

Enhancing the Interactions Between Neutral Molecular Tweezers and Anions

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Supporting Information

Cartesian coordinates (in Å) and energies (in hartrees) for the optimized structures at the MPW1B95/6-31+G* level

2-F Monomer

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NATOMS      58
Energy MPW1B95: -3146.689503
O      3.219764   -4.685034    0.000317
C      2.679179   -3.882486    1.087831
C      1.195341   -3.868454    0.703312
C      1.195445   -3.869371   -0.703278
C      2.679338   -3.882708   -1.087429
C     -0.000060   -3.847449    1.416172
C     -1.195452   -3.868482    0.703123
C     -1.195324   -3.869341   -0.703466
C      0.000063   -3.849353   -1.416368
C     -2.679156   -3.882554   -1.087853
C     -3.236063   -2.505073   -0.703924
C     -3.236862   -2.505409    0.703722
C     -2.679351   -3.882639    1.087407
C     -3.650843   -1.389937    1.405740
C     -4.094698   -0.252712    0.701198
C     -4.093804   -0.252321   -0.701188
C     -3.649123   -1.389175   -1.405813
O     -4.530339    0.831059   -1.443033
C     -4.979818    1.906511   -0.701829
C     -4.980671    1.906134    0.701928
O     -4.532110    0.830277    1.443098
C     -5.446821    3.028004   -1.395510
C     -5.914770    4.150915   -0.699009
C     -5.915611    4.150543    0.699178
C     -5.448508    3.027259    1.395643
O     -3.219768   -4.685027   -0.000312
C      3.236223   -2.505189   -0.703624
C      3.236712   -2.505293    0.704023
C      3.649428   -1.389408   -1.405613
C      4.093956   -0.252435   -0.701082
C      4.094546   -0.252593    0.701305
C      3.650538   -1.389700    1.405941
O      4.530647    0.830823   -1.443013
C      4.979964    1.906398   -0.701891
C      4.980522    1.906251    0.701867
O      4.531803    0.830517    1.443119
C      5.447111    3.027779   -1.395656
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C	5.914913	4.150804	-0.699242
C	5.915464	4.150660	0.698945
C	5.448214	3.027489	1.395496
F	-5.447977	3.031658	-2.743225
F	-6.361263	5.225014	-1.377762
F	-6.362930	5.224278	1.377965
F	-5.451300	3.030188	2.743356
F	-3.653993	-1.355435	-2.761872
F	-3.656924	-1.356779	2.761808
F	0.000229	-3.840660	-2.780433
F	-0.000224	-3.838016	2.780233
F	3.656353	-1.356326	2.762005
F	3.654560	-1.355883	-2.761675
F	5.448550	3.031212	-2.743372
F	6.361546	5.224793	-1.378077
F	6.362637	5.224506	1.377650
F	5.450723	3.030640	2.743210
H	2.954548	-4.293306	2.063863
H	2.955170	-4.293507	-2.063340
H	-2.954853	-4.293195	-2.063868
H	-2.954855	-4.293616	2.063335

2-CN Monomer

NATOMS 72

Energy MPW1B95: -3048.568927

O	-3.195145	0.000000	-4.863879
C	-2.675183	1.088146	-4.049435
C	-1.192282	0.700279	-4.001749
C	-1.192282	-0.700279	-4.001749
C	-2.675183	-1.088146	-4.049435
C	0.000000	1.450321	-3.979829
C	1.192282	0.700279	-4.001749
C	1.192282	-0.700279	-4.001749
C	0.000000	-1.450321	-3.979829
C	2.675183	-1.088146	-4.049435
C	3.269890	-0.699422	-2.689844
C	3.269890	0.699422	-2.689844
C	2.675183	1.088146	-4.049435
C	3.745928	1.437108	-1.598007
C	4.247651	0.698368	-0.496532
C	4.247651	-0.698368	-0.496532
C	3.745928	-1.437108	-1.598007
O	4.745869	-1.419659	0.573563
C	5.242966	-0.701391	1.631621
C	5.242966	0.701391	1.631621
O	4.745869	1.419659	0.573563
C	5.756570	-1.419612	2.725714
C	6.280807	-0.707418	3.843660
C	6.280807	0.707418	3.843660
C	5.756570	1.419612	2.725714
O	3.195145	0.000000	-4.863879
C	-3.269890	-0.699422	-2.689844
C	-3.269890	0.699422	-2.689844
C	-3.745928	-1.437108	-1.598007
C	-4.247651	-0.698368	-0.496532
C	-4.247651	0.698368	-0.496532

