4.258082	-10.541532
C	5.134015	-4.586613	-9.933229
C	5.267191	-4.514119	-8.537218
C	6.501490	-4.116028	-7.966468
C	7.585624	-3.795991	-8.799603
C	8.479626	-2.791004	-8.434695
C	8.303821	-2.089759	-7.230854
C	8.645204	-0.716476	-7.158662
C	8.095960	0.069658	-6.115321
C	7.776307	1.429917	-6.363003
C	6.929742	2.109599	-5.459530
C	6.037263	3.085233	-5.959132
C	6.019341	3.349910	-7.346438
C	4.787723	3.684698	-7.966846
C	3.617738	3.744083	-7.178009
C	2.386424	3.347554	-7.747847
C	2.363865	2.903949	-9.088501
C	1.453428	1.880388	-9.459123
C	0.597868	1.335937	-8.475902
C	0.257829	-0.034249	-8.546113
C	0.783389	-0.816761	-9.598007
C	1.102827	-2.176993	-9.350098
C	0.885857	-2.706780	-8.058905
C	1.778485	-3.682749	-7.560286
C	2.860321	-4.097321	-8.368220
C	4.092441	-4.432157	-7.748866
C	4.198997	-4.341451	-6.343454
C	5.430323	-3.944502	-5.774004
C	6.516475	-3.651030	-6.627877
C	7.426601	-2.627527	-6.256382
C	7.218428	-1.933020	-5.044244
C	7.558250	-0.562823	-4.972635
C	7.031865	0.221425	-3.921668
C	6.712934	1.577299	-4.168672
C	5.866064	2.258855	-3.265853
C	4.972884	3.235534	-3.765890
C	4.953414	3.501171	-5.153672

C	3.725979	3.835886	-5.772187
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CNT 39,1 Å Intermediate I

414

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CNT 39,1 Å Transition state TS

414			
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C	3.518525	-2.250185	23.204970
C	3.911993	-1.692270	24.441904
C	4.395153	-0.363050	24.473806
C	4.444988	0.320117	25.709633
C	4.201450	1.713662	25.734795
C	3.887279	2.333541	26.965113

C	2.977985	3.417648	26.976028
C	2.410485	3.849732	25.756232
C	1.079839	4.330639	25.749625
C	0.356440	4.366114	26.963069
C	-1.036096	4.115762	26.941082
C	-1.663771	3.836645	25.706381
C	-2.744881	2.924269	25.675463
C	-3.167261	2.318346	26.879998
C	-3.650240	0.988620	26.848435
C	-3.696939	0.304009	25.613263
C	-3.452732	-1.089499	25.589314
C	-3.167515	-1.757234	26.801236
C	-2.258158	-2.841272	26.791084
C	-1.661454	-3.225440	25.569159
C	-0.331015	-3.706786	25.575313
C	0.363189	-3.790090	26.803210
C	1.755693	-3.539745	26.824075
C	2.412386	-3.212872	25.616451
C	3.493053	-2.300093	25.646678
C	3.886486	-1.742002	26.883776
C	4.369436	-0.412327	26.915775
C	4.417812	0.271149	28.151604
C	4.172706	1.664593	28.176671
C	3.857744	2.284290	29.406904
C	2.947803	3.367943	29.417747
C	2.380193	3.799970	28.197996
C	1.049633	4.281560	28.191438
C	0.326336	4.317331	29.404865
C	-1.066449	4.068098	29.382913
C	-1.694605	3.789829	28.148173
C	-2.776191	2.877846	28.117143
C	-3.198329	2.271598	29.321715
C	-3.680967	0.941710	29.290075
C	-3.727498	0.257196	28.054796
C	-3.482228	-1.136261	28.030891
C	-3.196436	-1.803911	29.242839
C	-2.286480	-2.887558	29.232730
C	-1.689652	-3.271619	28.010880
C	-0.359151	-3.753301	28.017065
C	0.334971	-3.836974	29.244937
C	1.727756	-3.587703	29.265867
C	2.385049	-3.261532	28.058250
C	3.466529	-2.349443	28.088577
C	3.859555	-1.791120	29.325752
C	4.342174	-0.461267	29.357768
C	4.389750	0.222390	30.593557
C	4.143602	1.615664	30.618504
C	3.828122	2.235246	31.848677
C	2.917763	3.318458	31.859443
C	2.350056	3.750340	30.639689
C	1.019608	4.232295	30.633179
C	0.296438	4.268336	31.846635
C	-1.096423	4.019954	31.824754
C	-1.724972	3.742329	30.590020
C	-2.806942	2.830813	30.558961
C	-3.228832	2.224343	31.763552
C	-3.711201	0.894455	31.731841
C	-3.757679	0.210075	30.496468
C	-3.511520	-1.183237	30.472518

