Supporting Information: DFT

Molecular Tetrominoes: Selective Masking of Donor π-Face to Control Configuration of Donor-Acceptor Complex

Jenna Sartucci, Arindam Maity, Manikandan Mohanan, Jeffery Bertke, Miklos Kertesz, and Nagarjuna Gavvalapalli*

Department of Chemistry, Institute for Soft Matter Synthesis and Metrology, Georgetown University, 3700 O St NW, Washington, D.C., 20057, USA.

The default integration grid in Gaussian 16, Ultrafine, was used.

Optimized Geometry Coordinates

DDQ
Electronic Energy: -1485.329331 Hartrees
Free Energy: -1485.306750 Hartrees
Thermal Energy: 47.13 kcal/mol
Entropy: 112.545 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

C	-1.402582	0.67674	-0.000089
C	-1.402582	-0.676738	-0.00009
C	-0.120788	-1.458511	-0.000085
C	1.150702	-0.675079	-0.00001
C	1.150704	0.675081	-0.000023
C	-0.120788	1.458518	-0.000049
O	-0.139007	-2.66413	-0.000096
O	-0.139009	2.664138	0.000015
Cl	2.589165	-1.610534	0.00006
Cl	2.589177	1.610528	0.000015

C	-2.60251	1.438946	0.000017
C	-2.602508	-1.438946	0.000044
N	-3.578972	2.053698	0.000036
N	-3.578966	-2.053703	0.000117

PPP
Electronic Energy: -846.954836 Hartrees
Free Energy: -846.724244 Hartrees
Thermal Energy: 187.93 kcal/mol
Entropy: 146.98 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

C	6.173792	1.21095	-0.00011
C	7.562499	-1.205782	0.000136
C	5.459007	0.000033	0.000006
C	7.562351	1.206108	-0.000104
C	8.261717	0.000206	0.000019
C	6.173941	-1.210795	0.00013
C	4.038825	-0.000054	0.000001
C	2.828565	-0.000127	-0.000004
C	1.410725	-0.000153	-0.000011
C	-1.410725	-0.000206	-0.000026
C	0.691619	1.209569	0.000122
C	0.691664	-1.209902	-0.000152
C	-0.691619	-1.209927	-0.000159
C	-0.691664	1.209543	0.000115
C	-2.828565	-0.000232	-0.000034
C	-4.038824	-0.000249	-0.000041
C	-5.459007	-0.000054	-0.000012
C	-8.261717	0.000331	0.000043
C	-6.1737	1.210917	-0.000015
C	-6.174033	-1.210829	0.000019
C	-7.562591	-1.20571	0.000046
C	-7.562259	1.20618	0.000012
H	5.626617	-2.145114	0.000222
H	8.102028	-2.1457	0.000232
H	9.345292	0.000273	0.000023
H	8.101763	2.146094	-0.000196
H	5.626353	2.145201	-0.000206

H	1.236163	2.145387	0.000232
H	-1.236243	2.145341	0.00022
H	1.236243	-2.145699	-0.000256
H	-1.236163	-2.145745	-0.00027
H	-5.62678	-2.145188	0.000022
H	-8.10219	-2.145588	0.00007
H	-9.345292	0.00048	0.000064
H	-8.1016	2.146206	0.000009
H	-5.62619	2.145127	-0.00004

PCP
Electronic Energy: -2189.195090 Hartrees
Free Energy: -2188.660739 Hartrees
Thermal Energy: 396.86 kcal/mol
Entropy: 208.43 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	1.198247	0.257789	3.039696
S	-1.198204	0.257285	-3.039814
C	1.467202	-1.487799	2.477107
H	2.534518	-1.676213	2.382173
H	1.085579	-2.076596	3.31301
C	0.731718	-1.794683	1.208703
C	1.405409	-1.856286	-0.033131
C	0.65334	-1.868663	-1.217086
H	1.178938	-1.829752	-2.163462
C	-0.731587	-1.794902	-1.208539
C	-1.405272	-1.856347	0.033296
C	-0.6532	-1.868502	1.217256
H	-1.178805	-1.829464	2.163624
C	-1.467083	-1.488234	-2.476992
H	-2.534392	-1.676672	-2.382021
H	-1.085443	-2.077148	-3.312806
C	2.820736	-1.799707	-0.109892
C	4.024883	-1.707319	-0.190568
C	5.436618	-1.586076	-0.281721
C	6.21448	-1.414509	0.876905
H	5.724038	-1.380687	1.841796

C	7.594022	-1.288222	0.782117
H	8.183286	-1.155608	1.681856
C	8.220378	-1.331416	-0.46255
H	9.297151	-1.23285	-0.532571
C	7.457614	-1.501444	-1.61697
H	7.940639	-1.535154	-2.586491
C	6.077462	-1.627618	-1.532475
H	5.480247	-1.758489	-2.426163
C	-2.820603	-1.799816	0.110063
C	-4.024753	-1.707442	0.19073
C	-5.436481	-1.586188	0.281977
C	-6.077125	-1.626611	1.532872
H	-5.479759	-1.756631	2.426583
C	-7.457268	-1.500421	1.617473
H	-7.940136	-1.533257	2.587102
C	-8.220226	-1.331485	0.463019
H	-9.29699	-1.232894	0.533125
C	-7.59407	-1.289396	-0.781784
H	-8.183484	-1.157639	-1.681551
C	-6.214536	-1.415707	-0.876677
H	-5.724251	-1.38273	-1.841677
C	1.921454	1.273591	1.672762
H	2.655164	1.923765	2.154783
H	2.468805	0.599435	1.012632
C	0.939799	2.138351	0.861967
C	1.769815	3.035038	-0.083729
H	2.385045	2.406713	-0.737846
H	2.454273	3.659297	0.502204
C	0.841937	3.925245	-0.928586
H	1.448319	4.55142	-1.590868
C	-0.089866	3.042879	-1.775148
H	-0.745561	3.670977	-2.390232
H	0.497949	2.422114	-2.457686
C	-0.939989	2.13815	-0.862327
C	-0.000044	1.28007	-0.000135
H	-0.592747	0.637004	0.650284
H	0.592732	0.637002	-0.650489
C	0.08957	3.043092	1.774682
H	0.745184	3.67134	2.389698

H	-0.498173	2.422337	2.457288
C	-0.842334	3.925257	0.928022
H	-1.448787	4.551439	1.59023
C	-0.00025	4.815432	-0.000334
H	0.651233	5.466028	0.593426
H	-0.651809	5.465879	-0.594173
C	-1.77011	3.034849	0.083269
H	-2.454641	3.658964	-0.502732
H	-2.385268	2.406527	0.737457
C	-1.921543	1.27319	-1.673022
H	-2.655324	1.923221	-2.155129
H	-2.468814	0.599055	-1.012807

CPC (U Shape)

Electronic Energy: -3531.42911 Hartrees
Free Energy: -3530.590440 Hartrees
Thermal Energy: 605.43 kcal/mol
Entropy: 267.47 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	5.583185	-0.726139	-3.171117
S	7.566622	0.38859	2.943815
C	5.509057	-2.407597	-2.39028
H	4.471737	-2.730576	-2.33355
H	6.02734	-3.035177	-3.11736
C	6.18212	-2.447297	-1.053743
C	5.430853	-2.405637	0.143563
C	6.08377	-2.159513	1.359769
H	5.48646	-2.041517	2.255789
C	7.456404	-1.941187	1.410131
C	8.204105	-2.119779	0.242784
C	7.570539	-2.372982	-0.966963
H	8.155043	-2.424784	-1.878765
C	8.084307	-1.36579	2.643492
H	9.172808	-1.417211	2.602428
H	7.754843	-1.877916	3.549632
C	4.014123	-2.504082	0.122902
C	2.804493	-2.541562	0.099443
C	1.388209	-2.567535	0.050365
C	0.720354	-2.793472	-1.167697
H	1.302208	-2.956882	-2.066104

C	-0.661702	-2.805641	-1.222588
H	-1.16823	-2.978734	-2.163712
C	-1.426931	-2.592553	-0.061547
C	-0.75955	-2.366827	1.157251
H	-1.343451	-2.191666	2.052019
C	0.622433	-2.354774	1.211776
H	1.129049	-2.175669	2.151692
C	4.633955	0.349794	-2.001863
H	3.859899	0.823927	-2.609716
H	4.131779	-0.300562	-1.285079
C	5.438064	1.438266	-1.269291
C	4.444997	2.32478	-0.484786
H	3.879781	1.705454	0.220883
H	3.720352	2.772417	-1.174651
C	5.200235	3.431623	0.272674
H	4.480834	4.047036	0.822191
C	6.189284	2.79849	1.265163
H	6.721671	3.582931	1.816495
H	5.649347	2.194825	2.000313
C	7.199111	1.909388	0.513957
C	6.427291	0.830996	-0.262422
H	7.13179	0.190951	-0.794048
H	5.883431	0.205544	0.444726
C	6.214607	2.329196	-2.257807
H	5.519143	2.780213	-2.975787
H	6.915969	1.713789	-2.828934
C	6.973669	3.428962	-1.498384
H	7.531204	4.044121	-2.211908
C	5.971476	4.305376	-0.729755
H	5.276428	4.7816	-1.429897
H	6.497727	5.107678	-0.200958
C	7.959072	2.785271	-0.50724
H	8.522937	3.564558	0.018415
H	8.685937	2.169889	-1.0502
C	8.232434	1.287191	1.47062
H	8.870851	2.07627	1.87423
H	8.874007	0.592256	0.924548
H	9.281571	-1.999963	0.272471
C	-2.842681	-2.586299	-0.108972

C	-4.051723	-2.543329	-0.113367
C	-5.464157	-2.428846	-0.089406
C	-8.236301	-2.091988	-0.079138
C	-6.169177	-2.227017	-1.286228
C	-6.15978	-2.393528	1.139039
C	-7.551507	-2.295661	1.110424
C	-7.538083	-1.982259	-1.285766
H	-5.61282	-2.192632	-2.215535
H	-8.098497	-2.317335	2.046706
H	-9.308277	-1.93091	-0.065631
C	-5.424485	-2.312973	2.438677
H	-6.087786	-2.506413	3.281737
H	-4.594379	-3.01964	2.482105
C	-8.210725	-1.445036	-2.511511
H	-9.200643	-1.879864	-2.661831
H	-7.619846	-1.625539	-3.409925
S	-4.584959	-0.677901	2.691833
S	-8.566078	0.370104	-2.370588
C	-6.881283	1.122531	-2.23611
C	-6.55372	1.839122	-0.913872
C	-7.622776	2.89032	-0.558764
H	-8.594625	2.39989	-0.450276
H	-7.715009	3.61727	-1.374607
C	-7.245717	3.60927	0.746745
H	-8.021012	4.341558	0.993688
C	-7.136107	2.58352	1.889044
H	-6.894256	3.094814	2.827971
H	-8.099695	2.080847	2.033086
C	-6.047554	1.53558	1.567038
C	-6.427305	0.843173	0.249022
H	-5.66669	0.101724	0.006601
H	-7.373713	0.316895	0.373597
C	-5.194472	2.555686	-1.076288
H	-4.421159	1.822243	-1.332014
C	-4.81604	3.283775	0.226089
H	-3.851624	3.783624	0.091091
C	-5.896402	4.323126	0.565765
C	-4.704992	2.267183	1.373759
H	-4.422747	2.778505	2.301999

H	-3.921544	1.536336	1.154387
C	-5.982617	0.530342	2.731824
H	-5.873343	1.0746	3.672715
H	-6.9133	-0.038536	2.787921
H	-5.970913	5.067883	-0.234193
H	-5.625811	4.859353	1.481937
H	-5.247862	3.273259	-1.903187
H	-6.810225	1.834945	-3.061012
H	-6.152102	0.331077	-2.420728

CPC (Z shape)
Electronic Energy: -3531.428963 Hartrees
Free Energy: -3530.591754 Hartrees
Thermal Energy: 605.44 kcal/mol
Entropy: 270.58 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-8.042854	-0.89788	-3.093061
S	-5.946344	-0.443885	3.069763
C	-7.835909	-2.667529	-2.581877
H	-8.816948	-3.138271	-2.51025
H	-7.309933	-3.108408	-3.430968
C	-7.062226	-2.805124	-1.305449
C	-7.706623	-3.135512	-0.109942
C	-7.055437	-2.980575	1.106906
H	-7.593937	-3.160065	2.030739
C	-5.755057	-2.484875	1.172593
C	-5.053022	-2.278595	-0.037375
C	-5.717953	-2.451721	-1.259724
H	-5.194926	-2.204237	-2.175522
C	-5.189009	-2.032535	2.482509
H	-4.107578	-1.920443	2.442287
H	-5.434373	-2.729816	3.285412
C	-3.720455	-1.787088	-0.036734
C	-2.607281	-1.311714	-0.03731
C	-1.317269	-0.725103	-0.019341
C	-0.663253	-0.385422	-1.218061
H	-1.15243	-0.591391	-2.16168

C	0.586225	0.207566	-1.196423
H	1.082305	0.467073	-2.123084
C	1.228669	0.483668	0.02473
C	0.576353	0.140059	1.223594
H	1.063608	0.3473	2.168022
C	-0.672705	-0.453408	1.201995
H	-1.168237	-0.711531	2.129432
C	-9.043131	-0.168739	-1.718393
H	-9.92859	0.255855	-2.196708
H	-9.37615	-0.991523	-1.082016
C	-8.359868	0.913812	-0.86278
C	-9.429057	1.539149	0.061118
H	-9.876104	0.758215	0.687345
H	-10.235404	1.971079	-0.542832
C	-8.798885	2.626221	0.949437
H	-9.571415	3.055691	1.595271
C	-7.695059	2.004239	1.81958
H	-7.249782	2.770345	2.46561
H	-8.119332	1.236251	2.473187
C	-6.605574	1.376142	0.929534
C	-7.252419	0.318768	0.021151
H	-6.488569	-0.123407	-0.617446
H	-7.667676	-0.478504	0.638222
C	-7.752847	2.030662	-1.733793
H	-8.531584	2.476227	-2.364489
H	-7.000301	1.602181	-2.401952
C	-7.115331	3.109773	-0.84317
H	-6.675499	3.887187	-1.475963
C	-8.192997	3.726464	0.062999
H	-8.973775	4.193796	-0.547105
H	-7.757111	4.513477	0.68803
C	-6.012075	2.48002	0.025816
H	-5.537489	3.251414	0.643173
H	-5.231082	2.050384	-0.611766
C	-5.462521	0.78256	1.771153
H	-4.958292	1.588871	2.308842
H	-4.721754	0.308454	1.126915
H	-8.741877	-3.457993	-0.130187

S	7.981365	1.215844	-3.02302
S	5.940194	0.17218	3.085432
C	7.648685	2.925463	-2.388983
H	8.593339	3.460094	-2.284245
H	7.087629	3.385592	-3.204715
C	6.873466	2.915551	-1.10621
C	7.499025	3.201204	0.110654
C	6.865631	2.91262	1.312498
H	7.394877	3.059797	2.247323
C	5.601875	2.327005	1.340864
C	4.909096	2.16507	0.118846
C	5.556414	2.469254	-1.087246
H	5.046512	2.256521	-2.019082
C	5.072558	1.74273	2.613458
H	4.001421	1.55907	2.562838
H	5.271377	2.395035	3.465543
C	3.604376	1.60494	0.084453
C	2.508655	1.091752	0.049955
C	9.039845	0.470442	-1.701925
H	9.953285	0.148418	-2.206932
H	9.311468	1.269692	-1.008944
C	8.443073	-0.717173	-0.925076
C	9.557585	-1.318674	-0.039785
H	9.942185	-0.549624	0.640294
H	10.395391	-1.644532	-0.667017
C	9.014097	-2.50932	0.769506
H	9.817905	-2.92036	1.388623
C	7.865413	-2.036025	1.674463
H	7.481031	-2.876902	2.264125
H	8.228695	-1.284157	2.381283
C	6.730603	-1.434556	0.823496
C	7.293237	-0.271423	-0.008188
H	6.496851	0.153103	-0.618632
H	7.646307	0.511587	0.663227
C	7.924839	-1.816127	-1.872797
H	8.73596	-2.156354	-2.527819
H	7.141331	-1.403267	-2.514741
C	7.373087	-2.999089	-1.060219
H	6.994613	-3.763583	-1.746189

C	8.495736	-3.59048	-0.192665
H	9.310367	-3.95304	-0.829175
H	8.12276	-4.449816	0.375211
C	6.224404	-2.517212	-0.155961
H	5.811473	-3.363318	0.405261
H	5.412226	-2.107354	-0.767073
C	5.545799	-0.986651	1.697304
H	5.098157	-1.863274	2.171211
H	4.775101	-0.519439	1.083481
H	8.509515	3.594962	0.114672

PPP-DDQ-1
Electronic Energy: -2332.314911 Hartrees
Free Energy: -2332.039658 Hartrees
Thermal Energy: 236.992 kcal/mol
Entropy: 217.545 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