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C	-3.745928	1.437108	-1.598007
O	-4.745869	-1.419659	0.573563
C	-5.242966	-0.701391	1.631621
C	-5.242966	0.701391	1.631621
O	-4.745869	1.419659	0.573563
C	-5.756570	-1.419612	2.725714
C	-6.280807	-0.707418	3.843660
C	-6.280807	0.707418	3.843660
C	-5.756570	1.419612	2.725714
H	-2.938925	2.067051	-4.464651
H	-2.938925	-2.067051	-4.464651
H	2.938925	-2.067051	-4.464651
H	2.938925	2.067051	-4.464651
C	6.803681	1.428153	4.959281
N	7.233328	2.024698	5.876699
C	6.803681	-1.428153	4.959281
N	7.233328	-2.024698	5.876699
C	5.741480	-2.845800	2.696589
N	5.725324	-4.020858	2.666740
C	5.741480	2.845800	2.696589
N	5.725324	4.020858	2.666740
C	3.754281	2.865177	-1.587199
N	3.749215	4.040613	-1.613235
C	3.754281	-2.865177	-1.587199
N	3.749215	-4.040613	-1.613235
C	0.000000	2.880797	-3.977544
N	0.000000	4.056888	-3.974923
C	0.000000	-2.880797	-3.977544
N	0.000000	-4.056888	-3.974923
C	-3.754281	2.865177	-1.587199
N	-3.749215	4.040613	-1.613235
C	-3.754281	-2.865177	-1.587199
N	-3.749215	-4.040613	-1.613235
C	-5.741480	2.845800	2.696589
N	-5.725324	4.020858	2.666740
C	-6.803681	1.428153	4.959281
N	-7.233328	2.024698	5.876699
C	-6.803681	-1.428153	4.959281
N	-7.233328	-2.024698	5.876699
C	-5.741480	-2.845800	2.696589
N	-5.725324	-4.020858	2.666740

2-F...Cl- Complex

NATOMS 59

Energy MPW1B95: -3607.048180

Cl	-0.859839	0.000032	-0.000460
O	-0.877735	-3.236838	1.427218
C	-2.030814	-3.012881	0.701284
C	-2.031195	-3.012511	-0.701328
O	-0.878254	-3.236093	-1.427799
C	-3.219167	-2.782274	-1.394945
C	-4.412853	-2.554481	-0.697479
C	-4.412555	-2.554779	0.698159
C	-3.218693	-2.782913	1.395217
C	0.290075	-3.126419	0.701240
C	0.289755	-3.125972	-0.702287

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C	1.503084	-3.035144	-1.405047
C	2.693413	-2.960779	-0.704217
C	2.693663	-2.961246	0.702634
C	1.503541	-3.036037	1.403742
C	4.148142	-2.668650	1.085665
C	4.360122	-1.197458	0.703148
C	4.359979	-1.196986	-0.704051
C	4.147819	-2.667932	-1.087493
O	4.853616	-3.331573	-0.001238
C	4.361043	0.000365	-1.413184
C	4.360149	1.197207	-0.703182
C	4.360091	1.196731	0.704019
C	4.361134	-0.000618	1.413152
C	4.148011	2.667674	1.087487
C	2.693607	2.960591	0.704285
C	2.693789	2.961090	-0.702573
C	4.148230	2.668415	-1.085679
C	1.503275	3.035074	1.405083
C	0.289940	3.126075	0.702357
C	0.290163	3.126563	-0.701140
C	1.503659	3.036067	-1.403621
O	-0.878054	3.236144	1.428023
C	-2.030942	3.012782	0.701495
C	-2.030701	3.013201	-0.701140
O	-0.877586	3.237062	-1.427130
C	-3.218500	2.783225	-1.395262
C	-4.412264	2.554951	-0.698208
C	-4.412500	2.554490	0.697467
C	-3.218977	2.782362	1.395072
O	4.853796	3.331288	0.001199
F	-3.225448	-2.767132	2.747559
F	-3.225911	-2.765725	-2.747231
F	-3.225652	2.765771	2.747333
F	-3.224718	2.767458	-2.747537
F	-5.565691	-2.348488	-1.378242
F	-5.565106	-2.348981	1.379444
F	-5.565525	2.348239	1.377867
F	-5.565077	2.349258	-1.379131
F	1.477610	-3.014968	-2.765318
F	1.478342	-3.016635	2.764024
F	1.478456	3.016778	-2.763919
F	1.477755	3.014829	2.765363
F	4.330788	0.000873	-2.780767
F	4.330954	-0.001127	2.780739
H	4.508088	3.006793	2.063679
H	4.508509	3.008185	-2.061570
H	4.507828	-3.007078	-2.063701
H	4.508448	-3.008433	2.061542