C	-3.225246	-1.850811	31.684476
C	-2.314880	-2.934037	31.674354
C	-1.717950	-3.317936	30.452512
C	-0.387494	-3.799872	30.458744
C	0.306482	-3.883856	31.686662
C	1.699346	-3.635427	31.707692
C	2.357092	-3.309828	30.500114
C	3.439039	-2.398288	30.530540
C	3.831740	-1.839800	31.767748
C	4.314095	-0.509940	31.799747
C	4.360815	0.173818	33.035492
C	4.113975	1.566790	33.060330
C	3.797618	2.185789	34.290593
C	2.887123	3.268431	34.301292
C	2.319908	3.700597	33.081388
C	0.989692	4.182692	33.074913
C	0.266801	4.218249	34.288544
C	-1.125825	3.970546	34.266736
C	-1.754746	3.694090	33.031896
C	-2.836900	2.783080	33.000847
C	-3.257927	2.176279	34.205589
C	-3.740024	0.846676	34.173829
C	-3.787125	0.162689	32.938246
C	-3.540306	-1.230323	32.914225
C	-3.253162	-1.897346	34.126356
C	-2.342662	-2.980009	34.116208
C	-1.746225	-3.364166	32.894178
C	-0.415987	-3.846221	32.900455
C	0.277703	-3.929765	34.128593
C	1.670332	-3.682014	34.149704
C	2.328462	-3.357536	32.942012
C	3.410611	-2.446522	32.972515
C	3.802430	-1.887739	34.209866
C	4.284516	-0.558159	34.241837
C	4.331293	0.125924	35.477354
C	4.084164	1.517435	35.502096
C	3.769010	2.134882	36.732688
C	2.855370	3.220678	36.743374
C	2.289276	3.651038	35.523067
C	0.960405	4.132774	35.516619
C	0.239590	4.169041	36.730683
C	-1.157487	3.921031	36.708852
C	-1.784548	3.645080	35.473710
C	-2.865903	2.735285	35.442702
C	-3.286321	2.130431	36.647839
C	-3.769828	0.796633	36.615944
C	-3.816002	0.114577	35.380021
C	-3.568895	-1.276971	35.355965
C	-3.282944	-1.942466	36.568486
C	-2.369299	-3.028288	36.558280
C	-1.773997	-3.410615	35.335874
C	-0.445103	-3.892319	35.342174
C	0.246523	-3.976601	36.570692
C	1.643604	-3.728546	36.591920
C	2.299860	-3.404544	35.383874
C	3.381213	-2.494743	35.414394
C	3.772429	-1.937928	36.652046
C	4.255927	-0.604149	36.684100
C	4.326758	0.080048	37.923099

C	4.078558	1.474801	37.947871
C	3.738961	2.102473	39.157228
C	2.841551	3.168700	39.167697
C	2.269510	3.624325	37.968958
C	0.937481	4.107304	37.962500
C	0.196131	4.127991	39.154879
C	-1.175952	3.884652	39.133457
C	-1.828545	3.616613	37.919326
C	-2.912742	2.704957	37.888241
C	-3.329321	2.074432	39.071763
C	-3.804115	0.764529	39.040425
C	-3.869915	0.064295	37.825055
C	-3.621736	-1.330499	37.800922
C	-3.310825	-2.005408	38.992425
C	-2.413410	-3.071660	38.982387
C	-1.812675	-3.480073	37.780663
C	-0.480617	-3.963022	37.786986
C	0.232092	-4.030897	38.994958
C	1.604182	-3.787515	39.015823
C	2.285424	-3.472253	37.829065
C	3.369608	-2.560577	37.859668
C	3.757505	-1.977241	39.076645
C	4.232288	-0.667352	39.108115
C	0.538386	0.310734	19.746823
H	1.074702	-0.619323	19.611431
H	1.129207	1.197401	20.010070
H	-0.499067	0.351453	19.408440
Cl	0.992492	0.921619	17.209745
Cl	0.231928	-0.085987	21.872694

Table S6. Cartesian coordinates (Ångstroms) for the preliminary intermediate **I** and transition state **TS** computed at the M06-2X/UFF level for the chloride exchange S_N2 reaction occurring inside various CNTs of different radius.

CNT Chirality (4,4) Intermediate **I**

182			
C	1.245743	-3.691964	0.285078
C	1.245398	-2.335663	-0.044333
C	1.103121	-1.377236	0.974965
C	0.101814	-0.373331	0.842887
C	-0.714050	-0.371348	-0.302658
C	-2.101656	-0.336140	-0.156123
C	-2.659504	-0.303288	1.134494
C	-3.660054	-1.256580	1.477988
C	-4.059782	-2.201267	0.515916
C	-4.059493	-3.557562	0.845342
C	-3.659419	-3.955655	2.133543
C	-2.658209	-4.959601	2.265400
C	-2.100218	-5.521749	1.103282
C	-0.712673	-5.556745	0.956690
C	0.103015	-5.029332	1.973718
C	1.103826	-4.076277	1.630495
C	1.485124	-3.138041	2.625382

C	1.484756	-1.754653	2.289351
C	1.348003	-0.817776	3.339322
C	0.351255	0.181854	3.207667
C	-0.439306	0.174599	2.035522
C	-1.854638	0.210564	2.185005
C	-2.381736	0.251216	3.496395
C	-3.377665	-0.698084	3.838408
C	-3.777329	-1.621350	2.845064
C	-3.777027	-3.004749	3.181101
C	-3.377017	-3.369589	4.487388
C	-2.380435	-4.369303	4.618802
C	-1.853180	-4.934061	3.434576
C	-0.437903	-4.969718	3.285023
C	0.352479	-4.438278	4.330001
C	1.348705	-3.489196	3.988283
C	1.753477	-2.564260	4.979725
C	1.753170	-1.184905	4.644528
C	1.610814	-0.246854	5.694138
C	0.613514	0.754075	5.561842
C	-0.178157	0.752204	4.389290
C	-1.589398	0.787972	4.538578
C	-2.117438	0.822842	5.851014
C	-3.114284	-0.127350	6.193163
C	-3.519324	-1.051427	5.201285
C	-3.519002	-2.430837	5.536499
C	-3.113538	-2.796910	6.842073
C	-2.116122	-3.797516	6.973899
C	-1.587928	-4.367917	5.791245
C	-0.176739	-4.403550	5.641928
C	0.614694	-3.866973	6.684870
C	1.611357	-2.916393	6.343013
C	2.015258	-1.992264	7.335116
C	2.015197	-0.612709	6.999542
C	1.882905	0.329220	8.046825
C	0.881368	1.337829	7.912081
C	0.085418	1.324791	6.743112
C	-1.325983	1.359205	6.893563
C	-1.856630	1.402934	8.204769
C	-2.861925	0.448475	8.547892
C	-3.256184	-0.479459	7.555692
C	-3.255547	-1.859114	7.891322
C	-2.860352	-2.227652	9.199257
C	-1.855185	-3.233519	9.332465
C	-1.324484	-3.795582	8.146656
C	0.086919	-3.832825	7.996807
C	0.882735	-3.307805	9.041755
C	1.883012	-2.348280	8.698402
C	2.330838	-1.432513	9.682900
C	2.331647	-0.031499	9.341444
C	2.267453	0.952093	10.364033
C	1.204862	2.042882	10.213412
C	0.361270	1.956215	9.075186
C	-1.071368	1.983505	9.232011
C	-1.641441	2.087155	10.527676
C	-2.735608	1.075943	10.891244
C	-3.056994	0.104255	9.908190
C	-3.054987	-1.296606	10.249586
C	-2.729797	-1.705210	11.569353
C	-1.639802	-2.776656	11.711747