C	6.397792	-0.933609	-1.224914
C	7.76834	-0.746019	1.196043
C	5.692949	-1.061071	-0.015034
C	7.768911	-0.715117	-1.216665
C	8.45842	-0.620405	-0.008735
C	6.397221	-0.964673	1.198041
C	4.28971	-1.273681	-0.018117
C	3.091045	-1.436383	-0.020592
C	1.68101	-1.561833	-0.022584
C	-1.14233	-1.657162	-0.024048
C	0.961689	-1.576386	-1.231868
C	0.961752	-1.615802	1.185657
C	-0.422281	-1.661161	1.185692
C	-0.422387	-1.621744	-1.233302
C	-2.556975	-1.614699	-0.023242
C	-3.760583	-1.487567	-0.021175
C	-5.167494	-1.306839	-0.017925
C	-7.933453	-0.909473	-0.010534
C	-5.869074	-1.179564	-1.228823
C	-5.869092	-1.224459	1.19686
C	-7.243049	-1.027898	1.194768

C	-7.243043	-0.98321	-1.219394
H	5.856173	-1.063511	2.130775
H	8.301327	-0.673348	2.13674
H	9.528429	-0.449921	-0.006301
H	8.302349	-0.618406	-2.154939
H	5.857205	-1.008563	-2.160137
H	1.502982	-1.528419	-2.167832
H	-0.964975	-1.614412	-2.170193
H	1.503124	-1.598348	2.122637
H	-0.964886	-1.684288	2.122307
H	-5.32416	-1.298221	2.128542
H	-7.775953	-0.959189	2.135573
H	-9.005701	-0.752536	-0.007626
H	-7.775939	-0.879718	-2.157016
H	-5.324156	-1.218393	-2.162603
C	0.80063	1.645887	-0.649213
C	0.79778	1.625221	0.699726
C	-0.472209	1.562116	1.47943
C	-1.750671	1.523217	0.694105
C	-1.747706	1.542823	-0.657388
C	-0.466094	1.606171	-1.435815
O	-0.493933	1.553822	2.686196
O	-0.482778	1.634981	-2.642352
C	-2.947136	1.450229	1.457887
N	-3.910709	1.398835	2.090438
C	-2.94087	1.490259	-1.428007
N	-3.901728	1.454281	-2.065713
Cl	2.235144	1.688741	1.635364
Cl	2.241804	1.738437	-1.576467

PPP-DDQ-2
Electronic Energy: -2332.313811 Hartrees
Free Energy: -2332.038155 Hartrees
Thermal Energy: 237.11 kcal/mol
Entropy: 217.08 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

C	-8.542945	1.215203	0.133252
C	-9.904287	-1.187547	0.515122

C	-7.845354	-0.001659	0.035571
C	-9.901873	1.222994	0.418137
C	-10.586997	0.024173	0.609887
C	-8.54537	-1.205345	0.230683
C	-6.455504	-0.014952	-0.255789
C	-5.271205	-0.026677	-0.504525
C	-3.884042	-0.04109	-0.795172
C	-1.125148	-0.069856	-1.36683
C	-3.179064	1.16085	-0.994631
C	-3.182676	-1.257849	-0.890195
C	-1.828391	-1.27204	-1.170953
C	-1.824757	1.146789	-1.275375
C	0.267967	-0.083376	-1.622603
C	1.463992	-0.094435	-1.802337
C	2.874941	-0.103598	-1.945314
C	5.674486	-0.117585	-2.15326
C	3.590395	1.102117	-2.055679
C	3.587344	-1.316143	-1.935494
C	4.974646	-1.317581	-2.040406
C	4.977729	1.089583	-2.159364
H	-8.010562	-2.143885	0.155918
H	-10.43346	-2.121524	0.663496
H	-11.647483	0.034173	0.831982
H	-10.429181	2.166919	0.490955
H	-8.006293	2.143639	-0.016667
H	-3.711283	2.100973	-0.924574
H	-1.28864	2.075517	-1.423909
H	-3.717668	-2.186861	-0.739472
H	-1.295064	-2.211725	-1.23883
H	3.04399	-2.247571	-1.839324
H	5.511763	-2.257671	-2.017434
H	6.755215	-0.122091	-2.217923
H	5.517295	2.025953	-2.229316
H	3.049392	2.039855	-2.052827
C	2.085911	-0.583886	1.386885
C	2.104314	0.76273	1.31208

C	3.376071	1.52047	1.126655
C	4.639018	0.715857	1.048655
C	4.620352	-0.634811	1.12039
C	3.336078	-1.391547	1.282622
O	3.40862	2.725115	1.056795
O	3.335334	-2.597313	1.338941
C	5.848236	1.452728	0.917336
N	6.832437	2.046062	0.815968
C	5.808515	-1.414558	1.068088
N	6.775617	-2.042407	1.029647
Cl	0.684316	1.719863	1.410489
Cl	0.641548	-1.485595	1.592341

PPP-DDQ-3

Electronic Energy: -2332.313290 Hartrees
Free Energy: -2332.037137 Hartree
Thermal Energy: 237.014 kcal/mol
Entropy: 215.723 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

C	-8.605762	-1.271341	-0.008222
C	-10.105315	0.934567	-0.81988
C	-7.981256	-0.018777	-0.144925
C	-9.961008	-1.41144	-0.275193
C	-10.715134	-0.311419	-0.6812
C	-8.75065	1.084481	-0.555313
C	-6.595924	0.129249	0.126736
C	-5.41428	0.254386	0.357734
C	-4.031849	0.399917	0.628931
C	-1.286167	0.686749	1.162548
C	-3.261909	-0.705244	1.039976
C	-3.401446	1.650677	0.486374
C	-2.052031	1.791594	0.746817
C	-1.91269	-0.56622	1.302133
C	0.101237	0.821615	1.398944
C	1.297516	0.918627	1.563024
C	2.70364	0.972681	1.727935
C	5.496107	1.015603	1.962487
C	3.391259	-0.121784	2.284163

C	3.439329	2.088343	1.290107
C	4.822745	2.104518	1.410285
C	4.776864	-0.095006	2.397568
H	-8.271807	2.049746	-0.662087
H	-10.688228	1.791783	-1.135778
H	-11.772576	-0.424674	-0.888841
H	-10.43147	-2.381644	-0.166822
H	-8.015198	-2.122447	0.306812
H	-3.738195	-1.67202	1.139924
H	-1.323873	-1.42544	1.595462
H	-3.986683	2.501746	0.162747
H	-1.569395	2.752858	0.625744
H	2.915086	2.925551	0.847217
H	5.379282	2.965094	1.059917
H	6.575918	1.028292	2.042612
H	5.294836	-0.950394	2.813686
H	2.828604	-0.981899	2.624819
C	4.724651	-0.877852	-0.81173
C	4.356141	0.264197	-1.426404
C	2.921847	0.600899	-1.661386
C	1.907786	-0.410221	-1.218555
C	2.280049	-1.523204	-0.539721
C	3.716902	-1.856553	-0.303141
O	2.575358	1.631633	-2.185654
O	4.033045	-2.885933	0.245023
C	0.556966	-0.133699	-1.556806
N	-0.53659	0.061886	-1.87082
C	1.323082	-2.425786	-0.002467
N	0.531577	-3.121754	0.467648
Cl	5.48755	1.412337	-2.024226
Cl	6.367001	-1.32648	-0.581837

PPP-DDQ-4
Electronic Energy: -2332.311906 Hartrees
Free Energy: -2332.036528 Hartrees
Thermal Enegy: 237.04 kcal/mol
Entropy: 217.43 cal mol^{-1} $kelvin^{-1}$

Imaginary Frequencies: 0

C	9.033973	1.173744	0.29735
C	10.195067	-0.573296	-1.539008
C	8.250681	0.167657	-0.295538
C	10.377955	1.298634	-0.028032
C	10.963146	0.427444	-0.945669
C	8.850318	-0.705951	-1.219987
C	6.875941	0.035499	0.033701
C	5.703904	-0.078778	0.313424
C	4.331711	-0.213821	0.639643
C	1.60876	-0.483705	1.290133
C	3.726281	0.656745	1.566044
C	3.547573	-1.218599	0.040753
C	2.209404	-1.353926	0.360189
C	2.38695	0.526264	1.883693
C	0.235534	-0.628207	1.595411
C	-0.945998	-0.788404	1.806283
C	-2.344377	-0.97341	1.873611
C	-5.122762	-1.305123	1.757798
C	-3.20606	0.113306	2.125909
C	-2.904247	-2.242722	1.609606
C	-4.277643	-2.401438	1.553074
C	-4.582044	-0.057145	2.066078
H	8.249245	-1.481384	-1.678062
H	10.646385	-1.252322	-2.252868
H	12.01231	0.527933	-1.197166
H	10.971815	2.077849	0.435162
H	8.57456	1.847821	1.009408
H	4.323479	1.433373	2.026579
H	1.925625	1.20082	2.593789
H	4.005328	-1.885088	-0.679023
H	1.60408	-2.115887	-0.114211
H	-2.242361	-3.077091	1.418715
H	-4.69847	-3.371506	1.320038
H	-6.196325	-1.428675	1.684967
H	-5.236567	0.788377	2.240862
H	-2.778055	1.083436	2.34445
C	-3.477375	1.743167	-0.659916

C	-4.78032	1.444867	-0.839285
C	-5.228978	0.078784	-1.234864
C	-4.161725	-0.957087	-1.374063
C	-2.849681	-0.652537	-1.210524
C	-2.402464	0.732055	-0.873096
O	-6.390411	-0.190227	-1.436376
O	-1.227329	0.999354	-0.779845
C	-4.595143	-2.273066	-1.692122
N	-4.936389	-3.348241	-1.935095
C	-1.813148	-1.615342	-1.359387
N	-0.959348	-2.384236	-1.463295
Cl	-6.042162	2.588067	-0.593324
Cl	-2.933154	3.297405	-0.164406

PCP-DDQ-1

Electronic Energy: -3674.562133 Hartrees
Free Energy: -3673.980546 Hartrees
Thermal Energy: 445.87 kcal/mol
Entropy: 273.48 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-1.01232	2.032251	2.979589
S	-2.763966	0.105808	-3.004891
C	0.052656	0.542462	2.702816
C	-0.388487	-0.239143	1.505039
C	0.317666	-0.171657	0.279312
C	-0.271325	-0.676937	-0.89196
C	-1.540293	-1.229269	-0.886569
C	-2.187818	-1.417207	0.357431
C	-1.589751	-0.926605	1.529556
C	-2.251451	-1.473042	-2.181302
C	1.594837	0.416787	0.203059
C	2.713904	0.882948	0.122675
C	4.044375	1.343725	0.069178
C	4.749652	1.606308	1.262324
C	6.089143	1.95985	1.216133
C	6.742527	2.065004	-0.011043
C	6.046663	1.837456	-1.199335
C	4.71028	1.474932	-1.166532
C	-3.476134	-2.00154	0.428701
C	-4.594842	-2.460759	0.485485

C	-5.910506	-2.989732	0.537042
C	-6.55206	-3.192293	1.771585
C	-7.841656	-3.70476	1.813143
C	-8.510794	-4.021114	0.631656
C	-7.882944	-3.822888	-0.597281
C	-6.593099	-3.312253	-0.649423
C	-0.720012	3.060614	1.469373
C	-1.928503	3.273772	0.54035
C	-1.525811	4.299296	-0.543012
C	-2.699879	4.549202	-1.505934
C	-3.092437	3.232119	-2.19438
C	-3.506515	2.184818	-1.142864
C	-2.33845	1.972062	-0.16679
C	-3.144096	3.825665	1.309687
C	-4.317707	4.064839	0.346012
C	-3.902993	5.093145	-0.718877
C	-4.703025	2.741686	-0.339078
C	-3.947776	0.865354	-1.801209
C	4.999216	-1.642386	-1.218955
C	3.700245	-2.008439	-1.274705
C	2.89831	-2.249448	-0.046472
C	3.547463	-1.877929	1.242136
C	4.852679	-1.500952	1.304527
C	5.688736	-1.377982	0.07612
O	1.790511	-2.740757	-0.074117
O	6.857673	-1.067909	0.140148
C	2.726061	-1.96274	2.399487
N	2.044176	-1.997428	3.329692
C	5.494095	-1.205111	2.538971
N	6.005404	-0.959116	3.543889
Cl	2.870267	-2.280657	-2.759614
Cl	5.978958	-1.471136	-2.625517
H	-6.02718	-2.94434	2.685534
H	-8.327245	-3.858244	2.769571
H	-9.517251	-4.420719	0.668449
H	-8.400623	-4.067797	-1.51715
H	-0.062371	-0.035459	3.619645
H	1.092803	0.850686	2.629362
H	-2.135626	-1.004456	2.461361

H	4.238305	1.5095	2.211301
H	6.631101	2.124779	2.138464
H	7.794973	2.317327	-0.042051
H	6.558125	1.916975	-2.150154
H	-0.376963	4.02951	1.839213
H	0.107841	2.612519	0.9173
H	-1.223963	5.240675	-0.06972
H	-0.658707	3.924275	-1.099081
H	-2.394674	5.277324	-2.264199
H	-3.644118	6.044243	-0.240905
H	-4.737979	5.2908	-1.399891
H	-2.872375	4.76262	1.810414
H	-3.435848	3.114995	2.088453
H	-3.920749	3.405301	-2.891843
H	-2.251457	2.848482	-2.779504
H	-1.484288	1.57437	-0.715249
H	-2.623856	1.234324	0.583092
H	-4.863738	1.038916	-2.370514
H	-4.174723	0.117013	-1.040793
H	-5.013884	2.006847	0.412257
H	-5.556884	2.902154	-1.007263
H	-5.177254	4.442051	0.909044
H	-1.589783	-1.933223	-2.916962
H	-3.12073	-2.114051	-2.052046
H	-6.10089	-3.156207	-1.601269
H	0.252514	-0.555128	-1.831338
H	4.167858	1.273456	-2.081245

PCP-DDQ-2
Electronic Energy: -3674.561846 Hartrees
Free Energy: -3673.981039 Hartrees
Thermal Energy: 445.95 kcal/mol
Entropy: 275.29 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	0.506402	1.894798	3.021541
S	-1.853166	1.62339	-3.050184
C	1.124872	0.264072	2.400062
C	0.454985	-0.116568	1.118863

C	1.122282	-0.010784	-0.122479
C	0.3803	-0.133173	-1.30583
C	-0.99717	-0.331451	-1.296265
C	-1.640228	-0.565028	-0.060074
C	-0.895216	-0.45603	1.122313
C	-1.781462	-0.161472	-2.556918
C	2.514258	0.241061	-0.188045
C	3.711333	0.404108	-0.242309
C	5.121631	0.541744	-0.300182
C	5.875233	0.636324	0.882222
C	7.258073	0.744718	0.821891
C	7.908337	0.75902	-0.411276
C	7.168057	0.665568	-1.588972
C	5.784624	0.55817	-1.539237
C	-3.01286	-0.905026	0.013015
C	-4.162694	-1.264394	0.114739
C	-5.492386	-1.737977	0.26875
C	-5.778415	-2.687927	1.264935
C	-7.07497	-3.160269	1.41982
C	-8.09714	-2.696243	0.592892
C	-7.818511	-1.756839	-0.39866
C	-6.525274	-1.278828	-0.564771
C	1.011022	3.084005	1.69495
C	-0.12643	3.766064	0.913214
C	0.500566	4.841912	-0.001544
C	-0.594011	5.554653	-0.815689
C	-1.334707	4.53177	-1.692638
C	-1.979507	3.444556	-0.811628
C	-0.881112	2.767083	0.022602
C	-1.134899	4.449661	1.856343
C	-2.231282	5.153012	1.039348
C	-1.591781	6.225188	0.142254
C	-2.967021	4.122727	0.164012
C	-2.766921	2.423669	-1.653104
C	2.509453	-2.925684	0.714493
C	2.596772	-2.975018	-0.630634
C	1.386535	-3.14952	-1.487306
C	0.07984	-3.327382	-0.779142
C	0.001652	-3.330847	0.574535

C	1.210775	-3.105188	1.426759
O	1.445015	-3.16405	-2.69399
O	1.126229	-3.086779	2.63309
C	-1.060437	-3.514145	-1.6078
N	-1.98438	-3.653908	-2.28473
C	-1.220538	-3.566382	1.264444
N	-2.212176	-3.768649	1.818102
Cl	4.080048	-2.808161	-1.476816
Cl	3.870756	-2.652317	1.72535
H	-4.973089	-3.052063	1.890391
H	-7.288569	-3.895688	2.186479
H	-9.107255	-3.068063	0.718355
H	-8.610904	-1.397809	-1.044761
H	0.873415	-0.432704	3.201676
H	2.207346	0.295154	2.299081
H	-1.406766	-0.571227	2.069562
H	5.364756	0.620336	1.836982
H	7.831242	0.816695	1.738595
H	8.987754	0.842065	-0.454282
H	7.67118	0.676142	-2.548572
H	1.602944	3.847083	2.205371
H	1.679884	2.556571	1.012915
H	1.049809	5.571302	0.604702
H	1.2246	4.372369	-0.677312
H	-0.130319	6.311714	-1.455906
H	-1.080796	6.973396	0.757955
H	-2.364708	6.750677	-0.429039
H	-0.615485	5.176771	2.491881
H	-1.581273	3.701348	2.517869
H	-2.107225	5.035351	-2.285907
H	-0.638259	4.06613	-2.396209
H	-0.17505	2.277819	-0.648114
H	-1.33096	2.000011	0.652047
H	-3.619367	2.924575	-2.117499
H	-3.162961	1.630154	-1.017442
H	-3.438717	3.36202	0.796427
H	-3.76693	4.615911	-0.399985
H	-2.947104	5.621139	1.72225
H	-1.29005	-0.643282	-3.403394