2-F...Br- Complex

NATOMS 59

Energy MPW1B95: -5718.619972

Br	0.549092	-0.001189	-0.001912
O	0.877004	3.387460	1.418369
C	2.008554	3.047040	0.700994
C	2.008716	3.046366	-0.701223

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O	0.877487	3.386380	-1.419186
C	3.167067	2.697724	-1.395980
C	4.333652	2.359189	-0.697676
C	4.333459	2.360003	0.698787
C	3.166643	2.699140	1.396431
C	-0.299397	3.273239	0.700540
C	-0.299135	3.272626	-0.701711
C	-1.506461	3.139254	-1.406667
C	-2.691683	3.020585	-0.704474
C	-2.691920	3.021162	0.702617
C	-1.506971	3.140413	1.405157
C	-4.132761	2.670899	1.085611
C	-4.292164	1.193115	0.702928
C	-4.292031	1.192540	-0.703839
C	-4.132436	2.670023	-1.087639
O	-4.863957	3.307019	-0.001371
C	-4.288464	-0.003973	-1.413920
C	-4.290610	-1.199885	-0.702790
C	-4.290583	-1.199291	0.703981
C	-4.288604	-0.002766	1.414061
C	-4.127691	-2.676386	1.087834
C	-2.686080	-3.023487	0.704775
C	-2.686233	-3.024191	-0.702311
C	-4.127865	-2.677334	-1.085413
C	-1.500623	-3.139456	1.407048
C	-0.292993	-3.270291	0.702175
C	-0.293177	-3.271129	-0.700066
C	-1.500975	-3.141004	-1.404765
O	0.883752	-3.381793	1.419788
C	2.014730	-3.041389	0.701708
C	2.014519	-3.042197	-0.700524
O	0.883355	-3.383496	-1.417878
C	3.172647	-2.694383	-1.395946
C	4.339563	-2.355232	-0.698385
C	4.339806	-2.354540	0.698021
C	3.173096	-2.692803	1.396356
O	-4.857665	-3.315080	0.001548
F	3.171914	2.684744	2.748197
F	3.172609	2.681800	-2.747762
F	3.178765	-2.676839	2.748185
F	3.177919	-2.680086	-2.747793
F	5.468236	2.070082	-1.377551
F	5.467907	2.071820	1.379302
F	5.474644	-2.066309	1.377918
F	5.474157	-2.067656	-1.378969
F	-1.479069	3.108664	-2.766099
F	-1.480082	3.110954	2.764638
F	-1.474088	-3.111702	-2.764254
F	-1.473386	-3.108684	2.766505
F	-4.269001	-0.004568	-2.781517
F	-4.269222	-0.002135	2.781668
H	-4.499861	-3.001650	2.064263
H	-4.500225	-3.003403	-2.061501
H	-4.505305	2.994440	-2.064083
H	-4.505940	2.996060	2.061691