C	-1.069847	-3.279265	10.512196
C	0.363384	-3.325811	10.359712
C	1.207311	-2.879521	11.410872
C	2.264276	-1.834227	11.043644
C	2.674206	-0.908897	12.031737
C	2.685123	0.589175	11.665040
C	2.602172	1.576160	12.684271
C	1.542026	2.717247	12.525769
C	0.690577	2.657869	11.379681
C	-0.844658	2.634542	11.562148
C	-1.406870	2.687280	12.861528
C	-2.559197	1.705119	13.230044
C	-2.930151	0.734800	12.252133
C	-2.917889	-0.771421	12.618844
C	-2.537319	-1.175905	13.929997
C	-1.402213	-2.233382	14.060420
C	-0.842591	-2.791408	12.883024
C	0.694558	-2.894744	12.730569
C	1.546552	-2.416495	13.775343
C	2.584790	-1.311513	13.389073
C	2.961535	-0.344195	14.360813
C	2.970380	1.161657	13.994040
C	2.804113	2.097980	15.044185
C	1.734997	3.188560	14.901553
C	0.954677	3.235072	13.719222
C	-0.587253	3.222305	13.889473
C	-1.119140	3.235304	15.203489
C	-2.211829	2.222771	15.577516
C	-2.682370	1.311200	14.596957
C	-2.670238	-0.201121	14.963113
C	-2.203033	-0.560096	16.253171
C	-1.113150	-1.633227	16.388971
C	-0.583049	-2.235478	15.220145
C	0.959827	-2.328782	15.075673
C	1.736550	-1.731968	16.100425
C	2.799577	-0.693361	15.723450
C	3.117094	0.282275	16.704251
C	3.118383	1.681406	16.364007
C	2.934385	2.612567	17.415415
C	1.932716	3.619120	17.283452
C	1.150245	3.662330	16.104175
C	-0.281346	3.690249	16.254666
C	-0.803772	3.685170	17.571604
C	-1.807608	2.733154	17.917183
C	-2.258961	1.818762	16.935194
C	-2.255556	0.420910	17.274498
C	-1.804745	0.059759	18.567041
C	-0.800793	-0.944218	18.698011
C	-0.277588	-1.553619	17.531512
C	1.152923	-1.598734	17.385529
C	1.935136	-1.017984	18.412162
C	2.935119	-0.062198	18.066131
C	3.331999	0.865259	19.058035
C	3.331341	2.244320	18.722638
C	3.189482	3.182140	19.772426
C	2.191808	4.182239	19.640893
C	1.400876	4.180178	18.468073
C	-0.010214	4.215268	18.616529
C	-0.538374	4.251852	19.928765

C	-1.535436	3.302631	20.271550
C	-1.940272	2.378820	19.280260
C	-1.939092	0.999618	19.615463
C	-1.533971	0.633995	20.920317
C	-0.536326	-0.366070	21.051784
C	-0.007781	-0.935590	19.869656
C	1.403338	-0.972651	19.721869
C	2.194016	-0.435759	20.764183
C	3.190891	0.513780	20.421375
C	3.596389	1.438501	21.412457
C	3.595596	2.815809	21.077537
C	3.450945	3.749867	22.129092
C	2.449789	4.753194	21.997004
C	1.662648	4.753191	20.822472
C	0.253453	4.789406	20.971019
C	-0.270531	4.822843	22.283997
C	-1.270804	3.870000	22.627552
C	-1.677922	2.949934	21.634446
C	-1.677230	1.572485	21.969273
C	-1.269699	1.210955	23.273914
C	-0.268768	0.207334	23.406081
C	0.255479	-0.365169	22.224386
C	1.664761	-0.400893	22.075846
C	2.451702	0.138455	23.119087
C	3.452247	1.091070	22.775563
C	3.883301	2.008127	23.769793
C	3.882589	3.391783	23.433371
C	3.716948	4.341537	24.457242
C	2.735368	5.325252	24.327727
C	1.929272	5.349514	23.175582
C	0.513631	5.385902	23.324899
C	-0.034644	5.396012	24.619991
C	-1.015386	4.461776	24.956746
C	-1.438101	3.526866	23.995013
C	-1.437595	2.143121	24.331354
C	-1.014574	1.754034	25.614916
C	-0.033186	0.770035	25.744522
C	0.515445	0.185029	24.589261
C	1.931179	0.149355	24.439882
C	2.737113	0.700165	25.452201
C	3.718117	1.634158	25.115472
C	0.091012	0.319402	13.808149
H	0.350775	-0.588686	13.417712
H	0.435989	0.843709	12.991605
H	-0.840646	0.258142	13.400906
Cl	0.290947	0.730910	15.471721
Cl	-0.239727	-0.404898	10.885891

CNT Chirality (4,4) Transition state TS

182			
C	2.377034	-2.323196	0.195815
C	2.184424	-0.959247	-0.029005
C	1.851503	-0.121328	1.050376
C	0.714492	0.728564	0.938226
C	-0.040067	0.703505	-0.248400
C	-1.421394	0.516096	-0.178806
C	-2.034485	0.356304	1.076709
C	-2.890913	-0.761393	1.289081