H	-2.786868	-0.565451	-2.468067
H	-6.301161	-0.550804	-1.334532
H	0.884351	0.014321	-2.253005
H	5.203267	0.48223	-2.449445

PCP-DDQ-3
Electronic Energy: -3674.555831 Hartrees
Free Energy: -3673.976928 Hartrees
Thermal Energy: 445.93 kcal/mol
Entropy: 277.15 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-1.008323	-1.184401	-3.052216
S	-3.087303	0.828546	2.796992
C	-0.877786	0.658358	-3.188591
C	-1.575605	1.350887	-2.058824
C	-0.85118	1.930305	-0.991141
C	-1.52804	2.29909	0.18318
C	-2.89387	2.113201	0.325959
C	-3.636399	1.668286	-0.794813
C	-2.958243	1.301152	-1.966256
C	-3.529726	2.235453	1.6767
C	0.554232	2.084344	-1.044485
C	1.756589	2.231292	-1.042603
C	3.156679	2.395526	-0.95782
C	4.025824	1.690271	-1.817931
C	5.400624	1.841382	-1.702498
C	5.935968	2.673251	-0.720391
C	5.082752	3.386352	0.129265
C	3.708842	3.255701	0.01304
C	-5.040347	1.489356	-0.717851
C	-6.232537	1.296201	-0.636058
C	-7.627382	1.06254	-0.516672
C	-8.38031	0.635571	-1.624496
C	-9.743156	0.403229	-1.496407
C	-10.376017	0.590065	-0.26833
C	-9.637482	1.012174	0.836226
C	-8.274513	1.24831	0.717998

C	-0.116301	-1.564568	-1.475124
C	-0.962764	-2.156657	-0.335182
C	-0.00461	-2.579274	0.801734
C	-0.799283	-3.175315	1.976088
C	-1.776115	-2.121608	2.522658
C	-2.754288	-1.681445	1.416622
C	-1.946244	-1.122232	0.23513
C	-1.754169	-3.395242	-0.796341
C	-2.553124	-3.981985	0.378772
C	-1.585578	-4.405396	1.495808
C	-3.529332	-2.922512	0.9204
C	-3.778196	-0.659328	1.941363
C	5.23939	-1.222129	-0.552636
C	6.3892	-0.763403	-0.018462
C	6.40039	0.14932	1.162973
C	5.068849	0.586173	1.678748
C	3.911136	0.121549	1.14459
C	3.910616	-0.850345	0.010088
O	7.425439	0.519951	1.68521
O	2.875963	-1.307456	-0.416924
C	5.081115	1.504857	2.763194
N	5.078912	2.262722	3.633297
C	2.633267	0.50244	1.635722
N	1.585239	0.80568	2.011936
Cl	7.936025	-1.153515	-0.658208
Cl	5.189996	-2.243686	-1.934451
H	-7.883189	0.490728	-2.575434
H	-10.314355	0.074615	-2.356646
H	-11.439671	0.407149	-0.172361
H	-10.125915	1.157447	1.792547
H	-1.355077	0.873044	-4.146205
H	0.169958	0.945028	-3.254916
H	-3.528123	0.872829	-2.781612
H	3.604135	1.030161	-2.565455
H	6.05804	1.295307	-2.368262
H	7.009501	2.774087	-0.618042

H	5.497548	4.031791	0.89345
H	0.670196	-2.269323	-1.747565
H	0.379704	-0.65297	-1.143942
H	0.717108	-3.312322	0.42433
H	0.565607	-1.709503	1.137851
H	-0.103393	-3.46798	2.769194
H	-0.89748	-5.172824	1.124208
H	-2.141676	-4.846602	2.330475
H	-1.064056	-4.148712	-1.194791
H	-2.432464	-3.115014	-1.607913
H	-2.336432	-2.531716	3.371766
H	-1.222244	-1.251385	2.885979
H	-1.392204	-0.244169	0.567061
H	-2.630545	-0.809381	-0.553557
H	-4.419902	-1.143676	2.681144
H	-4.421286	-0.312277	1.131666
H	-4.233989	-2.62519	0.135145
H	-4.119821	-3.34461	1.741896
H	-3.121488	-4.85137	0.032598
H	-3.150163	3.104609	2.216397
H	-4.61217	2.319506	1.60658
H	-7.696279	1.574895	1.573349
H	-0.944809	2.641076	1.029227
H	3.045076	3.792903	0.677644

PCP-DDQ-4
Electronic Energy: -3674.554892 Hartrees
Free Energy: -3673.973535 Hartrees
Thermal Energy: 446.01 kcal/mol
Entropy: 274.327 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-1.503892	1.226976	3.309012
S	-2.783828	-0.784633	-2.767448
C	-1.313468	-0.611904	3.43559
C	-1.830581	-1.319369	2.221224
C	-0.949099	-1.826575	1.238429
C	-1.456532	-2.216729	-0.010083

C	-2.80571	-2.113585	-0.311986
C	-3.702768	-1.739014	0.717299
C	-3.193262	-1.356159	1.966772
C	-3.265963	-2.24328	-1.731682
C	0.449477	-1.850737	1.457116
C	1.648479	-1.831387	1.621828
C	3.051389	-1.718788	1.759064
C	3.607697	-0.761405	2.624388
C	4.985778	-0.609739	2.707042
C	5.835376	-1.426008	1.955683
C	5.295494	-2.389998	1.10757
C	3.917229	-2.52778	0.991875
C	-5.096549	-1.643976	0.475017
C	-6.280076	-1.51952	0.253949
C	-7.662472	-1.364161	-0.028481
C	-8.568235	-1.018495	0.989593
C	-9.917566	-0.86161	0.702182
C	-10.385583	-1.044205	-0.598246
C	-9.494812	-1.385991	-1.614754
C	-8.143967	-1.546323	-1.337135
C	-0.476259	1.691622	1.838982
C	-1.239304	2.260754	0.629386
C	-0.200883	2.796451	-0.381746
C	-0.909328	3.364912	-1.623209
C	-1.735198	2.257724	-2.299093
C	-2.789897	1.709906	-1.318581
C	-2.070367	1.173782	-0.071089
C	-2.170596	3.42004	1.032206
C	-2.882284	3.983559	-0.20887
C	-1.837591	4.515482	-1.203235
C	-3.708418	2.872163	-0.87982
C	-3.670701	0.633365	-1.976347
C	6.801308	0.212845	-0.736982
C	6.295873	-0.73431	-1.552107
C	4.826164	-0.910371	-1.732566
C	3.938537	-0.008363	-0.931094
C	4.448718	0.949729	-0.117841
C	5.9214	1.151819	0.023631

O	4.359232	-1.73362	-2.482355
O	6.366971	2.036829	0.714568
C	2.54198	-0.193656	-1.110474
N	1.406355	-0.341987	-1.251754
C	3.617355	1.817392	0.641685
N	2.939267	2.510856	1.266546
Cl	7.279984	-1.841505	-2.424622
Cl	8.487475	0.422111	-0.481277
H	-8.199051	-0.876368	1.997516
H	-10.607127	-0.595196	1.494555
H	-11.43921	-0.920167	-0.818573
H	-9.854656	-1.527564	-2.627058
H	-1.901069	-0.858473	4.321526
H	-0.272522	-0.857644	3.6352
H	-3.882085	-0.983833	2.715126
H	2.95019	-0.122893	3.199662
H	5.402355	0.150766	3.35636
H	6.909489	-1.310548	2.036427
H	5.948095	-3.027877	0.523221
H	0.234913	2.434023	2.203621
H	0.098695	0.814003	1.542191
H	0.41372	3.569607	0.091127
H	0.469171	1.985159	-0.675916
H	-0.157294	3.735654	-2.327595
H	-1.255901	5.320531	-0.740893
H	-2.33471	4.939334	-2.082996
H	-1.588791	4.209533	1.52283
H	-2.908598	3.062679	1.756353
H	-2.23033	2.651428	-3.19528
H	-1.079025	1.442911	-2.618026
H	-1.415455	0.352832	-0.362804
H	-2.80825	0.784213	0.630198
H	-4.256351	1.090506	-2.777447
H	-4.375728	0.223617	-1.252154
H	-4.467237	2.496488	-0.183677
H	-4.239217	3.275365	-1.750192
H	-3.550876	4.795696	0.094714
H	-2.769572	-3.07446	-2.23521

H	-4.341439	-2.395116	-1.795014
H	-7.447932	-1.809928	-2.123717
H	-0.757091	-2.49972	-0.786551
H	3.491904	-3.258749	0.315972

PCP-DDQ-5
Electronic Energy: -3674.554823 Hartrees
Free Energy: -3673.975370 Hartrees
Thermal Energy: 445.99 kcal/mol
Entropy: 278.28 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-0.957185	1.592679	2.9618
S	-3.243425	0.397591	-3.0357
C	-0.001305	0.093869	2.439577
C	-0.561474	-0.529882	1.198448
C	0.058573	-0.345068	-0.058348
C	-0.631833	-0.702076	-1.224921
C	-1.920359	-1.213819	-1.184401
C	-2.488779	-1.516356	0.075293
C	-1.787801	-1.176043	1.241831
C	-2.73451	-1.281871	-2.439687
C	1.337484	0.255712	-0.160843
C	2.433834	0.759598	-0.244964
C	3.750273	1.280728	-0.320673
C	4.42784	1.675025	0.846931
C	5.735098	2.144867	0.775351
C	6.387834	2.227565	-0.453425
C	5.724226	1.838855	-1.615866
C	4.41647	1.368373	-1.555767
C	-3.793948	-2.061253	0.179805
C	-4.924027	-2.484853	0.271014
C	-6.25539	-2.969189	0.364496
C	-6.823361	-3.264157	1.616134
C	-8.128372	-3.730896	1.699733
C	-8.886588	-3.90988	0.543666
C	-8.332184	-3.619231	-0.701975
C	-7.027758	-3.153055	-0.795992

C	-0.74329	2.765969	1.546437
C	-2.01282	3.118722	0.750923
C	-1.656988	4.24791	-0.241883
C	-2.893014	4.639934	-1.070712
C	-3.389807	3.421365	-1.865211
C	-3.760352	2.274725	-0.904935
C	-2.52766	1.918215	-0.059026
C	-3.141504	3.615768	1.674689
C	-4.377345	3.997578	0.84402
C	-4.008286	5.126883	-0.131383
C	-4.867089	2.772602	0.051513
C	-4.302457	1.051391	-1.665417
C	3.839875	-2.180408	-0.566066
C	3.845088	-2.022579	0.773377
C	5.016325	-1.439864	1.490094
C	6.21182	-1.084075	0.657554
C	6.210855	-1.250507	-0.68492
C	5.013239	-1.795812	-1.404234
O	5.024566	-1.267631	2.684808
O	5.022487	-1.926008	-2.604097
C	7.342659	-0.584583	1.360421
N	8.26443	-0.184067	1.926885
C	7.341554	-0.940077	-1.489603
N	8.263548	-0.692583	-2.137394
Cl	2.515193	-2.455917	1.767041
Cl	2.499318	-2.819879	-1.42317
H	-6.230373	-3.122155	2.510903
H	-8.556416	-3.95558	2.669543
H	-9.904733	-4.273941	0.613105
H	-8.91881	-3.756577	-1.602652
H	-0.097103	-0.570633	3.299901
H	1.048314	0.354443	2.3253
H	-2.269504	-1.333184	2.199194
H	3.923971	1.602075	1.802465
H	6.251243	2.430834	1.683376
H	7.411453	2.576744	-0.502804
H	6.23228	1.88612	-2.571043
H	-0.332238	3.67676	1.987737
H	0.01879	2.353173	0.883866

H	-1.282693	5.120281	0.30605
H	-0.851615	3.912632	-0.905479
H	-2.620617	5.439638	-1.766741
H	-3.675682	6.009584	0.425654
H	-4.886088	5.425172	-0.714935
H	-2.794925	4.481383	2.251883
H	-3.398631	2.830267	2.391269
H	-4.263121	3.697071	-2.468425
H	-2.613089	3.081326	-2.556428
H	-1.735872	1.560137	-0.717034
H	-2.781323	1.109366	0.626156
H	-5.251923	1.314889	-2.136895
H	-4.498876	0.229723	-0.97561
H	-5.146035	1.967106	0.740391
H	-5.764241	3.033162	-0.521673
H	-5.174265	4.334299	1.514634
H	-2.149587	-1.671021	-3.274814
H	-3.616923	-1.90604	-2.31671
H	-6.593279	-2.925201	-1.761393
H	-0.179118	-0.480348	-2.183684
H	3.903357	1.05764	-2.456959

PCP-DDQ-6
Electronic Energy: -3674.554426 Hartrees
Free Energy: -3673.975433 Hartrees
Thermal Energy: 445.87 kcal/mol
Entropy: 278.85 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-1.174213	1.666151	2.987609
S	-3.303918	0.236379	-3.024686
C	-0.172551	0.175933	2.529513
C	-0.695052	-0.491352	1.296828
C	-0.052542	-0.334701	0.047944
C	-0.705493	-0.746015	-1.12214
C	-1.984592	-1.279084	-1.092241
C	-2.5756	-1.550347	0.164654
C	-1.908422	-1.161286	1.334767
C	-2.764227	-1.409956	-2.363321

C	1.219235	0.280423	-0.049259
C	2.312224	0.792784	-0.139445
C	3.631615	1.299445	-0.246866
C	4.338475	1.707412	0.898477
C	5.652209	2.146772	0.791155
C	6.28364	2.186564	-0.451029
C	5.59164	1.784379	-1.59135
C	4.2764	1.343582	-1.496234
C	-3.871781	-2.118171	0.257069
C	-4.995269	-2.561496	0.335306
C	-6.318646	-3.069452	0.412737
C	-6.907927	-3.345328	1.658947
C	-8.205227	-3.835594	1.726541
C	-8.934962	-4.057533	0.559616
C	-8.359359	-3.786276	-0.680792
C	-7.062414	-3.296814	-0.75877
C	-0.961259	2.800294	1.540519
C	-2.220963	3.098469	0.707058
C	-1.869631	4.206925	-0.31044
C	-3.095129	4.545126	-1.177656
C	-3.544862	3.292631	-1.947139
C	-3.910221	2.165498	-0.962302
C	-2.689509	1.863231	-0.078638
C	-3.381825	3.594255	1.590604
C	-4.607014	3.922325	0.722009
C	-4.242542	5.031767	-0.277593
C	-5.049766	2.663955	-0.045493
C	-4.406896	0.908172	-1.698745
C	6.28649	-1.144833	0.717963
C	6.369185	-1.275017	-0.621554
C	5.198803	-1.706233	-1.441889
C	3.932268	-2.014665	-0.703281
C	3.856471	-1.912905	0.643465
C	5.022903	-1.433277	1.455878
O	5.25759	-1.828698	-2.641537
O	4.924577	-1.302343	2.651692
C	2.818587	-2.394162	-1.50072
N	1.910435	-2.683048	-2.151148
C	2.680882	-2.230989	1.375517

N	1.741347	-2.509532	1.984901
Cl	7.817842	-0.991334	-1.499664
Cl	7.617586	-0.671313	1.695778
H	-6.336776	-3.170448	2.562056
H	-8.649466	-4.045358	2.692458
H	-9.947156	-4.44002	0.616556
H	-8.923505	-3.957235	-1.590094
H	-0.265769	-0.472303	3.401337
H	0.872431	0.459022	2.427428
H	-2.404265	-1.30381	2.286844
H	3.850821	1.665474	1.864216
H	6.18845	2.448142	1.682592
H	7.311652	2.518077	-0.52782
H	6.079778	1.801325	-2.558077
H	-0.58161	3.734703	1.960311
H	-0.176027	2.386285	0.906321
H	-1.528353	5.103619	0.219748
H	-1.041797	3.87195	-0.946021
H	-2.825825	5.331159	-1.890457
H	-3.943399	5.937946	0.260604
H	-5.113714	5.291894	-0.888825
H	-3.069097	4.484073	2.150262
H	-3.636324	2.823229	2.323577
H	-4.410438	3.529816	-2.577382
H	-2.74497	2.951268	-2.610702
H	-1.874912	1.503485	-0.707214
H	-2.941101	1.06956	0.624388
H	-5.350652	1.137229	-2.199063
H	-4.602698	0.103521	-0.989081
H	-5.32558	1.87183	0.65989
H	-5.939465	2.886627	-0.645766
H	-5.426762	4.258893	1.364754
H	-2.145331	-1.80831	-3.168889
H	-3.63278	-2.053741	-2.243092
H	-6.611386	-3.084157	-1.720033
H	-0.228207	-0.565697	-2.076595
H	3.738164	1.026122	-2.380446