2-F...I- Complex

NATOMS 59

Energy MPW1B95: -3258.709251

I	0.000000	0.000000	0.701628
O	3.736785	1.428252	0.763551
C	3.596353	0.701621	1.928796
C	3.596353	-0.701621	1.928796
O	3.736785	-1.428252	0.763551
C	3.461288	-1.395675	3.132781
C	3.331726	-0.698195	4.340706
C	3.331726	0.698195	4.340706
C	3.461288	1.395675	3.132781
C	3.536920	0.700975	-0.395310
C	3.536920	-0.700975	-0.395310
C	3.311535	-1.405220	-1.590503
C	3.100974	-0.703476	-2.762491
C	3.100974	0.703476	-2.762491
C	3.311535	1.405220	-1.590503
C	2.677238	1.086893	-4.183287
C	1.195489	0.703236	-4.282797
C	1.195489	-0.703236	-4.282797
C	2.677238	-1.086893	-4.183287
O	3.280900	0.000000	-4.943746
C	0.000000	-1.414742	-4.270383
C	-1.195489	-0.703236	-4.282797
C	-1.195489	0.703236	-4.282797
C	0.000000	1.414742	-4.270383
C	-2.677238	1.086893	-4.183287
C	-3.100974	0.703476	-2.762491
C	-3.100974	-0.703476	-2.762491
C	-2.677238	-1.086893	-4.183287
C	-3.311535	1.405220	-1.590503
C	-3.536920	0.700975	-0.395310
C	-3.536920	-0.700975	-0.395310
C	-3.311535	-1.405220	-1.590503
O	-3.736785	1.428252	0.763551
C	-3.596353	0.701621	1.928796
C	-3.596353	-0.701621	1.928796
O	-3.736785	-1.428252	0.763551
C	-3.461288	-1.395675	3.132781
C	-3.331726	-0.698195	4.340706
C	-3.331726	0.698195	4.340706
C	-3.461288	1.395675	3.132781
O	-3.280900	0.000000	-4.943746
F	3.454095	2.747030	3.141001
F	3.454095	-2.747030	3.141001
F	-3.454095	2.747030	3.141001
F	-3.454095	-2.747030	3.141001
F	3.224034	-1.377915	5.506220
F	3.224034	1.377915	5.506220
F	-3.224034	1.377915	5.506220
F	-3.224034	-1.377915	5.506220
F	3.291673	-2.764071	-1.560377
F	3.291673	2.764071	-1.560377
F	-3.291673	-2.764071	-1.560377
F	-3.291673	2.764071	-1.560377

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F	0.000000	-2.781679	-4.257192
F	0.000000	2.781679	-4.257192
H	-2.984351	2.063366	-4.570458
H	-2.984351	-2.063366	-4.570458
H	2.984351	-2.063366	-4.570458
H	2.984351	2.063366	-4.570458

2-CN...Cl- Complex

NATOMS 73

Energy MPW1B95 : -3508.978953

C	-2.997328	2.815976	1.417030
C	-1.795849	2.898627	0.697894
C	-1.797030	2.894215	-0.708277
C	-3.000118	2.806698	-1.424173
C	-4.231240	2.704398	-0.708255
C	-4.229903	2.709083	0.704338
O	-0.635876	3.063935	1.404139
C	0.540278	2.986023	0.693299
C	0.539262	2.981937	-0.708230
O	-0.638211	3.055907	-1.417561
C	1.746334	2.960644	1.428331
C	2.939351	2.905372	0.689076
C	2.938678	2.901091	-0.706065
C	1.744677	2.952086	-1.444406
C	4.404613	2.664618	1.077917
O	5.088019	3.339777	-0.010382
C	4.403974	2.657771	-1.094016
C	4.635251	1.190986	-0.703661
C	4.635533	1.195337	0.696934
C	4.665919	-0.004694	-1.448153
C	4.635583	-1.195909	-0.696392
C	4.635069	-1.191536	0.704196
C	4.665718	0.004128	1.448694
C	4.404509	-2.665190	-1.077369
C	2.939168	-2.905821	-0.688655
C	2.938353	-2.901357	0.706476
C	4.403644	-2.658268	1.094566
O	5.087721	-3.340386	0.011039
C	1.744160	-2.951943	1.444486
C	0.538868	-2.981464	0.708086
C	0.539889	-2.985744	-0.693423
C	1.746238	-2.960920	-1.428038
O	-0.636322	-3.063427	-1.404341
C	-1.796305	-2.898157	-0.697967
C	-1.797424	-2.893561	0.708192
O	-0.638579	-3.054730	1.417490
C	-3.000351	-2.806092	1.424368
C	-4.231678	-2.704043	0.708840
C	-4.230569	-2.708977	-0.703735
C	-2.998140	-2.815992	-1.416619
C	4.718921	0.007437	2.878632
N	4.798365	0.009085	4.052304
C	4.719338	-0.008022	-2.878082
N	4.798976	-0.009713	-4.051741
C	1.737438	-2.986610	2.872033