C	-3.097608	-1.671276	0.236868
C	-2.905137	-3.035225	0.462070
C	-2.507171	-3.475579	1.737108
C	-1.370074	-4.325452	1.849206
C	-0.680570	-4.697907	0.681378
C	0.700752	-4.510433	0.611394
C	1.378896	-3.953066	1.710144
C	2.235475	-2.835495	1.497836
C	2.423602	-1.937384	2.581185
C	2.227187	-0.546182	2.351927
C	1.901430	0.268702	3.460746
C	0.769502	1.114830	3.349062
C	0.042550	1.086821	2.136433
C	-1.366360	0.895616	2.207358
C	-1.951268	0.746463	3.485741
C	-2.803879	-0.366364	3.697124
C	-3.012382	-1.252554	2.615536
C	-2.816171	-2.643752	2.845299
C	-2.423959	-3.052649	4.140901
C	-1.292006	-3.898743	4.252508
C	-0.631504	-4.276704	3.060706
C	0.777391	-4.085388	2.989260
C	1.428781	-3.530310	4.114586
C	2.281573	-2.417630	3.903289
C	2.495178	-1.528934	4.983556
C	2.299058	-0.141793	4.755339
C	1.967512	0.673073	5.864090
C	0.834599	1.520004	5.752230
C	0.106093	1.497507	4.538931
C	-1.298746	1.307096	4.609192
C	-1.884336	1.152567	5.887592
C	-2.737994	0.038683	6.098880
C	-2.951108	-0.849463	5.018761
C	-2.755129	-2.236458	5.248341
C	-2.357131	-2.645352	6.543628
C	-1.224185	-3.492273	6.655347
C	-0.562134	-3.875721	5.464602
C	0.842670	-3.685355	5.392955
C	1.494815	-3.125447	6.516503
C	2.348179	-2.011356	6.305324
C	2.563037	-1.124288	7.386129
C	2.365912	0.264070	7.158530
C	2.047311	1.086074	8.266272
C	0.904083	1.940743	8.153299
C	0.172355	1.903927	6.941878
C	-1.233850	1.714120	7.011154
C	-1.828446	1.573271	8.286764
C	-2.692034	0.450779	8.498709
C	-2.887617	-0.442560	7.420037
C	-2.689452	-1.830495	7.651205
C	-2.303800	-2.245193	8.948803
C	-1.159797	-3.100642	9.061628
C	-0.495323	-3.470831	7.867614
C	0.911173	-3.282379	7.794871
C	1.573091	-2.737781	8.919818
C	2.431743	-1.611572	8.707654
C	2.702377	-0.725052	9.781934
C	2.502326	0.689925	9.550788
C	2.231499	1.555733	10.645807

C	1.001029	2.475110	10.524246
C	0.239566	2.381489	9.327091
C	-1.193210	2.187577	9.396671
C	-1.835689	2.089449	10.660574
C	-2.768646	0.896269	10.884215
C	-2.902865	-0.030602	9.815197
C	-2.693597	-1.443065	10.053424
C	-2.339368	-1.890747	11.355119
C	-1.114803	-2.808167	11.476046
C	-0.426970	-3.138419	10.277061
C	1.006673	-2.953897	10.201256
C	1.718220	-2.459288	11.327803
C	2.625608	-1.246634	11.102073
C	2.856662	-0.365767	12.182051
C	2.660953	1.145656	11.935412
C	2.312081	1.974185	13.034074
C	1.075920	2.897890	12.911820
C	0.329203	2.887947	11.704880
C	-1.196590	2.666102	11.780590
C	-1.836614	2.535603	13.046372
C	-2.833617	1.357725	13.270117
C	-2.958019	0.423025	12.202612
C	-2.682076	-1.068796	12.455573
C	-2.288683	-1.499142	13.744414
C	-1.058052	-2.426978	13.867416
C	-0.376316	-2.798897	12.684136
C	1.153889	-2.654511	12.609552
C	1.875021	-2.164305	13.736579
C	2.746008	-0.893205	13.500450
C	2.911030	0.026186	14.569804
C	2.689136	1.528797	14.322808
C	2.345800	2.347895	15.425884
C	1.121235	3.263378	15.304778
C	0.385173	3.251956	14.094789
C	-1.139980	3.057740	14.168740
C	-1.721382	2.890206	15.447329
C	-2.664626	1.705920	15.678631
C	-2.947684	0.828423	14.600721
C	-2.649994	-0.676446	14.841774
C	-2.210844	-1.084775	16.127551
C	-0.984177	-2.003793	16.249709
C	-0.312497	-2.429868	15.074670
C	1.234004	-2.299368	15.015169
C	1.856134	-1.674438	16.126320
C	2.753108	-0.455864	15.890009
C	2.874317	0.473483	16.958848
C	2.670112	1.881379	16.725543
C	2.293034	2.683792	17.830649
C	1.153041	3.536094	17.717910
C	0.423806	3.560846	16.503393
C	-1.003583	3.372884	16.575317
C	-1.575065	3.180439	17.856354
C	-2.436511	2.063957	18.070534
C	-2.699300	1.179836	16.996175
C	-2.476198	-0.224110	17.221884
C	-2.032673	-0.623151	18.507367
C	-0.893597	-1.475046	18.620366
C	-0.229074	-1.905047	17.444884
C	1.198682	-1.734698	17.382331