PCP-DDQ-7
Electronic Energy: -3674.552521 Hartrees
Free Energy: -3673.969021 Hartrees
Thermal Energy: 445.34 kcal/mol
Entropy: 267.57 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 1

S	-0.937289	-0.907112	-3.050395
S	-3.009372	0.234604	3.018554
C	-0.299072	0.79811	-2.700646
C	-0.947939	1.408756	-1.494146
C	-0.215717	1.668688	-0.312278
C	-0.913825	1.902613	0.883491
C	-2.299775	1.945308	0.928181
C	-3.014524	1.892566	-0.29182
C	-2.31952	1.611178	-1.476539
C	-3.011374	1.919692	2.245706
C	1.20119	1.751532	-0.316425
C	2.39423	1.955893	-0.30022
C	3.776332	2.27721	-0.27499
C	4.557148	2.197705	-1.441354
C	5.900679	2.558686	-1.414125
C	6.488312	3.010789	-0.232276
C	5.727996	3.076863	0.932302
C	4.386486	2.704807	0.919028
C	-4.42764	2.003503	-0.324512
C	-5.636449	2.057056	-0.353324
C	-7.055312	2.10058	-0.368114
C	-7.761327	2.016837	-1.580909
C	-9.149355	2.051153	-1.586144
C	-9.854441	2.167967	-0.389186
C	-9.163	2.250965	0.818493
C	-7.775045	2.218512	0.834066
C	-0.426867	-1.879511	-1.56205
C	-1.542347	-2.447481	-0.66833
C	-0.889093	-3.427138	0.332942
C	-1.948703	-4.018297	1.276982
C	-2.624286	-2.882881	2.062246
C	-3.29925	-1.893928	1.09326
C	-2.241669	-1.335702	0.127859

C	-2.603388	-3.217533	-1.477474
C	-3.668417	-3.79986	-0.532547
C	-3.003314	-4.774141	0.452894
C	-4.344483	-2.66208	0.252678
C	-4.030988	-0.77536	1.853084
C	3.719806	-0.93859	0.608075
C	4.08013	-1.057584	-0.685966
C	5.477678	-0.794391	-1.140499
C	6.441527	-0.298714	-0.106848
C	6.067387	-0.130977	1.182398
C	4.680345	-0.458085	1.644432
O	5.833855	-0.977997	-2.278926
O	4.373045	-0.334812	2.804971
C	7.76223	-0.023559	-0.556063
N	8.834467	0.205189	-0.915268
C	6.965498	0.346457	2.176094
N	7.696477	0.743604	2.975368
Cl	2.989243	-1.522186	-1.9263
Cl	2.14312	-1.29036	1.184564
H	-7.208605	1.925206	-2.507472
H	-9.683801	1.986262	-2.52657
H	-10.937593	2.194201	-0.397487
H	-9.707798	2.34152	1.750803
H	-0.543199	1.34262	-3.614942
H	0.784377	0.768433	-2.600894
H	-2.888296	1.451657	-2.384272
H	4.100445	1.857924	-2.362463
H	6.492373	2.482364	-2.318255
H	7.535353	3.285548	-0.217405
H	6.18207	3.404658	1.859171
H	0.173393	-2.705417	-1.948592
H	0.233534	-1.2452	-0.972443
H	-0.381022	-4.230555	-0.212473
H	-0.12477	-2.90471	0.916437
H	-1.463603	-4.705804	1.977069
H	-2.534735	-5.59994	-0.093483
H	-3.755851	-5.212527	1.11731
H	-2.125407	-4.023729	-2.046803

H	-3.070527	-2.543169	-2.201012
H	-3.371902	-3.294741	2.750441
H	-1.883792	-2.35237	2.669058
H	-1.501201	-0.760911	0.68878
H	-2.722608	-0.655481	-0.572211
H	-4.820148	-1.217269	2.465852
H	-4.508365	-0.08951	1.153548
H	-4.837814	-1.969089	-0.438155
H	-5.121058	-3.071781	0.908708
H	-4.423878	-4.328877	-1.122039
H	-2.496593	2.531974	2.987662
H	-4.037139	2.272545	2.159895
H	-7.233678	2.282275	1.769772
H	-0.348666	2.000598	1.802585
H	3.795981	2.751919	1.825228

CPC-DDQ-1
Electronic Energy: -5016.795998 Hartrees
Free Energy: -5015.908793 Hartrees
Thermal Energy: 654.66 kcal/mol
Entropy: 330.44 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	8.434426	-1.47606	-1.732741
S	5.286764	3.673497	0.734618
C	8.357464	-0.305752	-3.166813
H	9.362421	0.049896	-3.397245
H	8.026956	-0.943913	-3.988498
C	7.412028	0.832099	-2.924664
C	7.893441	2.109308	-2.619536
C	7.044289	3.083562	-2.11125
H	7.449164	4.038022	-1.794241
C	5.694269	2.819023	-1.892255
C	5.175727	1.582572	-2.340832
C	6.042362	0.604388	-2.849431
H	5.640869	-0.373501	-3.084292
C	4.862792	3.752438	-1.069234
H	3.797903	3.570678	-1.198798
H	5.066764	4.794809	-1.320091

C	3.799336	1.276237	-2.191183
C	2.633112	0.997895	-2.026981
C	1.303136	0.619834	-1.739664
C	0.669396	-0.409469	-2.467996
H	1.206891	-0.889428	-3.275712
C	-0.617894	-0.811933	-2.152565
H	-1.09663	-1.599028	-2.721538
C	-1.307313	-0.222304	-1.079408
C	-0.672452	0.802718	-0.347879
H	-1.193667	1.254054	0.486895
C	0.601811	1.225384	-0.681223
H	1.083913	2.003263	-0.103806
C	9.114126	-0.429108	-0.368651
H	10.012278	-0.945314	-0.021845
H	9.430032	0.519511	-0.808221
C	8.183336	-0.16799	0.828647
C	9.004219	0.549534	1.923337
H	9.411845	1.485226	1.522661
H	9.855851	-0.074421	2.218819
C	8.120839	0.845288	3.147958
H	8.720686	1.3534	3.910014
C	6.951046	1.752409	2.732484
H	6.32245	1.97718	3.602335
H	7.332593	2.704875	2.352997
C	6.105778	1.064234	1.643839
C	7.005353	0.739113	0.44152
H	6.412291	0.242748	-0.326168
H	7.387707	1.669042	0.020324
C	7.624124	-1.479671	1.412942
H	8.450319	-2.140478	1.702825
H	7.042254	-1.999019	0.646286
C	6.737145	-1.177847	2.632591
H	6.336679	-2.11712	3.028164
C	7.572486	-0.474595	3.713869
H	8.397683	-1.121023	4.033171
H	6.956364	-0.27572	4.597551
C	5.568962	-0.268705	2.212071
H	4.915227	-0.071902	3.068235
H	4.965385	-0.768887	1.450975

C	4.903218	1.927919	1.223611
H	4.200607	2.004954	2.054372
H	4.372609	1.457221	0.39568
H	8.952463	2.319703	-2.721871
S	-8.697273	-0.728643	-2.25971
S	-5.031041	1.12853	2.807049
C	-8.315549	-2.328759	-1.406163
H	-9.228303	-2.727223	-0.962128
H	-8.025339	-2.98426	-2.229572
C	-7.223963	-2.182676	-0.38943
C	-7.51244	-2.184214	0.97822
C	-6.564131	-1.76199	1.901242
H	-6.829266	-1.691159	2.950083
C	-5.308893	-1.314713	1.494479
C	-4.967603	-1.441353	0.128038
C	-5.926591	-1.883957	-0.792413
H	-5.673622	-1.892286	-1.845691
C	-4.420543	-0.58647	2.454179
H	-3.38764	-0.546084	2.119037
H	-4.43151	-1.055406	3.439267
C	-3.689002	-1.036356	-0.336392
C	-2.601202	-0.662505	-0.710178
C	-9.315721	0.349006	-0.888966
H	-10.309004	0.677607	-1.202558
H	-9.441942	-0.281928	-0.006444
C	-8.460897	1.580017	-0.53671
C	-9.258232	2.445509	0.464723
H	-9.492665	1.853615	1.357208
H	-10.211913	2.748295	0.017292
C	-8.445703	3.690885	0.86065
H	-9.027056	4.289305	1.569224
C	-7.127489	3.257545	1.521681
H	-6.54842	4.140144	1.818464
H	-7.333007	2.684721	2.430735
C	-6.301505	2.396101	0.547263
C	-7.136684	1.175606	0.129821
H	-6.561233	0.566721	-0.566702

H	-7.343121	0.564885	1.009065
C	-8.149467	2.433616	-1.781287
H	-9.084118	2.742382	-2.264646
H	-7.593389	1.831682	-2.505852
C	-7.329062	3.671651	-1.382947
H	-7.102769	4.258764	-2.27858
C	-8.139413	4.524833	-0.393858
H	-9.071057	4.859627	-0.862949
H	-7.575834	5.422792	-0.118261
C	-6.011541	3.229761	-0.720931
H	-5.412207	4.109335	-0.45923
H	-5.420122	2.632828	-1.424642
C	-4.955355	1.978544	1.165478
H	-4.34612	2.8705	1.330167
H	-4.407622	1.331645	0.479701
H	-8.50521	-2.461517	1.315392
C	-1.101081	-3.174869	0.756151
C	-0.522741	-3.711511	-0.338308
C	0.831862	-3.290626	-0.799831
C	1.516537	-2.223043	0.00028
C	-0.461513	-2.050465	1.501734
C	0.905507	-1.636445	1.059312
O	1.375584	-3.79179	-1.754146
O	-1.008061	-1.496421	2.426454
Cl	-2.608814	-3.707825	1.374077
Cl	-1.270834	-4.938249	-1.280346
C	2.838949	-1.895313	-0.399632
C	1.53063	-0.611928	1.821693
N	3.919828	-1.63657	-0.711403
N	2.0394	0.223303	2.433698

CPC-DDQ-2
Electronic Energy: -5016.795950 Hartrees
Free Energy: -5015.909918 Hartrees
Thermal Energy: 654.58 kcal/mol
Entropy: 332.661 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	7.575809	-1.540604	-2.442569

S	5.947811	3.668101	1.072722
C	7.280066	-0.250433	-3.741374
H	8.232066	0.014889	-4.20204
H	6.676713	-0.773132	-4.485799
C	6.573009	0.947289	-3.183174
C	7.25348	2.140501	-2.919471
C	6.674174	3.121068	-2.12469
H	7.249844	3.997627	-1.850439
C	5.408587	2.948255	-1.565778
C	4.656117	1.821417	-1.964185
C	5.252424	0.838126	-2.768922
H	4.689068	-0.058246	-2.99456
C	4.938058	3.853824	-0.46904
H	3.887211	3.693431	-0.233933
H	5.07377	4.905148	-0.729892
C	3.317944	1.604208	-1.548151
C	2.169072	1.329222	-1.280589
C	0.852836	0.895678	-1.012557
C	0.318113	-0.186702	-1.741764
H	0.925485	-0.65643	-2.504707
C	-0.951945	-0.656588	-1.477875
H	-1.34879	-1.500936	-2.026778
C	-1.751124	-0.052293	-0.480725
C	-1.227697	1.045314	0.231886
H	-1.828848	1.510196	1.002413
C	0.05015	1.504824	-0.02253
H	0.454464	2.330327	0.548685
C	8.776441	-0.698423	-1.314745
H	9.658188	-1.342453	-1.289524
H	9.066757	0.237616	-1.796313
C	8.306895	-0.422171	0.122781
C	9.510129	0.149731	0.907198
H	9.86434	1.064889	0.418375
H	10.338835	-0.567632	0.891083
C	9.107602	0.453982	2.360283
H	9.972535	0.858274	2.895824
C	7.970345	1.488346	2.373075
H	7.684523	1.719601	3.406022
H	8.307955	2.422277	1.913817

C	6.749484	0.947364	1.604663
C	7.17471	0.616284	0.165273
H	6.313872	0.239908	-0.389046
H	7.507545	1.530498	-0.324734
C	7.832899	-1.709101	0.824113
H	8.634246	-2.457662	0.809139
H	6.98394	-2.132188	0.278965
C	7.425189	-1.399781	2.274395
H	7.076747	-2.319793	2.754873
C	8.63508	-0.841348	3.039803
H	9.445995	-1.578079	3.054695
H	8.361925	-0.640255	4.081286
C	6.288088	-0.363886	2.28113
H	5.975789	-0.157996	3.31131
H	5.417091	-0.75618	1.752895
C	5.574979	1.94182	1.625794
H	5.201013	2.038621	2.647048
H	4.752002	1.568234	1.019089
H	8.266366	2.272628	-3.283785
S	-8.874534	-1.79634	-2.239085
S	-6.101025	1.379884	2.738081
C	-8.352183	-3.165572	-1.103925
H	-9.238312	-3.639726	-0.680829
H	-7.87648	-3.878579	-1.780022
C	-7.415309	-2.690317	-0.035156
C	-7.854965	-2.524522	1.281791
C	-7.089109	-1.818904	2.200703
H	-7.479505	-1.630879	3.194364
C	-5.87192	-1.247127	1.838003
C	-5.359567	-1.533153	0.550985
C	-6.135677	-2.258419	-0.364541
H	-5.762244	-2.394814	-1.372204
C	-5.210658	-0.247392	2.732812
H	-4.165782	-0.096295	2.477923
H	-5.258213	-0.557699	3.77741
C	-4.102901	-1.019795	0.14558
C	-3.034711	-0.555023	-0.184471
C	-9.793086	-0.643321	-1.121514
H	-	-0.53425	-1.566066

	10.784806		
H	-9.917459	-1.147	-0.160502
C	-9.175656	0.750641	-0.907481
C	-10.195865	1.612774	-0.130641
H	-10.432798	1.130409	0.824851
H	-11.13097	1.683923	-0.698083
C	-9.62583	3.020025	0.120156
H	-10.362501	3.613652	0.670754
C	-8.335708	2.91359	0.948654
H	-7.930364	3.913898	1.14242
H	-8.548489	2.456857	1.919574
C	-7.290777	2.063825	0.200328
C	-7.885155	0.674305	-0.077059
H	-7.153953	0.069472	-0.61281
H	-8.092319	0.178232	0.871237
C	-8.864836	1.447869	-2.246001
H	-9.778395	1.522894	-2.847997
H	-8.151008	0.844109	-2.813833
C	-8.286097	2.84941	-1.990965
H	-8.055933	3.325388	-2.94946
C	-9.315944	3.695738	-1.225378
H	-10.231829	3.79818	-1.817682
H	-8.925961	4.705396	-1.05651
C	-6.995433	2.734514	-1.15996
H	-6.565728	3.729907	-0.998703
H	-6.249736	2.14463	-1.705311
C	-5.972177	1.968916	0.988656
H	-5.52006	2.961701	1.05012
H	-5.26516	1.320996	0.469418
H	-8.829616	-2.901991	1.57138
C	1.540138	-2.929141	-0.336372
C	2.502886	-2.033976	-0.032188
C	2.295301	-0.995024	1.015242
C	0.987327	-0.998298	1.720348
C	0.230408	-2.95475	0.379338
C	0.026428	-1.915802	1.434168

O	3.148285	-0.180783	1.291546
O	-0.62647	-3.771843	0.135223
Cl	1.720971	-4.1023	-1.580589
Cl	4.028185	-1.98084	-0.82504
C	0.806903	-0.003818	2.720281
C	-1.207122	-1.958821	2.136112
N	0.646658	0.806523	3.526036
N	-2.20595	-1.985608	2.713649

CPC-DDQ-3
Electronic Energy: -5016.794728 Hartrees
Free Energy: -5015.909061 Hartrees
Thermal Energy: 654.59 kcal/mol
Entropy: 333.46 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	7.575057	-1.312006	-3.236332
S	6.292828	0.219626	2.972933
C	7.653166	0.539805	-3.232554
H	8.683723	0.857153	-3.394642
H	7.071804	0.812962	-4.115282
C	7.083619	1.129376	-1.977893
C	7.920077	1.660158	-0.990854
C	7.430678	1.938181	0.278673
H	8.108889	2.274049	1.054767
C	6.101763	1.685279	0.611382
C	5.223174	1.280499	-0.421011
C	5.725628	1.018325	-1.704
H	5.051784	0.631104	-2.458452
C	5.666999	1.6977	2.042619
H	4.58832	1.771177	2.147859
H	6.110621	2.533687	2.584991
C	3.853427	1.043336	-0.152086
C	2.693312	0.808828	0.104389
C	1.332371	0.657697	0.435991
C	0.348049	0.572086	-0.571187
H	0.656781	0.566266	-1.608704
C	-0.991995	0.524459	-0.241232
H	-1.744057	0.478222	-1.018427