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N	1.782450	-3.047770	4.045593
C	1.742014	-3.004395	-2.855358
N	1.789780	-3.072589	-4.028423
C	-2.973527	-2.864490	-2.841577
N	-2.961956	-2.928533	-4.015597
C	-5.461250	-2.643029	-1.424169
N	-6.474814	-2.604914	-2.019407
C	-5.463506	-2.633850	1.426898
N	-6.478069	-2.593033	2.020252
C	-2.977808	-2.843769	2.849692
N	-2.968007	-2.898293	4.024208
C	1.738551	2.987193	-2.871934
N	1.784121	3.048779	-4.045450
C	1.741673	3.003559	2.855651
N	1.788936	3.071210	4.028769
C	-2.978111	2.844829	-2.849485
N	-2.968742	2.899872	-4.023981
C	-5.463226	2.634066	-1.426044
N	-6.477908	2.593112	-2.019184
C	-5.460469	2.643105	1.424961
N	-6.473895	2.605006	2.020437
C	-2.972161	2.863735	2.841985
N	-2.960114	2.926952	4.016046
Cl	-0.613794	0.000221	-0.004825
H	4.751535	3.013387	2.056394
H	4.750952	2.999715	-2.074877
H	4.751562	-3.013992	-2.055787
H	4.750506	-3.000173	2.075481

2-CN...Br- Complex

NATOMS 73

Energy MPW1B95: -5620.548603

Br	0.000000	0.000000	0.449647
O	3.211571	1.407154	0.624923
C	2.991318	0.703036	1.778563
C	2.991318	-0.703036	1.778563
O	3.211571	-1.407154	0.624923
C	2.851963	-1.421356	2.975398
C	2.693258	-0.706352	4.201069
C	2.693258	0.706352	4.201069
C	2.851963	1.421356	2.975398
C	3.110181	0.700537	-0.554499
C	3.110181	-0.700537	-0.554499
C	3.037350	-1.437682	-1.756818
C	2.944079	-0.697430	-2.945807
C	2.944079	0.697430	-2.945807
C	3.037350	1.437682	-1.756818
C	2.666558	1.086067	-4.403007
C	1.193616	0.700362	-4.606238
C	1.193616	-0.700362	-4.606238
C	2.666558	-1.086067	-4.403007
O	3.330146	0.000000	-5.102671
C	0.000000	-1.448180	-4.631902
C	-1.193616	-0.700362	-4.606238
C	-1.193616	0.700362	-4.606238
C	0.000000	1.448180	-4.631902

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C	-2.666558	1.086067	-4.403007
C	-2.944079	0.697430	-2.945807
C	-2.944079	-0.697430	-2.945807
C	-2.666558	-1.086067	-4.403007
C	-3.037350	1.437682	-1.756818
C	-3.110181	0.700537	-0.554499
C	-3.110181	-0.700537	-0.554499
C	-3.037350	-1.437682	-1.756818
O	-3.211571	1.407154	0.624923
C	-2.991318	0.703036	1.778563
C	-2.991318	-0.703036	1.778563
O	-3.211571	-1.407154	0.624923
C	-2.851963	-1.421356	2.975398
C	-2.693258	-0.706352	4.201069
C	-2.693258	0.706352	4.201069
C	-2.851963	1.421356	2.975398
O	-3.330146	0.000000	-5.102671
H	-3.008010	2.065847	-4.753652
H	-3.008010	-2.065847	-4.753652
H	3.008010	-2.065847	-4.753652
H	3.008010	2.065847	-4.753652
C	-3.053993	2.865216	-1.756493
N	-3.097784	4.039242	-1.809254
C	-3.053993	-2.865216	-1.756493
N	-3.097784	-4.039242	-1.809254
C	0.000000	2.877976	-4.691109
N	0.000000	4.050851	-4.780687
C	0.000000	-2.877976	-4.691109
N	0.000000	-4.050851	-4.780687
C	3.053993	-2.865216	-1.756493
N	3.097784	-4.039242	-1.809254
C	3.053993	2.865216	-1.756493
N	3.097784	4.039242	-1.809254
C	-2.897600	-2.846283	2.954119
N	-2.960132	-4.020455	2.947098
C	-2.897600	2.846283	2.954119
N	-2.960132	4.020455	2.947098
C	-2.567082	1.424734	5.428238
N	-2.472854	2.016838	6.439988
C	-2.567082	-1.424734	5.428238
N	-2.472854	-2.016838	6.439988
C	2.897600	2.846283	2.954119
N	2.960132	4.020455	2.947098
C	2.897600	-2.846283	2.954119
N	2.960132	-4.020455	2.947098
C	2.567082	-1.424734	5.428238
N	2.472854	-2.016838	6.439988
C	2.567082	1.424734	5.428238
N	2.472854	2.016838	6.439988