C	1.833477	-1.128059	18.493205
C	2.687116	-0.005755	18.277975
C	2.887732	0.887344	19.357156
C	2.684428	2.273343	19.126588
C	2.352656	3.089006	20.233883
C	1.219819	3.935835	20.121853
C	0.490791	3.913229	18.909638
C	-0.915209	3.730122	18.981015
C	-1.499553	3.577366	20.260160
C	-2.353365	2.464271	20.472492
C	-2.567567	1.577314	19.391863
C	-2.360806	0.191208	19.617422
C	-1.962979	-0.218275	20.911956
C	-0.830339	-1.064949	21.024146
C	-0.167263	-1.448675	19.834736
C	1.239165	-1.268256	19.768745
C	1.889210	-0.706856	20.892357
C	2.741801	0.407125	20.679747
C	2.953475	1.297586	21.758698
C	2.753243	2.681848	21.528511
C	2.420242	3.493499	22.637345
C	1.283549	4.343061	22.524932
C	0.558232	4.322505	21.311409
C	-0.845227	4.136882	21.382936
C	-1.425273	3.981320	22.662912
C	-2.281353	2.863961	22.875687
C	-2.498064	1.980071	21.793705
C	-2.297663	0.595290	22.020664
C	-1.898469	0.190404	23.315246
C	-0.761846	-0.659086	23.427757
C	-0.102754	-1.045253	22.237946
C	1.300846	-0.859342	22.169691
C	1.947120	-0.296443	23.294114
C	2.803407	0.820741	23.081264
C	3.042381	1.706619	24.164516
C	2.843994	3.097657	23.933290
C	2.489529	3.924140	25.014534
C	1.375024	4.757044	24.904317
C	0.626173	4.755185	23.713935
C	-0.783369	4.565956	23.786064
C	-1.382830	4.384682	25.045325
C	-2.222124	3.289093	25.253889
C	-2.453718	2.385784	24.201092
C	-2.255717	0.994292	24.429753
C	-1.836507	0.566081	25.702018
C	-0.722030	-0.266793	25.812314
C	-0.037999	-0.663139	24.649231
C	1.371544	-0.473165	24.579633
C	2.035944	0.106680	25.675222
C	2.875649	1.201944	25.466623
C	0.031832	0.249442	13.214831
H	0.406683	-0.487253	13.790875
H	0.378005	0.575910	12.277840
H	-0.824312	0.482865	13.695673
Cl	0.074412	0.628413	15.706657
Cl	-0.082807	-0.258454	10.593646

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C	2.032147	-4.986241	0.883485
C	1.640956	-3.723454	0.440198
C	1.350359	-2.711509	1.370612
C	0.230969	-1.865501	1.155929
C	-0.568998	-2.052974	0.016229
C	-1.957121	-1.970194	0.117921
C	-2.555253	-1.699322	1.360043
C	-3.723207	-2.409508	1.742651
C	-4.262711	-3.372737	0.873580
C	-4.730167	-4.584669	1.380457
C	-4.661404	-4.841915	2.759981
C	-4.263281	-6.127284	3.212006
C	-3.944870	-7.122694	2.272924
C	-2.845353	-7.953782	2.484011
C	-2.056345	-7.795408	3.635682
C	-0.643153	-7.879800	3.531503
C	-0.054990	-8.119812	2.278286
C	1.092295	-7.422341	1.901906
C	1.659586	-6.479936	2.776099
C	2.135549	-5.246027	2.260339
C	2.239793	-4.142353	3.144656
C	1.840889	-2.855958	2.693154
C	1.552125	-1.860963	3.653899
C	0.436346	-1.017786	3.439953
C	-0.339988	-1.207603	2.274858
C	-1.754163	-1.123018	2.378370
C	-2.325261	-0.852487	3.642106
C	-3.489701	-1.559836	4.023191
C	-4.029615	-2.506315	3.123692
C	-4.505807	-3.740994	3.640040
C	-4.419495	-3.970600	5.031331
C	-4.021769	-5.251455	5.481795
C	-3.729683	-6.244932	4.520481
C	-2.609405	-7.091479	4.735469
C	-1.833956	-6.904579	5.901575
C	-0.425466	-6.989549	5.797854
C	0.143853	-7.256328	4.532697
C	1.312857	-6.546072	4.149339
C	1.857242	-5.602823	5.049402
C	2.331224	-4.372838	4.535516
C	2.461089	-3.274043	5.415658
C	2.062897	-1.991581	4.965572
C	1.771393	-0.995566	5.925653
C	0.654216	-0.151323	5.711393
C	-0.123990	-0.338898	4.546215
C	-1.533976	-0.254313	4.649464
C	-2.107195	0.014229	5.913809
C	-3.273764	-0.693092	6.294901
C	-3.816352	-1.640226	5.396187
C	-4.291311	-2.871242	5.910834
C	-4.203990	-3.103282	7.302401
C	-3.803809	-4.385171	7.753299
C	-3.511031	-5.381267	6.793509
C	-2.393796	-6.225031	7.007715
C	-1.615271	-6.037716	8.172700
C	-0.205079	-6.124960	8.069159