C	-1.402774	0.557955	1.106492
C	-0.414412	0.583979	2.117195
H	-0.724169	0.601041	3.153708
C	0.923466	0.631988	1.789212
H	1.6748	0.687339	2.565994
C	8.661969	-1.789152	-1.817158
H	9.417669	-2.454705	-2.240213
H	9.173394	-0.886235	-1.476549
C	7.978738	-2.487059	-0.626904
C	9.081339	-2.991507	0.330825
H	9.695066	-2.146016	0.662906
H	9.744811	-3.684924	-0.198713
C	8.453069	-3.692923	1.548063
H	9.249496	-4.042353	2.212711
C	7.554375	-2.702852	2.306143
H	7.112621	-3.1919	3.182561
H	8.14761	-1.859237	2.67091
C	6.436954	-2.182731	1.381669
C	7.075875	-1.518172	0.152402
H	6.29081	-1.155428	-0.510423
H	7.659954	-0.655979	0.474917
C	7.135788	-3.694138	-1.081684
H	7.767017	-4.403914	-1.629765
H	6.356229	-3.355045	-1.770024
C	6.501307	-4.385709	0.136181
H	5.893874	-5.230584	-0.203575
C	7.610939	-4.888388	1.073681
H	8.243714	-5.61376	0.55063
H	7.173594	-5.403852	1.935671
C	5.604224	-3.387995	0.890689
H	5.129358	-3.885017	1.744444
H	4.800851	-3.034955	0.233884
C	5.495326	-1.217511	2.123687
H	4.970592	-1.764443	2.910643
H	4.740239	-0.824941	1.442094
H	8.974046	1.802251	-1.203579
S	-7.305758	-3.494696	2.33092
S	-6.1597	1.576127	-1.611236
C	-7.712296	-2.037243	3.402207

H	-8.786844	-2.013386	3.585919
H	-7.212641	-2.27557	4.343133
C	-7.222107	-0.749434	2.812444
C	-8.109954	0.158216	2.227984
C	-7.638841	1.191148	1.428398
H	-8.342228	1.840931	0.920125
C	-6.277966	1.341759	1.168112
C	-5.371561	0.510715	1.863984
C	-5.857495	-0.512618	2.690138
H	-5.149736	-1.193707	3.146751
C	-5.816481	2.257944	0.079266
H	-4.763825	2.510156	0.16542
H	-6.384515	3.189839	0.081236
C	-3.96982	0.591225	1.643682
C	-2.77909	0.563534	1.425658
C	-8.256884	-3.161178	0.779868
H	-8.899741	-4.032822	0.638786
H	-8.904673	-2.302772	0.970253
C	-7.436238	-2.923543	-0.501235
C	-8.416612	-2.891084	-1.695275
H	-9.157887	-2.098348	-1.540986
H	-8.963746	-3.839073	-1.75245
C	-7.653284	-2.646053	-3.008477
H	-8.364704	-2.627058	-3.840144
C	-6.920671	-1.297185	-2.934105
H	-6.384574	-1.108769	-3.872069
H	-7.640688	-0.484005	-2.803816
C	-5.926655	-1.295533	-1.756942
C	-6.693629	-1.578767	-0.455309
H	-5.994523	-1.589105	0.38033
H	-7.407637	-0.774247	-0.277635
C	-6.410018	-4.047806	-0.740989
H	-6.922299	-5.016137	-0.789165
H	-5.713764	-4.091161	0.101557
C	-5.642086	-3.79371	-2.048923
H	-4.907279	-4.591267	-2.197389
C	-6.630712	-3.772913	-3.22612
H	-7.142011	-4.738634	-3.303244
H	-6.094415	-3.615555	-4.168284

C	-4.91169	-2.440923	-1.968298
H	-4.342671	-2.269383	-2.889518
H	-4.193286	-2.451429	-1.140378
C	-5.147999	0.029766	-1.681751
H	-4.526842	0.130028	-2.575596
H	-4.482701	0.030148	-0.818485
H	-9.178128	0.019252	2.354159
C	-1.536132	3.540603	-1.054709
C	-0.296389	3.562696	-1.587392
C	0.923976	3.680022	-0.740783
C	0.703673	3.712583	0.735297
C	-0.544611	3.702099	1.271642
C	-1.759893	3.654527	0.413701
O	-2.868133	3.698332	0.902377
O	2.040198	3.73445	-1.204597
Cl	-2.961875	3.332082	-1.993905
Cl	-0.006702	3.407494	-3.276544
C	-0.763349	3.735176	2.676078
C	1.874344	3.760228	1.540372
N	-0.92972	3.74717	3.817844
N	2.826362	3.780778	2.191939

CPC-DDQ-4
Electronic Energy: -5016.794317 Hartrees
Free Energy: -5015.909671 Hartrees
Thermal Energy: 654.67 kcal/mol
Entropy: 335.87 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-9.163944	-0.036984	-3.002222
S	-6.684906	-1.75891	2.782875
C	-9.182758	-1.889216	-3.071201
H	-10.215221	-2.239574	-3.052892
H	-8.76993	-2.103018	-4.058991
C	-8.369361	-2.50646	-1.973883
C	-8.98858	-3.108699	-0.874947
C	-8.258008	-3.413894	0.26616
H	-8.766137	-3.803865	1.140971

C	-6.898779	-3.121146	0.352901
C	-6.241334	-2.639882	-0.802675
C	-6.987691	-2.348928	-1.953201
H	-6.484459	-1.897401	-2.799587
C	-6.201767	-3.167611	1.676786
H	-5.119487	-3.184378	1.567077
H	-6.502932	-4.042728	2.255122
C	-4.853696	-2.33791	-0.779981
C	-3.684514	-2.028271	-0.737818
C	-2.324108	-1.641859	-0.649419
C	-1.580653	-1.33846	-1.804928
H	-2.057054	-1.416237	-2.77388
C	-0.258593	-0.943017	-1.708324
H	0.307264	-0.706513	-2.600384
C	0.364428	-0.833221	-0.452285
C	-0.376257	-1.139578	0.703581
H	0.097368	-1.054274	1.673406
C	-1.69655	-1.538992	0.606646
H	-2.262993	-1.769064	1.500204
C	-9.982117	0.337816	-1.38615
H	-10.824958	0.988293	-1.630102
H	-10.390923	-0.598395	-0.999941
C	-9.113275	1.01454	-0.310385
C	-10.035668	1.42819	0.858272
H	-10.545457	0.542643	1.255438
H	-10.811074	2.112631	0.495433
C	-9.217706	2.10534	1.971987
H	-9.888492	2.390136	2.788758
C	-8.158127	1.125796	2.501015
H	-7.579128	1.596929	3.304331
H	-8.642101	0.241742	2.92645
C	-7.214273	0.69604	1.361627
C	-8.046095	0.055229	0.239496
H	-7.385248	-0.243681	-0.573656
H	-8.52819	-0.845368	0.620469

C	-8.414096	2.276376	-0.852257
H	-9.161577	2.979526	-1.238779
H	-7.764191	2.002096	-1.688286
C	-7.589748	2.944164	0.260752
H	-7.087467	3.829029	-0.142803
C	-8.523263	3.356549	1.410389
H	-9.268704	4.073546	1.049414
H	-7.952434	3.85508	2.201341
C	-6.531901	1.957417	0.786477
H	-5.925459	2.439175	1.562088
H	-5.852097	1.669225	-0.023466
C	-6.115083	-0.254289	1.868011
H	-5.473316	0.283337	2.569978
H	-5.487429	-0.585338	1.040271
H	-10.058723	-3.283616	-0.892245
S	7.495936	-0.471932	-2.850305
S	4.876771	-1.239328	3.061797
C	7.11639	1.266672	-2.333774
H	8.042479	1.81244	-2.15835
H	6.631757	1.697368	-3.21148
C	6.222768	1.28603	-1.134768
C	6.719644	1.619769	0.127499
C	5.960206	1.381039	1.26397
H	6.375003	1.594248	2.241899
C	4.695614	0.78923	1.1847
C	4.14037	0.561484	-0.094873
C	4.906536	0.832606	-1.23653
H	4.495274	0.59671	-2.210201
C	4.032047	0.280832	2.422935
H	2.975816	0.074348	2.266218
H	4.124927	0.993483	3.244194
C	2.833637	0.029965	-0.237226
C	1.705444	-0.391929	-0.345994
C	8.43673	-1.151235	-1.408422
H	9.389169	-1.492421	-1.819867
H	8.651672	-0.319467	-0.734249
C	7.776655	-2.30495	-0.631282
C	8.803736	-2.844067	0.389698

H	9.114042	-2.035262	1.061411
H	9.701397	-3.191805	-0.134045
C	8.19224	-3.99733	1.204852
H	8.934232	-4.364167	1.920892
C	6.95608	-3.492848	1.966794
H	6.523243	-4.306589	2.560651
H	7.242374	-2.699849	2.66411
C	5.905373	-2.953367	0.977348
C	6.539166	-1.828489	0.14487
H	5.803423	-1.446508	-0.562061
H	6.821402	-1.010292	0.807164
C	7.362053	-3.458072	-1.565336
H	8.235995	-3.820861	-2.119217
H	6.641453	-3.090148	-2.301672
C	6.743444	-4.604551	-0.748313
H	6.440864	-5.408883	-1.426049
C	7.779971	-5.134188	0.255925
H	8.656218	-5.518761	-0.277125
H	7.359768	-5.967421	0.829473
C	5.506978	-4.092127	0.011983
H	5.047789	-4.91328	0.57407
H	4.755808	-3.725771	-0.69709
C	4.635689	-2.476158	1.704762
H	4.152	-3.33221	2.180623
H	3.923824	-2.055074	0.993621
H	7.714587	2.038032	0.221689
C	1.987594	3.097191	-0.696532
C	2.034505	3.072535	0.651409
C	3.24191	3.517723	1.405874
C	4.408885	3.982377	0.592584
C	3.169903	3.501193	-1.513105
C	4.384744	3.949354	-0.762566
O	3.284034	3.524337	2.614469
O	3.157913	3.485066	-2.721037
Cl	0.597649	2.636538	-1.590927
Cl	0.72194	2.530085	1.617089
C	5.529737	4.472651	1.31803
C	5.493289	4.361472	-1.552374
N	6.438805	4.881621	1.899098

N	6.396214	4.683499	-2.194754

CPC-DDQ-5
Electronic Energy: -5016.793393 Hartrees
Free Energy: -5015.909642 Hartrees
Thermal Energy: 654.67 kcal/mol
Entropy: 337.74 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-8.967326	-1.382803	-3.000684
S	-6.927257	-0.370481	3.113477
C	-9.031195	-3.075285	-2.247695
H	-10.071721	-3.386177	-2.149059
H	-8.561428	-3.701352	-3.008791
C	-8.307296	-3.141641	-0.936812
C	-9.011952	-3.204297	0.268755
C	-8.365471	-2.972999	1.476014
H	-8.939619	-2.941772	2.39521
C	-7.007876	-2.663352	1.520654
C	-6.264411	-2.733597	0.31996
C	-6.926689	-2.981538	-0.89077
H	-6.358017	-2.943913	-1.812004
C	-6.401979	-2.117174	2.775813
H	-5.315366	-2.16912	2.760201
H	-6.759886	-2.652413	3.656951
C	-4.874358	-2.443541	0.302438
C	-3.702873	-2.140364	0.279271
C	-2.340957	-1.74982	0.270085
C	-1.572931	-1.838943	-0.905724
H	-2.031922	-2.22453	-1.807099
C	-0.249877	-1.435184	-0.914922
H	0.334492	-1.501184	-1.823879
C	0.349945	-0.929078	0.251528
C	-0.415485	-0.840251	1.428856
H	0.038417	-0.433192	2.323344
C	-1.737662	-1.244611	1.437728
H	-2.32413	-1.167268	2.344449
C	-9.878658	-0.337079	-1.77684

H	-10.685094	0.135997	-2.341528
H	-10.33807	-1.008838	-1.048516
C	-9.063851	0.747963	-1.049499
C	-10.049839	1.632131	-0.253358
H	-10.610742	1.011228	0.45494
H	-10.778834	2.083485	-0.936167
C	-9.288662	2.733917	0.504449
H	-10.003831	3.347784	1.061125
C	-8.295792	2.091876	1.486355
H	-7.758418	2.870992	2.040137
H	-8.832776	1.484387	2.220832
C	-7.290576	1.206742	0.72474
C	-8.063937	0.133545	-0.057413
H	-7.359353	-0.491266	-0.605436
H	-8.596151	-0.508289	0.645033
C	-8.293976	1.643292	-2.039557
H	-8.993235	2.100728	-2.749738
H	-7.597957	1.029954	-2.619107
C	-7.52669	2.736816	-1.278073
H	-6.973236	3.354352	-1.992582
C	-8.522121	3.611214	-0.498559
H	-9.22072	4.092935	-1.191377
H	-7.99082	4.40932	0.031269
C	-6.535414	2.087069	-0.2962
H	-5.968207	2.863632	0.229768
H	-5.811948	1.473016	-0.844613
C	-6.255113	0.582064	1.676174
H	-5.647788	1.376697	2.115783
H	-5.581846	-0.076335	1.12662
H	-10.082703	-3.375832	0.255309
S	7.064354	-0.009977	-3.037431
S	5.338404	-1.719944	3.010767
C	6.742905	1.613132	-2.202865
H	7.679179	2.155611	-2.076085

H	6.127379	2.15999	-2.920409
C	6.033422	1.41682	-0.902319
C	6.702679	1.588407	0.317129
C	6.123678	1.161966	1.49965
H	6.671375	1.245429	2.430481
C	4.864506	0.554431	1.512834
C	4.134853	0.487486	0.30269
C	4.730172	0.924534	-0.886886
H	4.195091	0.792511	-1.819339
C	4.390473	-0.148054	2.742588
H	3.324993	-0.362497	2.711176
H	4.603279	0.434308	3.640534
C	2.823086	-0.05003	0.268416
C	1.69325	-0.480954	0.245034
C	8.204604	-0.875298	-1.862916
H	9.087361	-1.127556	-2.454478
H	8.513982	-0.14761	-1.109736
C	7.671847	-2.148806	-1.180247
C	8.84196	-2.801082	-0.409712
H	9.241092	-2.090318	0.323194
H	9.655795	-3.041844	-1.103104
C	8.365988	-4.078488	0.304192
H	9.208169	-4.524264	0.842567
C	7.251823	-3.727363	1.303583
H	6.917606	-4.631451	1.826149
H	7.631512	-3.036562	2.062312
C	6.062586	-3.080543	0.568004
C	6.557614	-1.828463	-0.172001
H	5.722481	-1.373306	-0.70257
H	6.924813	-1.105008	0.555573
C	7.132747	-3.164119	-2.20596
H	7.917813	-3.416431	-2.92862
H	6.308689	-2.713163	-2.766827
C	6.650112	-4.435644	-1.487864
H	6.257297	-5.140894	-2.22694
C	7.827425	-5.075626	-0.734308
H	8.618704	-5.351783	-1.439648
H	7.502713	-5.996011	-0.237082
C	5.535472	-4.077494	-0.488262

H	5.171305	-4.985566	0.005504
H	4.684534	-3.634155	-1.018128
C	4.90984	-2.752499	1.53446
H	4.509111	-3.683022	1.94282
H	4.096653	-2.254663	1.004825
H	7.691972	2.029405	0.326105
C	2.496804	3.331099	-1.112944
C	1.843133	3.013878	0.024186
C	2.530286	3.044123	1.348715
C	3.926369	3.586513	1.370527
C	3.89467	3.853323	-1.102674
C	4.547971	3.993019	0.235853
O	1.996825	2.664593	2.364021
O	4.47087	4.181959	-2.114033
Cl	1.776729	3.196278	-2.668161
Cl	0.198793	2.525489	0.054362
C	4.537539	3.67939	2.651398
C	5.843466	4.579011	0.245522
N	5.029684	3.74218	3.693212
N	6.88864	5.068015	0.255063

CPC-DDQ-6
Electronic Energy: -5016.794223 Hartrees
Free Energy: -5015.908730 Hartrees
Thermal Energy: 654.733 kcal/mol
Entropy: 334.3 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-9.08052	-0.76536	-2.832187
S	-6.968644	0.180672	3.267165
C	-9.187257	-2.45516	-2.078533
H	-10.235592	-2.736104	-1.972933
H	-8.740574	-3.09486	-2.842152
C	-8.456771	-2.541761	-0.772496
C	-9.153997	-2.583416	0.438347
C	-8.491577	-2.372357	1.640665
H	-9.057802	-2.321432	2.563884
C	-7.124084	-2.107928	1.67551