2-CN...I- Complex

NATOMS 73

Energy MPW1B95: -3160.634049

I	0.000000	0.000000	0.453816
O	3.540112	1.405192	0.576160
C	3.336154	0.702806	1.735773

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C	3.336154	-0.702806	1.735773
O	3.540112	-1.405192	0.576160
C	3.212731	-1.422166	2.934656
C	3.053306	-0.706584	4.159449
C	3.053306	0.706584	4.159449
C	3.212731	1.422166	2.934656
C	3.378017	0.700153	-0.599665
C	3.378017	-0.700153	-0.599665
C	3.222966	-1.437965	-1.794951
C	3.045001	-0.697856	-2.973299
C	3.045001	0.697856	-2.973299
C	3.222966	1.437965	-1.794951
C	2.673636	1.086428	-4.408404
C	1.192497	0.700200	-4.532336
C	1.192497	-0.700200	-4.532336
C	2.673636	-1.086428	-4.408404
O	3.294250	0.000000	-5.148474
C	0.000000	-1.449323	-4.536072
C	-1.192497	-0.700200	-4.532336
C	-1.192497	0.700200	-4.532336
C	0.000000	1.449323	-4.536072
C	-2.673636	1.086428	-4.408404
C	-3.045001	0.697856	-2.973299
C	-3.045001	-0.697856	-2.973299
C	-2.673636	-1.086428	-4.408404
C	-3.222966	1.437965	-1.794951
C	-3.378017	0.700153	-0.599665
C	-3.378017	-0.700153	-0.599665
C	-3.222966	-1.437965	-1.794951
O	-3.540112	1.405192	0.576160
C	-3.336154	0.702806	1.735773
C	-3.336154	-0.702806	1.735773
O	-3.540112	-1.405192	0.576160
C	-3.212731	-1.422166	2.934656
C	-3.053306	-0.706584	4.159449
C	-3.053306	0.706584	4.159449
C	-3.212731	1.422166	2.934656
O	-3.294250	0.000000	-5.148474
H	-2.990663	2.065599	-4.783015
H	-2.990663	-2.065599	-4.783015
H	2.990663	-2.065599	-4.783015
H	2.990663	2.065599	-4.783015
C	-3.236800	2.865507	-1.794030
N	-3.275580	4.039690	-1.846118
C	-3.236800	-2.865507	-1.794030
N	-3.275580	-4.039690	-1.846118
C	0.000000	2.879758	-4.570389
N	0.000000	4.054129	-4.636164
C	0.000000	-2.879758	-4.570389
N	0.000000	-4.054129	-4.636164
C	3.236800	-2.865507	-1.794030
N	3.275580	-4.039690	-1.846118
C	3.236800	2.865507	-1.794030
N	3.275580	4.039690	-1.846118
C	-3.256395	-2.846821	2.912161
N	-3.318278	-4.021069	2.902173
C	-3.256395	2.846821	2.912161

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N	-3.318278	4.021069	2.902173
C	-2.912690	1.424522	5.385247
N	-2.800072	2.017845	6.394362
C	-2.912690	-1.424522	5.385247
N	-2.800072	-2.017845	6.394362
C	3.256395	2.846821	2.912161
N	3.318278	4.021069	2.902173
C	3.256395	-2.846821	2.912161
N	3.318278	-4.021069	2.902173
C	2.912690	-1.424522	5.385247
N	2.800072	-2.017845	6.394362
C	2.912690	1.424522	5.385247
N	2.800072	2.017845	6.394362