C	0.366886	-6.392454	6.804641
C	1.532753	-5.684699	6.422609
C	2.077796	-4.739211	7.321319
C	2.551169	-3.507106	6.807149
C	2.679673	-2.408612	7.688041
C	2.281596	-1.125938	7.237591
C	1.989843	-0.129735	8.197168
C	0.872963	0.715022	7.982516
C	0.094269	0.527354	6.817938
C	-1.315988	0.611407	6.921894
C	-1.888828	0.878589	8.186799
C	-3.056868	0.172848	8.567286
C	-3.600799	-0.772995	7.667960
C	-4.077025	-2.003947	8.182229
C	-3.989932	-2.236152	9.573579
C	-3.584906	-3.516706	10.023824
C	-3.291823	-4.513232	9.064556
C	-2.173747	-5.356444	9.278394
C	-1.394168	-5.168096	10.442201
C	0.015650	-5.260885	10.340029
C	0.587703	-5.529202	9.076261
C	1.753976	-4.821470	8.694558
C	2.297969	-3.875514	9.593374
C	2.768357	-2.641947	9.079673
C	2.895264	-1.543498	9.960841
C	2.500230	-0.259518	9.508919
C	2.213011	0.740905	10.465823
C	1.096409	1.588598	10.249767
C	0.313966	1.395317	9.088263
C	-1.097201	1.475824	9.194551
C	-1.670091	1.742875	10.459482
C	-2.841822	1.038693	10.839873
C	-3.386405	0.093729	9.940093
C	-3.866700	-1.136653	10.453825
C	-3.784257	-1.369950	11.845913
C	-3.368362	-2.649012	12.294474
C	-3.070389	-3.642609	11.333877
C	-1.950598	-4.483990	11.546541
C	-1.171501	-4.299899	12.710999
C	0.238402	-4.404581	12.612896
C	0.809840	-4.669199	11.348148
C	1.975688	-3.960347	10.966917
C	2.518928	-3.015252	11.866674
C	2.983675	-1.777738	11.352588
C	3.107783	-0.678838	12.233112
C	2.723103	0.610420	11.777784
C	2.444382	1.618262	12.730481
C	1.326874	2.474195	12.511560
C	0.538105	2.271862	11.354308
C	-0.876445	2.340171	11.466104
C	-1.450306	2.604996	12.730496
C	-2.627506	1.903322	13.111089
C	-3.174932	0.959065	12.212901
C	-3.667277	-0.270324	12.727215
C	-3.594693	-0.506799	14.121642
C	-3.162441	-1.789231	14.568556
C	-2.851911	-2.776119	13.604122
C	-1.728140	-3.618380	13.815949
C	-0.951888	-3.451920	14.986908

C	0.464971	-3.574829	14.896226
C	1.035975	-3.824538	13.625498
C	2.199334	-3.106398	13.241977
C	2.743290	-2.161237	14.141000
C	3.196753	-0.915879	13.624262
C	3.327324	0.183654	14.502162
C	2.947120	1.477221	14.046770
C	2.653639	2.473655	15.005999
C	1.537598	3.326435	14.789019
C	0.759654	3.148424	13.620976
C	-0.658176	3.210213	13.733046
C	-1.233613	3.473681	14.997609
C	-2.407938	2.769756	15.379757
C	-2.967504	1.828823	14.482673
C	-3.466905	0.598253	15.000686
C	-3.353036	0.359266	16.390674
C	-2.930822	-0.922938	16.835722
C	-2.636959	-1.918393	15.876159
C	-1.511894	-2.765269	16.089212
C	-0.732842	-2.585753	17.255830
C	0.681816	-2.697483	17.164741
C	1.266795	-2.986908	15.908295
C	2.430570	-2.259045	15.519155
C	2.960756	-1.296077	16.411544
C	3.418524	-0.053651	15.893096
C	3.546823	1.046654	16.772364
C	3.155650	2.333917	16.320890
C	2.862885	3.328698	17.281358
C	1.748079	4.176647	17.066130
C	0.971633	3.995579	15.898918
C	-0.441183	4.072736	16.004155
C	-1.014009	4.338497	17.269088
C	-2.181396	3.632031	17.651300
C	-2.731575	2.688674	16.753235
C	-3.211338	1.457777	17.269312
C	-3.110713	1.222245	18.659194
C	-2.703948	-0.059286	19.105770
C	-2.410199	-1.052205	18.143956
C	-1.292423	-1.898955	18.358240
C	-0.517347	-1.716971	19.526168
C	0.892929	-1.812107	19.429174
C	1.471069	-2.090329	18.169272
C	2.634846	-1.375924	17.784855
C	3.170539	-0.421157	18.680125
C	3.636830	0.813445	18.163718
C	3.766276	1.912373	19.043984
C	3.370574	3.195799	18.593733
C	3.079893	4.191858	19.553885
C	1.964879	5.038187	19.339182
C	1.187396	4.853202	18.173185
C	-0.222804	4.936858	18.276511
C	-0.795140	5.204400	19.541339
C	-1.960363	4.496242	19.923549
C	-2.505295	3.550964	19.024867
C	-2.979262	2.319541	19.539644
C	-2.886709	2.085270	20.930343
C	-2.486616	0.802923	21.378754
C	-2.193437	-0.191143	20.417209
C	-1.077921	-1.037098	20.631965

C	-0.302190	-0.853014	21.799502
C	1.107616	-0.941024	21.699103
C	1.682352	-1.211931	20.436288
C	2.846269	-0.501407	20.053624
C	3.386436	0.447987	20.951108
C	3.856917	1.680157	20.435602
C	3.986411	2.779238	21.315524
C	3.589860	4.060561	20.865669
C	3.299076	5.054174	21.827206
C	2.180106	5.902398	21.612073
C	1.405022	5.717102	20.445437
C	-0.003362	5.802104	20.548614
C	-0.572757	6.068256	21.814097
C	-1.741000	5.356952	22.197467
C	-2.284625	4.413804	21.297059
C	-2.757276	3.183284	21.810765
C	-2.665626	2.951880	23.201313
C	-2.266855	1.665163	23.652109
C	-1.977381	0.670847	22.690777
C	-0.863034	-0.173848	22.905517
C	-0.087835	0.014572	24.071732
C	1.326368	-0.070876	23.969426
C	1.898146	-0.342005	22.706258
C	3.061365	0.366907	22.324489
C	3.600225	1.314197	23.223566
C	4.074457	2.549421	22.706858
C	4.230448	3.650155	23.587145
C	3.832484	4.935689	23.135655
C	3.514632	5.930894	24.075134
C	2.415976	6.763095	23.864099
C	1.627288	6.606166	22.712002
C	0.214157	6.691253	22.815773
C	-0.373944	6.930265	24.069236
C	-1.520581	6.231790	24.445533
C	-2.087279	5.289573	23.570913
C	-2.562142	4.054997	24.086151
C	-2.459291	3.794435	25.462890
C	-2.068716	2.531253	25.905722
C	-1.777751	1.519651	24.975013
C	-0.659208	0.672719	25.190363
C	0.140175	0.859840	26.330548
C	1.528360	0.777047	26.229532
C	2.126979	0.506056	24.987688
C	3.294412	1.217030	24.604790
C	3.833511	2.180549	25.473674
C	4.300042	3.392730	24.966623
C	-0.072461	-0.042829	14.674658
H	0.315618	-1.032704	14.611248
H	-1.088190	-0.066660	14.390930
H	0.401521	0.571647	13.944040
Cl	0.088167	0.596020	16.352940
Cl	-0.418327	-1.216259	11.730701