C	-6.391973	-2.203851	0.469915
C	-7.071638	-2.425157	-0.736475
H	-6.508522	-2.4075	-1.66171
C	-6.491529	-1.578978	2.924853
H	-5.406695	-1.657538	2.897359
H	-6.853493	-2.105088	3.809854
C	-4.989217	-1.983741	0.441382
C	-3.799447	-1.765541	0.398702
C	-2.407758	-1.504695	0.345823
C	-1.745997	-1.405737	-0.892642
H	-2.314419	-1.531861	-1.805243
C	-0.387794	-1.153217	-0.947035
H	0.115574	-1.083857	-1.902924
C	0.35759	-0.990167	0.234797
C	-0.302198	-1.084491	1.473041
H	0.267334	-0.962178	2.385534
C	-1.661241	-1.337328	1.527265
H	-2.162995	-1.411293	2.483724
C	-9.956336	0.302127	-1.601768
H	-10.752928	0.798169	-2.160715
H	-10.429591	-0.358693	-0.872337
C	-9.109058	1.362994	-0.87639
C	-10.067289	2.266071	-0.067722
H	-10.636486	1.654879	0.642397
H	-10.791347	2.737576	-0.74213
C	-9.274349	3.346141	0.688579
H	-9.970284	3.973852	1.254153
C	-8.288549	2.676514	1.659125
H	-7.728441	3.440239	2.211849
H	-8.833649	2.078417	2.395267
C	-7.310806	1.771461	0.884894
C	-8.115749	0.72062	0.104399
H	-7.430327	0.08182	-0.451971
H	-8.656924	0.088392	0.808543
C	-8.326778	2.244721	-1.868807

H	-9.021074	2.72178	-2.570891
H	-7.650232	1.618068	-2.457186
C	-7.527774	3.316381	-1.108771
H	-6.965957	3.924266	-1.825024
C	-8.496116	4.210039	-0.316905
H	-9.189091	4.71105	-1.001648
H	-7.941982	4.993181	0.211899
C	-6.543791	2.638994	-0.138172
H	-5.954395	3.399593	0.38668
H	-5.839122	2.011231	-0.695473
C	-6.283337	1.115566	1.824236
H	-5.647913	1.890931	2.258351
H	-5.635371	0.438188	1.266754
H	-10.229609	-2.721736	0.432977
S	6.831852	1.896088	2.831011
S	4.219146	1.554289	-3.121637
C	7.297231	0.192566	2.270448
H	8.372493	0.136257	2.10641
H	7.053157	-0.437534	3.127243
C	6.52677	-0.198634	1.049835
C	7.13758	-0.229282	-0.206041
C	6.368182	-0.332066	-1.356227
H	6.847132	-0.300739	-2.327596
C	4.972386	-0.389658	-1.296679
C	4.357932	-0.481106	-0.02704
C	5.147971	-0.403387	1.12786
H	4.661883	-0.412661	2.095577
C	4.165348	-0.204325	-2.540398
H	3.131318	-0.51385	-2.407455
H	4.588216	-0.76599	-3.375058
C	2.951241	-0.615192	0.090297
C	1.753586	-0.763287	0.170301
C	7.369959	2.972685	1.42471
H	8.056737	3.699685	1.863554
H	7.947236	2.351709	0.736468
C	6.260048	3.717863	0.660775
C	6.930507	4.703584	-0.322232
H	7.585292	4.152192	-1.006996

H	7.561108	5.409076	0.230627
C	5.862078	5.47045	-1.121927
H	6.356638	6.162098	-1.811012
C	5.005861	4.477643	-1.924618
H	4.250915	5.018679	-2.507312
H	5.632124	3.929879	-2.635137
C	4.31521	3.481635	-0.973745
C	5.389848	2.749897	-0.155336
H	4.907817	2.048364	0.524554
H	6.024244	2.176732	-0.831255
C	5.350993	4.517482	1.613907
H	5.95319	5.224425	2.196844
H	4.875935	3.834064	2.323833
C	4.279564	5.274857	0.812143
H	3.633465	5.825591	1.502879
C	4.962549	6.256175	-0.153966
H	5.557049	6.983976	0.40882
H	4.209815	6.819714	-0.715779
C	3.426725	4.274914	0.010727
H	2.644811	4.80925	-0.540805
H	2.92405	3.579585	0.692709
C	3.417709	2.495697	-1.742634
H	2.598253	3.046141	-2.210333
H	2.973353	1.770889	-1.059352
H	8.214542	-0.140663	-0.283722
C	3.658737	-3.657965	-0.88863
C	3.599547	-3.736824	0.456731
C	4.818522	-3.576246	1.303277
C	6.118648	-3.39515	0.584088
C	6.1833	-3.374807	-0.769961
C	4.950512	-3.476117	-1.611884
O	5.015637	-3.428096	-2.818524
O	4.776014	-3.602313	2.510283
Cl	2.264751	-3.757667	-1.887298
Cl	2.135199	-3.988725	1.31426
C	7.418728	-3.273942	-1.467412
C	7.276014	-3.275296	1.401801
N	8.425896	-3.202346	-2.025796
N	8.212475	-3.165803	2.067139

CPC-DDQ-7
Electronic Energy: -5016.792703 Hartrees
Free Energy: -5015.908367 Hartrees
Thermal Energy: 654.552 kcal/mol
Entropy: 336.12 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-9.117765	-0.635552	-3.123287
S	-6.925151	-1.066658	3.006785
C	-9.199105	-2.454119	-2.773491
H	-10.243327	-2.764262	-2.722368
H	-8.757451	-2.897174	-3.668225
C	-8.449459	-2.827442	-1.530279
C	-9.129346	-3.150911	-0.352482
C	-8.452555	-3.208026	0.859077
H	-9.00598	-3.37699	1.776017
C	-7.088438	-2.93608	0.937803
C	-6.372381	-2.744269	-0.266186
C	-7.065249	-2.702556	-1.48442
H	-6.515566	-2.46473	-2.387059
C	-6.44308	-2.698023	2.267253
H	-5.358392	-2.760646	2.210554
H	-6.791188	-3.414256	3.013514
C	-4.977774	-2.477534	-0.253338
C	-3.801905	-2.190945	-0.240279
C	-2.435167	-1.820381	-0.204191
C	-1.663364	-1.80196	-1.380382
H	-2.12314	-2.086528	-2.317956
C	-0.33776	-1.413081	-1.34374
H	0.249096	-1.387078	-2.252742
C	0.259574	-1.029493	-0.129439
C	-0.509817	-1.046094	1.048493
H	-0.064784	-0.722584	1.980077
C	-1.834551	-1.438018	1.010655
H	-2.427073	-1.437543	1.916663
C	-9.985121	0.114219	-1.672015
H	-10.795448	0.713056	-2.093782

H	-10.439875	-0.701066	-1.105124
C	-9.137755	0.994824	-0.735776
C	-10.09336	1.67808	0.268003
H	-10.645834	0.914085	0.827491
H	-10.831975	2.28051	-0.273387
C	-9.300838	2.568933	1.240466
H	-9.995005	3.042732	1.94192
C	-8.293942	1.709823	2.021558
H	-7.733531	2.335621	2.72639
H	-8.82182	0.95301	2.609258
C	-7.318352	1.017377	1.050737
C	-8.123523	0.159934	0.06166
H	-7.439543	-0.32601	-0.633529
H	-8.647636	-0.623104	0.610078
C	-8.378614	2.088763	-1.511448
H	-9.087881	2.703375	-2.078878
H	-7.703733	1.621189	-2.234228
C	-7.57987	2.970699	-0.537184
H	-7.034677	3.732371	-1.103437
C	-8.546059	3.648445	0.447833
H	-9.254096	4.28247	-0.097186
H	-7.992319	4.298464	1.13402
C	-6.574624	2.1041	0.242374
H	-5.985659	2.733631	0.919106
H	-5.870961	1.629401	-0.450583
C	-6.270718	0.180791	1.805928
H	-5.639502	0.846977	2.398451
H	-5.621696	-0.341731	1.102807
H	-10.203441	-3.298953	-0.37709
S	7.189306	-0.500375	-3.097143
S	5.162318	-1.310787	3.03953
C	6.755842	1.219144	-2.560471
H	7.664079	1.815924	-2.47559
H	6.169367	1.605662	-3.396017
C	5.972937	1.214069	-1.285366
C	6.563202	1.59346	-0.076314

C	5.924903	1.33338	1.126746
H	6.416017	1.576417	2.061592
C	4.689918	0.6807	1.169544
C	4.033008	0.410275	-0.053403
C	4.681295	0.694811	-1.26312
H	4.194144	0.424717	-2.191933
C	4.173265	0.147616	2.467503
H	3.122813	-0.128069	2.411429
H	4.294971	0.873992	3.2732
C	2.733857	-0.155315	-0.078231
C	1.603054	-0.587283	-0.100811
C	8.285976	-1.107686	-1.735832
H	9.216277	-1.404642	-2.22499
H	8.512373	-0.255658	-1.091257
C	7.759419	-2.281939	-0.890788
C	8.902143	-2.750672	0.037721
H	9.227985	-1.916324	0.669842
H	9.766187	-3.058742	-0.562092
C	8.430236	-3.921567	0.917687
H	9.252986	-4.238011	1.566456
C	7.243136	-3.470811	1.78409
H	6.90996	-4.296786	2.42348
H	7.548447	-2.653293	2.443981
C	6.07966	-3.002199	0.88926
C	6.573491	-1.858732	-0.010272
H	5.75688	-1.527722	-0.651115
H	6.868657	-1.015449	0.6139
C	7.324264	-3.469303	-1.771126
H	8.162469	-3.794634	-2.39878
H	6.520998	-3.15105	-2.442137
C	6.844801	-4.633755	-0.888369
H	6.525463	-5.463282	-1.52692
C	7.995217	-5.092736	0.022119
H	8.838906	-5.439019	-0.584735
H	7.674147	-5.93801	0.640324
C	5.65695	-4.175212	-0.023198
H	5.295769	-5.010502	0.587365
H	4.825528	-3.860256	-0.664052
C	4.858746	-2.578663	1.725129

H	4.462829	-3.450294	2.251002
H	4.065006	-2.202215	1.078094
H	7.542964	2.056498	-0.078743
C	4.392981	4.057928	0.551148
C	4.139622	3.980704	-0.772011
C	2.880288	3.380343	-1.297663
C	1.895974	2.882468	-0.282599
C	3.453948	3.493586	1.56338
C	2.188658	2.893214	1.040162
O	2.640619	3.300255	-2.478818
O	3.672551	3.536243	2.752328
Cl	5.79121	4.827099	1.190465
Cl	5.21012	4.604026	-1.965619
C	0.664815	2.388274	-0.790198
C	1.320692	2.315121	2.005652
N	-0.351848	2.022623	-1.196631
N	0.632573	1.803335	2.777621

CPC-DDQ-8
Electronic Energy: -5016.792620 Hartrees
Free Energy: -5015.907714 Hartrees
Thermal Energy: 654.617 kcal/mol
Entropy: 335.14 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-9.166957	-0.890403	-2.814892
S	-7.053606	0.155645	3.269451
C	-9.270142	-2.568795	-2.03488
H	-10.317975	-2.850398	-1.925815
H	-8.821263	-3.218836	-2.788403
C	-8.54041	-2.633804	-0.727231
C	-9.238536	-2.655591	0.483682
C	-8.576834	-2.424088	1.68269
H	-9.143372	-2.359248	2.604872
C	-7.209775	-2.157204	1.713579
C	-6.476558	-2.272152	0.51016
C	-7.155384	-2.516031	-0.692495
H	-6.591524	-2.513562	-1.617431

C	-6.57731	-1.609458	2.954678
H	-5.492627	-1.689693	2.92871
H	-6.939949	-2.121419	3.847657
C	-5.075113	-2.046886	0.478181
C	-3.886773	-1.821297	0.430714
C	-2.498208	-1.548261	0.370117
C	-1.799162	-1.674883	-0.84528
H	-2.333195	-1.994439	-1.730824
C	-0.445234	-1.406891	-0.910081
H	0.089155	-1.531796	-1.842405
C	0.254886	-0.999939	0.240866
C	-0.439732	-0.878326	1.457799
H	0.09975	-0.579131	2.347107
C	-1.794166	-1.147083	1.520952
H	-2.324436	-1.055683	2.460219
C	-10.044793	0.194654	-1.601606
H	-10.84235	0.680547	-2.168129
H	-10.51676	-0.455526	-0.861839
C	-9.199748	1.26835	-0.892553
C	-10.159957	2.180488	-0.096484
H	-10.727133	1.578018	0.622664
H	-10.885618	2.640347	-0.777253
C	-9.369523	3.273363	0.643843
H	-10.066851	3.907362	1.20074
C	-8.381438	2.620294	1.623272
H	-7.822984	3.393404	2.164595
H	-8.924423	2.031415	2.368321
C	-7.401684	1.706685	0.861768
C	-8.204323	0.642652	0.096884
H	-7.517765	-0.002532	-0.450615
H	-8.743695	0.019318	0.810218
C	-8.420149	2.137646	-1.89798
H	-9.115997	2.602732	-2.606604
H	-7.742098	1.504405	-2.47746
C	-7.623631	3.222223	-1.153711

H	-7.063693	3.821169	-1.878926
C	-8.594086	4.124668	-0.374397
H	-9.288704	4.613912	-1.066031
H	-8.041756	4.916823	0.142826
C	-6.637422	2.561355	-0.174015
H	-6.049844	3.331007	0.339637
H	-5.931355	1.927649	-0.722578
C	-6.372004	1.067622	1.810301
H	-5.737496	1.851262	2.230771
H	-5.7235	0.382597	1.263004
H	-10.314048	-2.794975	0.479965
S	6.725875	1.972618	2.856833
S	4.164693	1.591706	-3.117465
C	7.164948	0.256994	2.312827
H	8.241792	0.185732	2.159233
H	6.901177	-0.357111	3.17585
C	6.402477	-0.144045	1.089465
C	7.026336	-0.197039	-0.160146
C	6.269897	-0.305133	-1.317168
H	6.757803	-0.285076	-2.28454
C	4.874179	-0.352283	-1.272157
C	4.247153	-0.427229	-0.006304
C	5.024591	-0.335383	1.156222
H	4.526595	-0.330281	2.11798
C	4.081336	-0.162109	-2.525586
H	3.040501	-0.452066	-2.403761
H	4.502816	-0.734299	-3.354085
C	2.841842	-0.576814	0.101154
C	1.645559	-0.748318	0.174123
C	7.277122	3.028603	1.440037
H	7.967137	3.755732	1.87367
H	7.852202	2.3954	0.76104
C	6.175954	3.772728	0.662538
C	6.858319	4.748665	-0.322158
H	7.515634	4.189583	-0.998364
H	7.487903	5.455304	0.230582
C	5.799422	5.514554	-1.135381
H	6.30242	6.199296	-1.82535

C	4.945339	4.519669	-1.937517
H	4.197147	5.059551	-2.529802
H	5.574663	3.964298	-2.639391
C	4.243163	3.532994	-0.98528
C	5.307992	2.802329	-0.153013
H	4.817172	2.108214	0.5282
H	5.944525	2.220208	-0.819381
C	5.263389	4.583436	1.602866
H	5.864144	5.292355	2.18507
H	4.780016	3.907372	2.314123
C	4.201179	5.339208	0.7874
H	3.552152	5.897448	1.469305
C	4.895793	6.310938	-0.180066
H	5.488873	7.040371	0.382226
H	4.149897	6.873448	-0.75187
C	3.350492	4.336964	-0.013517
H	2.575033	4.870413	-0.574825
H	2.839555	3.648665	0.6694
C	3.349463	2.544859	-1.755485
H	2.535161	3.093515	-2.23394
H	2.897529	1.825368	-1.071339
H	8.104671	-0.112253	-0.226019
C	6.130705	-3.463184	0.651591
C	6.328207	-3.425306	-0.682718
C	5.187697	-3.415646	-1.643661
C	3.81643	-3.511443	-1.055276
C	3.617135	-3.623678	0.280043
C	4.76473	-3.555295	1.242242
O	4.571794	-3.586265	2.434118
O	5.343613	-3.36325	-2.84199
Cl	7.422818	-3.458335	1.787121
Cl	7.892765	-3.411849	-1.394958
C	2.326859	-3.790544	0.850339
C	2.734018	-3.454922	-1.974385
N	1.281313	-3.963197	1.307982
N	1.850067	-3.363518	-2.710333

CPC-DDQ-9

Electronic Energy: -5016.790888 Hartrees
Free Energy: -5015.906363 Hartrees
Thermal Energy: 654.59 kcal/mol
Entropy: 335.86 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	8.259782	-1.451812	-2.950642
S	5.970019	0.055603	2.973047
C	8.481292	0.386387	-2.869757
H	9.545639	0.619832	-2.828442
H	8.097732	0.723595	-3.834661
C	7.735863	0.996692	-1.721438
C	8.413065	1.439318	-0.581589
C	7.717125	1.727711	0.585355
H	8.26222	1.990345	1.485026
C	6.334411	1.57493	0.657207
C	5.632681	1.259489	-0.529021
C	6.345134	0.985147	-1.704483
H	5.79825	0.65866	-2.580736
C	5.642248	1.590331	1.984497
H	4.568089	1.729327	1.881693
H	6.032404	2.380621	2.628201
C	4.220466	1.114049	-0.519287
C	3.021866	0.955167	-0.484231
C	1.615127	0.820719	-0.403673
C	0.811466	0.922911	-1.553463
H	1.283143	1.07158	-2.516072
C	-0.568535	0.868608	-1.457951
H	-1.178276	0.970265	-2.346844
C	-1.196608	0.705621	-0.208517
C	-0.391761	0.57654	0.93892
H	-0.864259	0.449762	1.904749
C	0.988325	0.633329	0.842298
H	1.59705	0.554447	1.733829
C	9.027409	-2.043752	-1.375076
H	9.794694	-2.760307	-1.6764
H	9.535217	-1.192443	-0.916593
C	8.086555	-2.707296	-0.352938
C	8.954785	-3.317816	0.770094
H	9.5601	-2.531287	1.235739