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C	1.724417	-2.950820	-0.190568
C	1.355874	-1.623274	-0.404973
C	1.074153	-0.787470	0.688674

C	-0.030861	0.101086	0.622474
C	-0.825537	0.131456	-0.535815
C	-2.213012	0.216547	-0.426947
C	-2.815758	0.271827	0.840992
C	-3.996605	-0.476712	1.086476
C	-4.544173	-1.261777	0.057895
C	-5.033472	-2.536736	0.339587
C	-4.978785	-3.035688	1.651886
C	-4.603820	-4.387211	1.870612
C	-4.293486	-5.205324	0.771364
C	-3.208071	-6.078113	0.836849
C	-2.425233	-6.138902	2.002000
C	-1.012732	-6.225100	1.890949
C	-0.419283	-6.248222	0.617649
C	0.740633	-5.513113	0.376004
C	1.315457	-4.749682	1.405959
C	1.813869	-3.451934	1.118987
C	1.928683	-2.524241	2.185266
C	1.553073	-1.171842	1.966842
C	1.272854	-0.358160	3.087299
C	0.171199	0.527126	3.021374
C	-0.599871	0.559005	1.837868
C	-2.013394	0.645673	1.948824
C	-2.589124	0.696231	3.238106
C	-3.766424	-0.049312	3.482632
C	-4.314165	-0.812236	2.427069
C	-4.812847	-2.111057	2.713996
C	-4.740429	-2.585328	4.042864
C	-4.366101	-3.932199	4.260897
C	-4.081880	-4.743814	3.139981
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CNT Chirality (6,6) Intermediate I

270			
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C	1.175330	0.335883	8.184227
C	0.649247	1.120462	9.234680
C	0.329735	2.476461	8.987014
C	-0.514382	3.158806	9.891309
C	-1.404849	4.139111	9.393980
C	-1.424926	4.408866	8.006681
C	-2.651893	4.749439	7.390404
C	-3.822411	4.806856	8.179857
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C	-6.835390	2.392119	6.884578
C	-7.171399	1.019733	6.814887
C	-6.643926	0.236303	5.763988
C	-6.326287	-1.120207	6.010691
C	-6.544216	-1.652773	7.301276
C	-5.654157	-2.632843	7.799882
C	-4.572616	-3.052177	6.992994
C	-3.345642	-3.391042	7.610649
C	-3.237138	-3.299014	9.016621
C	-2.004624	-2.901980	9.586204
C	-0.917075	-2.609016	8.732944
C	-0.012543	-1.584998	9.100450
C	-0.221680	-0.885835	10.310509
C	0.114488	0.486692	10.378719
C	-0.410818	1.271533	11.429573
C	-0.729348	2.626469	11.182608
C	-1.572915	3.307286	12.087848
C	-2.467098	4.289702	11.588678
C	-2.485974	4.557164	10.201794
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C	-7.897616	2.542535	9.079440
C	-8.235857	1.166158	9.008878
C	-7.708425	0.384572	7.957345
C	-7.390405	-0.970499	8.203932
C	-7.609209	-1.501398	9.494405
C	-6.715443	-2.483512	9.994912
C	-5.634608	-2.900664	9.187116
C	-4.408630	-3.238244	9.804366
C	-4.302120	-3.146526	11.209787
C	-3.065736	-2.748140	11.781154
C	-1.979619	-2.455997	10.926860
C	-1.075238	-1.433620	11.294204
C	-1.284474	-0.736793	12.504811
C	-0.945951	0.639692	12.573849
C	-1.450709	1.427478	13.638153
C	-1.769557	2.785760	13.390845
C	-2.626874	3.472561	14.265539
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C	-3.540934	4.729448	12.402097

C	-4.770898	5.066550	11.784672
C	-5.948462	5.104511	12.548711
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C	-9.297260	1.328568	11.183265
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C	-8.477017	-0.829752	10.390980
C	-8.663838	-1.369120	11.674000
C	-7.785498	-2.333024	12.165732
C	-6.706487	-2.773015	11.382152
C	-5.477239	-3.110273	12.001029
C	-5.343919	-3.001417	13.394707
C	-4.129626	-2.610175	13.955851
C	-3.029513	-2.321771	13.132157
C	-2.122265	-1.297615	13.500714
C	-2.326854	-0.576943	14.688422
C	-1.993625	0.774649	14.756639
Cl	-1.015142	1.258951	2.907909
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H	1.077077	-0.369659	1.107704
H	-0.176531	0.714432	0.600124
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CNT Chirality (6,6) Transition state TS