H	9.64921	-4.051806	0.345398
C	8.064286	-3.990353	1.829582
H	8.697593	-4.415568	2.614591
C	7.119731	-2.946607	2.446827
H	6.490436	-3.41601	3.212381
H	7.698741	-2.160708	2.940843
C	6.231936	-2.320695	1.354178
C	7.132267	-1.684651	0.283561
H	6.510454	-1.246884	-0.496648
H	7.711269	-0.878673	0.735085
C	7.251893	-3.833473	-0.993076
H	7.917018	-4.580494	-1.442602
H	6.638131	-3.419472	-1.798289
C	6.356187	-4.496314	0.066442
H	5.759029	-5.282685	-0.405876
C	7.235397	-5.104933	1.170744
H	7.896792	-5.867875	0.745856
H	6.610874	-5.601091	1.921578
C	5.414203	-3.44554	0.680576
H	4.75607	-3.919943	1.417573
H	4.772624	-3.016404	-0.097518
C	5.242787	-1.300759	1.945077
H	4.546175	-1.820747	2.606907
H	4.655099	-0.838439	1.151603
H	9.495748	1.50059	-0.591911
S	-7.789289	-1.133313	3.012036
S	-5.916625	-0.542491	-3.211686
C	-7.889534	0.69339	2.710009
H	-8.934744	1.003616	2.726917
H	-7.394286	1.116914	3.585733
C	-7.212704	1.093734	1.435081
C	-7.957521	1.432243	0.301641
C	-7.349228	1.524993	-0.943288
H	-7.951924	1.710854	-1.824855
C	-5.988308	1.274827	-1.100321
C	-5.209899	1.071294	0.06137
C	-5.831486	0.991509	1.314598
H	-5.228185	0.770248	2.185499
C	-5.410803	1.078284	-2.465623

H	-4.32606	1.150657	-2.464908
H	-5.798781	1.813857	-3.170781
C	-3.806506	0.890182	-0.027755
C	-2.607048	0.74783	-0.105538
C	-8.724512	-1.854497	1.588157
H	-9.509278	-2.468784	2.035329
H	-9.211885	-1.030057	1.063293
C	-7.917931	-2.707393	0.591613
C	-8.912877	-3.382257	-0.378961
H	-9.500602	-2.614305	-0.895277
H	-9.617389	-4.005111	0.184257
C	-8.157412	-4.24323	-1.406854
H	-8.879028	-4.711703	-2.083691
C	-7.19936	-3.356447	-2.218145
H	-6.666306	-3.961465	-2.961401
H	-7.763414	-2.595011	-2.76467
C	-6.186802	-2.670513	-1.281154
C	-6.954174	-1.844426	-0.237546
H	-6.244461	-1.361346	0.433384
H	-7.514383	-1.059143	-0.745032
C	-7.109706	-3.807084	1.306834
H	-7.783616	-4.442046	1.89448
H	-6.407158	-3.345343	2.006562
C	-6.34857	-4.658767	0.277606
H	-5.767677	-5.42495	0.800916
C	-7.352749	-5.328895	-0.673981
H	-8.02604	-5.982622	-0.108718
H	-6.825261	-5.958082	-1.399255
C	-5.392564	-3.763574	-0.53156
H	-4.828678	-4.371917	-1.24814
H	-4.663515	-3.292693	0.137853
C	-5.188368	-1.802653	-2.068174
H	-4.574152	-2.447553	-2.700961
H	-4.516442	-1.282466	-1.384381
H	-9.029912	1.569426	0.387926
C	0.648093	4.06672	-0.556099
C	0.737037	3.888818	0.778182
C	-0.476053	3.725402	1.630544
C	-1.805749	3.777546	0.936743

C	-1.895672	3.956732	-0.40018
C	-0.670528	4.108678	-1.253222
O	-0.770242	4.267011	-2.445524
O	-0.414274	3.568439	2.825607
Cl	2.021572	4.276857	-1.562603
Cl	2.23538	3.857477	1.617148
C	-3.140072	3.993197	-1.086044
C	-2.948344	3.609672	1.765428
N	-4.145279	4.028093	-1.651356
N	-3.87041	3.47695	2.446232

CPC-DDQ-10

Electronic Energy: -5016.790607 Hartrees
Free Energy: -5015.907769 Hartrees
Thermal Energy: 654.56 kcal/mol
Entropy: 339.311 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-9.338341	-0.970072	-2.882983
S	-7.260151	-0.030059	3.2279
C	-9.423482	-2.664584	-2.137191
H	-10.468106	-2.960385	-2.035287
H	-8.966469	-3.294325	-2.903001
C	-8.694872	-2.74809	-0.829919
C	-9.394611	-2.808043	0.378696
C	-8.738441	-2.595982	1.584225
H	-9.30781	-2.55948	2.5062
C	-7.375016	-2.312015	1.624664
C	-6.638418	-2.388225	0.420248
C	-7.311765	-2.610903	-0.789474
H	-6.746467	-2.578585	-1.712976
C	-6.754486	-1.780533	2.879065
H	-5.668456	-1.84144	2.85505
H	-7.111224	-2.316856	3.760024
C	-5.239668	-2.143773	0.397337
C	-4.054308	-1.900807	0.362397
C	-2.669549	-1.604226	0.323522
C	-2.033801	-1.322834	-0.90085
H	-2.615954	-1.341389	-1.813296
C	-0.68429	-1.026433	-0.940328

H	-0.199978	-0.812774	-1.884751
C	0.075309	-1.00037	0.243794
C	-0.556147	-1.287485	1.468756
H	0.033468	-1.290715	2.376467
C	-1.906185	-1.582975	1.506461
H	-2.387471	-1.808108	2.449618
C	-10.228284	0.08162	-1.648981
H	-11.029347	0.571159	-2.207303
H	-10.695442	-0.587777	-0.923425
C	-9.394166	1.14879	-0.917382
C	-10.363871	2.041353	-0.110749
H	-10.930586	1.423478	0.595561
H	-11.089243	2.507964	-0.78719
C	-9.583762	3.126674	0.651454
H	-10.287675	3.74684	1.215506
C	-8.596062	2.463521	1.624531
H	-8.045175	3.230857	2.181478
H	-9.138794	1.858674	2.356949
C	-7.606909	1.569239	0.852384
C	-8.399065	0.513087	0.065954
H	-7.705589	-0.117806	-0.489267
H	-8.937133	-0.126148	0.766238
C	-8.615766	2.039949	-1.904449
H	-9.311423	2.512429	-2.60834
H	-7.931273	1.420685	-2.491399
C	-7.829504	3.11684	-1.138627
H	-7.270233	3.731456	-1.851179
C	-8.809034	3.999926	-0.348752
H	-9.503639	4.496371	-1.035215
H	-8.264105	4.786663	0.18427
C	-6.843556	2.44602	-0.165517
H	-6.263004	3.210536	0.363465
H	-6.131079	1.825712	-0.72123

C	-6.577371	0.921058	1.794674
H	-5.953781	1.701675	2.236434
H	-5.917937	0.254383	1.237891
H	-10.468125	-2.961749	0.369436
S	6.189126	2.540481	2.999973
S	4.333456	1.21787	-3.106558
C	6.666871	0.766567	2.784489
H	7.752893	0.677836	2.764971
H	6.309965	0.288268	3.697892
C	6.043344	0.169035	1.560825
C	6.821179	-0.121788	0.42877
C	6.218977	-0.392244	-0.793262
H	6.832227	-0.516574	-1.678521
C	4.833555	-0.426186	-0.921958
C	4.047851	-0.31102	0.254298
C	4.669233	0.004174	1.476279
H	4.047616	0.176052	2.345658
C	4.196232	-0.432884	-2.274285
H	3.153602	-0.739885	-2.231917
H	4.722255	-1.094861	-2.96251
C	2.646124	-0.476692	0.211373
C	1.457542	-0.706974	0.211857
C	6.914405	3.364743	1.510187
H	7.556436	4.157145	1.901005
H	7.559788	2.638253	1.011444
C	5.919192	3.96871	0.502715
C	6.719761	4.785638	-0.536112
H	7.445267	4.13415	-1.037206
H	7.288596	5.57403	-0.030228
C	5.769516	5.408086	-1.574535
H	6.355367	5.981755	-2.299548
C	5.004497	4.29376	-2.306765
H	4.334907	4.728939	-3.058114
H	5.706029	3.642282	-2.836354
C	4.187836	3.460381	-1.30056
C	5.14117	2.876252	-0.246849
H	4.566017	2.296067	0.473774
H	5.843487	2.198947	-0.734368

C	4.91173	4.908166	1.193448
H	5.448299	5.703856	1.723731
H	4.343278	4.347088	1.940685
C	3.958147	5.519339	0.153719
H	3.239705	6.170577	0.661213
C	4.769042	6.335314	-0.865507
H	5.300204	7.147825	-0.358019
H	4.100032	6.796359	-1.600185
C	3.196438	4.397772	-0.575122
H	2.496612	4.831072	-1.298751
H	2.6031	3.819822	0.142592
C	3.377649	2.35731	-2.004463
H	2.625981	2.818455	-2.649006
H	2.847228	1.746337	-1.27266
H	7.901858	-0.072744	0.497555
C	6.705483	-3.617922	-0.974445
C	5.398935	-3.700249	-1.298311
C	4.321682	-3.498529	-0.286008
C	4.767063	-3.183005	1.104193
C	6.082365	-3.091908	1.427886
C	7.156184	-3.327696	0.41853
O	8.324726	-3.293869	0.727169
O	3.147202	-3.584744	-0.559834
Cl	7.966929	-3.815702	-2.126344
Cl	4.852157	-4.037764	-2.894476
C	6.509108	-2.77119	2.745412
C	3.731886	-2.99306	2.060889
N	6.838934	-2.491006	3.81528
N	2.885421	-2.831036	2.82791

CPC-DDQ-11
Electronic Energy: -5016.782086 Hartrees
Free Energy: -5015.902224 Hartrees
Thermal Energy: 654.54 kcal/mol
Entropy: 345.49 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-8.411031	-1.183766	2.584801
S	-	0.350669	-3.356369

	10.625941		
C	-7.640823	-2.477315	1.500708
H	-6.562534	-2.333851	1.482411
H	-7.85706	-3.402997	2.036858
C	-8.228021	-2.491222	0.123738
C	-7.551138	-1.895035	-0.965196
C	-8.2388	-1.671338	-2.166571
H	-7.73559	-1.13397	-2.961286
C	-9.579633	-2.01354	-2.304666
C	-10.196554	-2.725107	-1.271805
C	-9.52398	-2.960398	-0.079673
H	-10.042529	-3.437936	0.744182
C	-10.378893	-1.483684	-3.456621
H	-11.350352	-1.973389	-3.531679
H	-9.860888	-1.610821	-4.409204
C	-6.215859	-1.429422	-0.833402
C	-5.09051	-0.999556	-0.715341
C	-3.774217	-0.497016	-0.56126
C	-3.080195	-0.670176	0.651168
H	-3.562482	-1.196339	1.465349
C	-1.796395	-0.179866	0.805237
H	-1.262637	-0.325236	1.735974
C	-1.159296	0.501602	-0.249307
C	-1.852115	0.675638	-1.460658
H	-1.367954	1.199405	-2.275275
C	-3.136941	0.185733	-1.613753
H	-3.665558	0.323732	-2.54846
C	-7.980003	0.410266	1.749015
H	-7.475597	1.008836	2.511059
H	-7.248178	0.190246	0.970962
C	-9.15554	1.216651	1.169165
C	-8.611343	2.575841	0.675556
H	-7.834504	2.407251	-0.078896
H	-8.142589	3.113682	1.50764
C	-9.750289	3.422802	0.079406
H	-9.344857	4.37943	-0.265181

C	-10.380568	2.680383	-1.11038
H	-11.184839	3.28498	-1.546654
H	-9.633018	2.521956	-1.893035
C	-10.938685	1.319428	-0.651262
C	-9.796447	0.500429	-0.029541
H	-10.177865	-0.468115	0.294314
H	-9.036622	0.317708	-0.788822
C	-10.239401	1.480314	2.232098
H	-9.79874	2.003239	3.089346
H	-10.628763	0.526427	2.599924
C	-11.378786	2.319909	1.632306
H	-12.146768	2.486221	2.394471
C	-10.822203	3.670269	1.153089
H	-10.392236	4.219333	1.997888
H	-11.628499	4.288247	0.742948
C	-12.001359	1.568933	0.442359
H	-12.832682	2.150388	0.027186
H	-12.413335	0.610777	0.780063
C	-11.61487	0.561061	-1.80765
H	-12.518812	1.095163	-2.108878
H	-11.916737	-0.433981	-1.473813
H	-11.227862	-3.042457	-1.380683
C	0.162734	0.981715	-0.078509
C	1.300309	1.341178	0.12151
C	2.646497	1.682044	0.403735

C	5.324818	2.254055	0.929104
C	3.560058	1.86493	-0.645525
C	3.108155	1.710505	1.739835
C	4.434712	2.068262	1.975928
C	4.912637	2.07213	-0.392697
H	3.203536	1.774786	-1.664907
H	4.792075	2.143474	2.996272
H	6.356693	2.486245	1.146869
C	2.245096	1.244003	2.868618
H	2.671247	1.525778	3.831128
H	1.234891	1.651194	2.803837
C	5.91954	1.94283	-1.490888
H	6.754746	2.636058	-1.369205
H	5.484438	2.112436	-2.475777
S	1.950594	-0.58636	2.848185
S	6.747618	0.275419	-1.523347
C	5.35877	-0.930516	-1.727863
C	5.087356	-1.885675	-0.555114
C	6.36285	-2.626846	-0.11839
H	7.110794	-1.907442	0.216716
H	6.793921	-3.169633	-0.968086
C	6.045972	-3.600462	1.027022
H	6.968304	-4.102482	1.333794
C	5.471589	-2.819983	2.223423
H	5.264737	-3.508499	3.050669
H	6.204794	-2.09151	2.583739
C	4.171823	-2.093143	1.812835
C	4.501361	-1.141087	0.653003
H	3.590321	-0.628016	0.349631
H	5.209881	-0.385712	0.994762
C	4.0479	-2.929313	-1.024322
H	3.130803	-2.419876	-1.341504
C	3.732941	-3.912585	0.117714
H	2.995445	-4.641624	-0.232424
C	5.01992	-4.637298	0.543442
C	3.157454	-3.142458	1.317
H	2.917553	-3.838989	2.129111
H	2.227116	-2.643635	1.031432
C	3.638526	-1.317639	3.031659

H	3.572054	-1.991969	3.888239
H	4.32996	-0.516061	3.298893
H	5.429887	-5.208331	-0.296971
H	4.799069	-5.352833	1.342738
H	4.434347	-3.476211	-1.892145
H	5.625425	-1.50565	-2.616924
H	4.464238	-0.350255	-1.959652
C	10.382481	1.182497	-1.651243
C	10.102313	-0.073778	-1.246613
C	9.446768	-0.341659	0.063981
C	8.929938	0.849184	0.811201
C	9.256402	2.110198	0.433589
C	10.006985	2.371885	-0.833175
C	8.859216	3.252122	1.180106
C	8.162985	0.569363	1.975092
N	8.519283	4.169169	1.793349
N	7.51393	0.343287	2.901866
O	10.25944	3.502732	-1.176712
O	9.353807	-1.450554	0.532863
Cl	10.488726	-1.466253	-2.169995
Cl	11.163865	1.530992	-3.140256

CONTROL MOLECULES

PLP-DDQ-center
Electronic Energy: -3286.082687 Hartrees
Free Energy: -3285.703642 Hartrees
Thermal Energy: 314.624 kcal/mol
Entropy: 259.472 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	1.924709	4.162808	0.408492
S	-2.175608	-2.481463	2.182701
C	1.314341	2.811719	-0.684777
H	0.748725	3.253946	-1.503761
H	2.215192	2.357696	-1.097344
C	0.489325	1.809733	0.063547
C	1.103935	0.849944	0.912774