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C	7.612305	5.232114	-9.979369
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C	3.614083	1.330162	-12.822022
C	3.857980	-0.042041	-12.818125
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C	4.311823	-1.922301	-11.328796
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C	2.143915	3.029976	-9.251553
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C	2.364352	1.126791	-10.753902
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C	2.253539	-1.026276	-9.612126
C	3.060347	-2.124567	-9.236794
C	4.200394	-2.432759	-10.011479
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C	5.327455	-3.131957	-7.963794
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C	7.685009	-2.526909	-7.902714
C	8.590979	-1.644034	-7.259614
C	8.291994	-1.184871	-5.957768
C	8.671102	0.126191	-5.589864
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C	6.921519	2.652157	-3.517303
C	6.112511	3.750357	-3.892852
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C	1.098976	0.905503	-8.676129
C	1.346630	-0.487291	-8.672117
C	0.988104	-1.245058	-7.534568
C	1.796096	-2.343988	-7.158634
C	2.937815	-2.652579	-7.931894
C	4.088133	-3.163191	-7.285869
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C	5.248345	-3.136479	-5.142454
C	6.423060	-2.743473	-5.822282
C	7.326691	-1.864060	-5.180973
C	7.029561	-1.403834	-3.878302
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C	6.813664	0.502142	-2.374541
C	6.565569	1.894808	-2.378547
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C	-0.276149	-1.463796	-5.456232
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C	6.063734	-2.082140	-3.101479
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C	5.303141	1.675364	-0.298772
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C	1.560750	-3.597599	-3.128490
C	1.536141	-3.782585	-1.728165
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C	4.504450	-1.839839	0.280814
C	4.888393	-0.529863	0.651798
C	4.294340	0.063826	1.788377
C	4.042747	1.456494	1.782200
C	3.133271	1.993817	2.720827
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C	-2.802164	-1.900615	-1.298540
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C	3.627974	-0.749796	2.732858
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C	2.775547	1.236895	3.858815
C	1.865703	1.774392	4.796999
C	1.056449	2.870976	4.419699

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C	-3.209203	2.614634	0.363905
C	-4.174997	1.936040	1.140164
C	-4.554101	0.624208	0.771689
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C	-3.708384	-1.362122	-0.358033
C	-4.065898	-2.119339	0.779696
C	-3.257860	-3.217655	1.155204
C	-2.116615	-3.526060	0.381753
C	-0.965972	-4.034885	1.027592
C	-0.990826	-4.221263	2.427465
C	0.193500	-4.007142	3.170068
C	1.368090	-3.612787	2.491166
C	2.272851	-2.736216	3.134097
C	1.974268	-2.277519	4.436128
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C	1.756781	-0.373849	5.940230
C	1.508344	1.018312	5.935484
C	0.601126	1.557059	6.875369
C	-0.207171	2.655217	6.498765
C	-0.084604	3.181232	5.193256
C	-1.234617	3.692281	4.547433
C	-2.473815	3.662510	5.225728
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C	-5.220643	-0.188420	1.715849
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C	-5.330202	-2.338692	2.857753
C	-4.522029	-3.437487	3.233209
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C	-6.236536	-1.800066	3.798460
C	-6.593098	-2.557174	4.937039

C	-5.785266	-3.656202	5.312231
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C	-3.493779	-4.476403	5.183593
C	-3.518638	-4.663362	6.583977
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C	-1.158627	-4.057205	6.647921
C	-0.255418	-3.178008	7.290386
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C	-0.774725	-0.811262	10.094904
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C	-6.098385	2.839310	7.240350
C	-7.000743	1.960120	6.599375
C	-7.965010	1.282076	7.377444
C	-8.344724	-0.034476	7.008148
C	-7.746992	-0.626520	5.873658
C	-7.499326	-2.018169	5.877659
C	-7.857325	-2.773813	7.015950
C	-7.047260	-3.876622	7.392100
C	-5.907499	-4.184765	6.616912
C	-4.758085	-4.695718	7.261785
C	-4.784868	-4.883016	8.661447
C	-3.596276	-4.669778	9.406859
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C	-1.520585	-3.397671	9.368114
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C	-1.441729	-1.622274	11.039462
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C	-3.980682	1.999155	12.725587
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C	-5.023672	3.063046	10.791813
C	-6.267936	3.017844	11.441161
C	-7.435296	2.808348	10.709228
C	-7.377026	2.640769	9.316256
C	-8.281217	1.759001	8.673893
C	-9.230700	1.056625	9.433547
C	-9.603432	-0.236438	9.070956
C	-9.032670	-0.847660	7.942895
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C	-8.315304	-4.090405	9.447991
C	-7.181055	-4.426403	8.691347
C	-6.029032	-4.939071	9.337656
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C	-3.065614	-3.147959	12.740392
C	-2.693202	-1.854934	13.103418
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H	0.109029	0.977634	0.268530
H	0.225468	-0.884101	0.056613
Cl	1.995392	0.289098	-1.242241

CNT Chirality (7,7) Intermediate I

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C	6.330673	0.567687	3.343583
C	5.128134	1.072162	2.852884
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C	0.320056	0.041883	2.956338
C	-0.526206	-1.092124	2.988496
C	-0.476556	-2.036410	1.950978
C	-0.769891	-3.375458	2.200473
C	-1.118798	-3.798301	3.492740
C	-0.812391	-5.113791	3.915613
C	-0.158417	-5.998694	3.043959
C	0.675420	-6.996308	3.544973
C	0.872508	-7.130699	4.928338
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C	4.450781	-7.929398	4.915359
C	4.796958	-7.464532	6.193896
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C	8.000161	-3.166153	6.081832
C	7.630488	-2.190948	7.040467
C	7.324945	-0.872597	6.615672
C	6.684520	0.010391	7.512629
C	5.841973	1.023266	7.002178
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C	7.997321	-1.373010	12.332544
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C	1.733338	2.185346	8.953181
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CNT Chirality (8,8) Intermediate I

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CNT Chirality (9,9) Intermediate I

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CNT Chirality (10,10) Intermediate I

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CNT Chirality (12,12) Intermediate I

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CNT Chirality (14,14) Intermediate I

622			
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Graphene Transition state TS

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C	18.800188	27.686257	-0.402115
C	20.790602	26.278240	-0.590731
C	21.624786	27.404489	-0.623679
C	23.596607	25.998198	-0.815786
C	23.005011	27.266717	-0.733987
C	24.993900	25.858781	-0.927691
C	25.828084	26.985078	-0.957098
C	27.799285	25.579049	-1.151842
C	27.208127	26.847461	-1.066991
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C	33.399830	25.021415	-1.582957
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C	36.206736	24.742170	-1.785009
C	35.615019	26.010437	-1.703442
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C	60.911401	23.448943	-3.234662
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