C	0.301661	0.011387	1.697808
H	0.786758	-0.69632	2.359563
C	-1.08669	0.082654	1.675773
C	-1.700913	0.988571	0.772656
C	-0.897507	1.842593	-0.000858
H	-1.382854	2.543992	-0.667957
C	-1.896982	-0.72584	2.653681
H	-2.865939	-0.261402	2.83384
H	-1.365539	-0.778408	3.604566
C	2.514083	0.755128	0.972994
C	3.72	0.674164	0.942761
C	5.132193	0.567336	0.845818
C	5.748186	0.647523	-0.415565
H	5.129643	0.776289	-1.29443
C	7.128004	0.535718	-0.522378
H	7.596143	0.596099	-1.497772
C	7.908851	0.344272	0.616823
H	8.985445	0.258546	0.528355
C	7.303507	0.261098	1.869696
H	7.908524	0.111567	2.756148
C	5.923898	0.369593	1.988502
H	5.44668	0.307532	2.958435
C	-3.110268	1.040836	0.647952
C	-4.309187	1.010671	0.491853
C	-5.709948	0.916292	0.274544
C	-6.205009	0.746728	-1.030051
H	-5.504653	0.682935	-1.852473
C	-7.572959	0.635007	-1.242269
H	-7.948224	0.499861	-2.249793
C	-8.460315	0.690698	-0.168414
H	-9.5266	0.603189	-0.340539
C	-7.974888	0.855361	1.127839
H	-8.662402	0.897201	1.96438
C	-6.60884	0.966468	1.353034
H	-6.224875	1.097386	2.357217
C	0.339273	4.981383	0.780776
H	0.572488	5.837022	1.414673
H	-0.141134	5.336887	-0.132481
C	-3.665878	-2.347385	1.13841

H	-4.49631	-1.932379	1.709359
H	-3.484707	-1.751029	0.24972
H	-0.332733	4.313453	1.320875
H	-3.903614	-3.366422	0.834429
C	1.989997	-1.883611	-1.083171
C	0.958882	-2.646169	-0.658026
C	-0.449126	-2.345566	-1.036968
C	-0.685169	-1.085853	-1.793898
C	0.349253	-0.309685	-2.210455
C	1.766288	-0.650954	-1.887798
O	-1.363858	-3.090764	-0.77
O	2.675096	0.054788	-2.267539
Cl	1.170563	-4.042483	0.316811
Cl	3.62974	-2.262173	-0.746655
C	-2.035292	-0.768136	-2.100512
C	0.140243	0.846065	-3.010562
N	-0.041756	1.784546	-3.656879
N	-3.130868	-0.497212	-2.342505

PLP-DDQ-edge-CO-parallel

Electronic Energy: -3286.078867 Hartrees
Free Energy: -3285.702818 Hartrees
Thermal Energy: 314.604 kcal/mol
Entropy: 265.715 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	0.081719	3.71259	-0.616001
S	3.832355	-3.33191	-1.199798
C	0.579492	2.346726	0.512867
H	1.07095	2.781539	1.384447
H	-0.358876	1.900417	0.840591
C	1.465152	1.324112	-0.135502
C	0.946081	0.37701	-1.055299
C	1.797823	-0.576251	-1.625049
H	1.379815	-1.308358	-2.305315
C	3.156856	-0.614485	-1.337467
C	3.680104	0.330337	-0.426768
C	2.818298	1.280617	0.155326

H	3.234145	1.989199	0.861332
C	4.030876	-1.663504	-1.960263
H	5.080142	-1.375943	-1.917223
H	3.760395	-1.819372	-3.005662
C	-0.428631	0.398538	-1.381973
C	-1.612136	0.477746	-1.621244
C	-3.01094	0.616969	-1.750385
C	-3.606547	1.884757	-1.559871
H	-2.967817	2.737921	-1.370868
C	-4.984736	2.020471	-1.594947
H	-5.435307	2.990659	-1.426882
C	-5.793723	0.901566	-1.803797
H	-6.871901	1.004174	-1.797992
C	-5.213494	-0.350888	-2.023811
H	-5.843966	-1.215016	-2.19611
C	-3.834445	-0.495154	-2.00739
H	-3.377658	-1.463866	-2.165014
C	5.054323	0.327188	-0.07894
C	6.223758	0.298237	0.231525
C	7.595056	0.232243	0.592488
C	8.149705	1.167609	1.483411
H	7.517879	1.947115	1.890314
C	9.490612	1.089244	1.835112
H	9.907988	1.815502	2.522571
C	10.298356	0.082407	1.308403
H	11.344204	0.024704	1.585579
C	9.757568	-0.849922	0.424228
H	10.38226	-1.63393	0.012778
C	8.418039	-0.779482	0.065855
H	7.99412	-1.501207	-0.621399
C	1.718569	4.430704	-0.970845
H	1.551387	5.270067	-1.645935
H	2.189779	4.799313	-0.05777
C	4.251313	-2.961596	0.536356
H	4.159574	-3.902845	1.078477
H	5.271199	-2.589289	0.625726
H	2.369338	3.705058	-1.459721
H	3.554546	-2.23769	0.958685
C	-5.288004	0.433647	1.3066

C	-3.961223	0.710629	1.383138
C	-2.931411	-0.356438	1.243476
C	-3.42626	-1.728743	0.940473
C	-4.744425	-2.008379	0.878971
C	-5.783537	-0.957922	1.082206
O	-1.752927	-0.10636	1.364091
O	-6.96706	-1.204256	1.065479
Cl	-2.201974	-2.899268	0.654051
Cl	-5.34769	-3.57568	0.509127
C	-3.465702	2.021104	1.626863
C	-6.278642	1.442713	1.4527
N	-7.074974	2.270918	1.560331
N	-3.045305	3.077528	1.824368

PLP-DDQ-edge-CO-perpendicular

Electronic Energy: -3286.081449 Hartrees
Free Energy: -3285.704075 Hartrees
Thermal Energy: 314.601 kcal/mol
Entropy: 262.912 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-0.097941	3.931323	-0.796492
S	3.316523	-3.261131	-1.060629
C	0.441495	2.642864	0.402191
H	0.991196	3.128396	1.209867
H	-0.481951	2.244328	0.820739
C	1.269152	1.555811	-0.215623
C	0.684382	0.570227	-1.05098
C	1.482543	-0.446579	-1.59093
H	1.012923	-1.213172	-2.194888
C	2.846348	-0.519754	-1.342926
C	3.431926	0.457774	-0.508738
C	2.627517	1.481988	0.030832
H	3.092711	2.214566	0.679059
C	3.654763	-1.654717	-1.899586
H	4.72001	-1.436399	-1.847028

H	3.392813	-1.840443	-2.94248
C	-0.704464	0.571535	-1.297415
C	-1.90304	0.556497	-1.475282
C	-3.304348	0.566973	-1.66483
C	-4.054105	1.707592	-1.323028
H	-3.539019	2.583024	-0.948228
C	-5.434285	1.699398	-1.461289
H	-6.004985	2.578767	-1.188731
C	-6.088376	0.561876	-1.936389
H	-7.167142	0.556879	-2.030937
C	-5.35503	-0.571383	-2.27763
H	-5.860684	-1.460544	-2.633196
C	-3.970558	-0.574779	-2.145909
H	-3.393757	-1.449824	-2.418605
C	4.809069	0.409251	-0.181373
C	5.980089	0.343345	0.118642
C	7.351794	0.235105	0.465682
C	7.977976	1.227443	1.240175
H	7.400499	2.082562	1.568379
C	9.319315	1.108464	1.578201
H	9.792413	1.878983	2.175493
C	10.056235	0.00385	1.153359
H	11.10267	-0.08559	1.419796
C	9.443981	-0.985839	0.38563
H	10.013445	-1.846282	0.05469
C	8.10353	-0.875582	0.041613
H	7.623086	-1.642397	-0.553287
C	1.527952	4.616065	-1.254689
H	1.34253	5.40483	-1.98375
H	2.030707	5.045459	-0.38617
C	3.577412	-2.788857	0.682955
H	3.456757	-3.704871	1.261633
H	4.58185	-2.394562	0.836401
H	2.157907	3.851346	-1.710061
H	2.827386	-2.067284	1.003769
C	-2.241152	-1.079445	1.127074
C	-3.012739	-2.067264	0.603398
C	-4.503932	-1.989682	0.619899
C	-5.10374	-0.738874	1.176451

C	-4.337297	0.273039	1.631533
C	-2.849302	0.184805	1.647442
O	-5.179989	-2.913263	0.23302
O	-2.156484	1.08372	2.064847
Cl	-6.819373	-0.697826	1.215146
Cl	-4.991924	1.732889	2.260994
C	-2.449899	-3.240344	0.033897
C	-0.832166	-1.197562	1.256218
N	0.307884	-1.303475	1.402214
N	-1.986616	-4.177955	-0.454686

PLP-DDQ-edge-Cl-in

Electronic Energy: -3286.081127 Hartrees
Free Energy: -3285.702253 Hartrees
Thermal Energy: 314.644 kcal/mol
Entropy: 259.903 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	1.130093	-4.337612	0.134211
S	2.553203	3.311333	0.305022
C	0.350379	-3.0209	1.128198
H	-0.649059	-2.837557	0.729902
H	0.213448	-3.460874	2.120197
C	1.095703	-1.709053	1.252342
C	0.388463	-0.557444	1.677607
C	1.063957	0.660344	1.823956
H	0.501987	1.53234	2.134249
C	2.412253	0.792029	1.525447
C	3.112836	-0.3464	1.068069
C	2.441456	-1.580028	0.960885
H	2.99074	-2.448442	0.621082
C	3.078533	2.133218	1.626026
H	4.162057	2.034221	1.600399
H	2.800394	2.636311	2.55345
C	-1.015668	-0.588765	1.8584
C	-2.224446	-0.571505	1.903046
C	-3.638973	-0.499694	1.855169
C	-4.402334	-1.617376	1.474125

H	-3.901321	-2.552438	1.257957
C	-5.784054	-1.515207	1.357374
H	-6.35937	-2.377146	1.043396
C	-6.424528	-0.304125	1.611975
H	-7.49784	-0.221355	1.496893
C	-5.675825	0.80882	1.993339
H	-6.167819	1.756049	2.176764
C	-4.294175	0.716439	2.117912
H	-3.709728	1.58104	2.406009
C	4.475593	-0.259839	0.685874
C	5.62861	-0.172533	0.32838
C	6.977822	-0.053146	-0.097219
C	7.706167	-1.187542	-0.495954
H	7.226427	-2.157892	-0.470201
C	9.023684	-1.060964	-0.915536
H	9.576382	-1.941889	-1.220057
C	9.635094	0.191565	-0.945592
H	10.663417	0.285973	-1.273643
C	8.920849	1.322328	-0.552276
H	9.392867	2.297482	-0.574218
C	7.603158	1.206036	-0.130413
H	7.044645	2.081789	0.176245
C	0.936633	-3.622082	-1.532968
H	-0.108323	-3.381314	-1.729098
H	1.554234	-2.731062	-1.652925
C	2.855099	2.296271	-1.179702
H	2.613868	2.926395	-2.035671
H	3.898274	1.987294	-1.238538
H	1.26971	-4.381996	-2.239714
H	2.205333	1.421572	-1.186192
C	-3.660134	2.003148	-0.739355
C	-4.74614	1.04052	-1.128425
C	-4.464613	-0.23583	-1.478035
C	-3.051393	-0.736866	-1.519405
C	-1.976724	0.266511	-1.2817
C	-2.25498	1.518408	-0.86243
O	-3.931437	3.123597	-0.381899
O	-2.814753	-1.899795	-1.746627
Cl	-1.028169	2.647372	-0.456806

Cl	-0.376512	-0.293689	-1.546779
C	-6.072695	1.552427	-1.125359
C	-5.473942	-1.166489	-1.848649
N	-7.148396	1.96919	-1.142913
N	-6.291311	-1.918437	-2.160726

PLP-DDQ-edge-CO-in

Electronic Energy: - -3286.081570 Hartrees
Free Energy: -3285.703247 Hartrees
Thermal Energy: 314.736 kcal/mol
Entropy: 261.368 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	0.783866	-4.08309	-0.723279
S	2.760998	2.882998	-0.4333
C	0.87294	-3.402094	0.986003
H	-0.12079	-3.427974	1.431429
H	1.504342	-4.112833	1.521444
C	1.460257	-2.021248	1.053869
C	0.649004	-0.887823	1.290196
C	1.237233	0.385647	1.341377
H	0.599911	1.245316	1.504991
C	2.594249	0.577651	1.137014
C	3.406858	-0.553855	0.884313
C	2.820449	-1.829467	0.856813
H	3.450815	-2.686034	0.65195
C	3.159944	1.967203	1.118322
H	4.239396	1.957961	1.259183
H	2.714793	2.577999	1.905025
C	-0.757669	-0.99748	1.429095
C	-1.96418	-1.054633	1.492612
C	-3.38077	-1.113101	1.539908
C	-4.076934	-2.13377	0.868082
H	-3.519403	-2.88683	0.325574
C	-5.467128	-2.172671	0.895897
H	-5.990643	-2.955272	0.361089
C	-6.183632	-1.195909	1.582756

H	-7.265996	-1.214339	1.58489
C	-5.502083	-0.174764	2.245539
H	-6.055622	0.598071	2.764699
C	-4.112178	-0.131015	2.229558
H	-3.581345	0.658494	2.74653
C	4.797125	-0.412913	0.642571
C	5.975979	-0.274889	0.407144
C	7.353365	-0.090199	0.116455
C	8.186031	-1.192444	-0.143945
H	7.764985	-2.189575	-0.115753
C	9.530189	-1.000518	-0.434322
H	10.163284	-1.857103	-0.633501
C	10.065305	0.286294	-0.470784
H	11.114676	0.431623	-0.698077
C	9.247455	1.385683	-0.214284
H	9.659809	2.387386	-0.241805
C	7.902279	1.204001	0.077893
H	7.263654	2.055308	0.278829
C	-0.29525	-2.8435	-1.50966
H	-1.278218	-2.820066	-1.042426
H	0.150811	-1.851516	-1.470207
C	3.508653	1.77686	-1.676255
H	3.313119	2.233136	-2.646715
H	4.584002	1.685961	-1.528321
H	-0.406752	-3.139392	-2.552142
H	3.050111	0.788109	-1.647023
C	-4.289033	2.100596	0.046371
C	-5.157585	1.1032	-0.662413
C	-4.623865	0.125242	-1.430112
C	-3.144648	0.028542	-1.656479
C	-2.293346	1.073708	-1.018839
C	-2.8194	1.99126	-0.180257
O	-4.777571	2.961848	0.736917
O	-2.684737	-0.854805	-2.339303
Cl	-1.855831	3.143357	0.654155
Cl	-0.626311	1.026895	-1.412601
C	-6.56109	1.257422	-0.494415
C	-5.425755	-0.841792	-2.096793
N	-7.70095	1.388383	-0.373245

N	-6.078263	-1.625944	-2.635486

LPL-DDQ-center-parallel

Electronic Energy: -4239.844532 Hartrees
Free Energy: -4239.366173 Hartrees
Thermal Energy: 391.802 kcal/mol
Entropy: 309.306 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-8.518129	-3.578908	0.43341
S	-4.254834	3.141712	0.951093
C	-8.668957	-2.00802	1.382675
H	-9.697069	-1.64812	1.31141
H	-8.489304	-2.304371	2.417854
C	-7.700837	-0.94431	0.945404
C	-8.146425	0.195083	0.274587
C	-7.246351	1.168839	-0.156192
H	-7.612724	2.039861	-0.687985
C	-5.880122	1.042284	0.069956
C	-5.422007	-0.110591	0.757968
C	-6.333418	-1.088777	1.172836
H	-5.960702	-1.974829	1.672219
C	-4.919078	2.089239	-0.405035
H	-5.384209	2.740225	-1.14658
H	-4.043165	1.632998	-0.863526
C	-4.040883	-0.260535	1.026295
C	-2.853163	-0.316691	1.254683
C	-1.45657	-0.309442	1.43092
C	-0.742237	-1.508654	1.652641
H	-1.291362	-2.436994	1.736098
C	0.632894	-1.502332	1.71293
H	1.181004	-2.426221	1.841788
C	1.351452	-0.295926	1.55778
C	0.638106	0.911715	1.411835
H	1.192678	1.837518	1.320833
C	-0.742158	0.904257	1.344664
H	-1.293123	1.827726	1.215639
C	-8.819732	-2.949348	-1.250359

H	-8.749854	-3.806175	-1.920311
H	-9.817239	-2.514305	-1.332532
C	-5.782685	4.003751	1.442007
H	-5.51783	4.668537	2.264282
H	-6.175238	4.600199	0.616309
H	-9.206524	0.322074	0.083823
S	8.400402	-3.497326	0.290071
S	3.994221	3.158411	0.751043
C	8.029242	-2.086944	-0.834439
H	8.960616	-1.740371	-1.286084
H	7.418382	-2.528631	-1.623874
C	7.307599	-0.953158	-0.161687
C	7.951926	0.259328	0.085708
C	7.284831	1.30477	0.721796
H	7.80446	2.238732	0.904549
C	5.961405	1.177677	1.130395
C	5.302615	-0.050191	0.880314
C	5.98383	-1.096934	0.248931
H	5.462173	-2.030053	0.076111
C	5.258656	2.321615	1.800246
H	5.983845	3.065222	2.134069
H	4.694451	1.980182	2.669808
C	3.938612	-0.206473	1.2234
C	2.758415	-0.290439	1.475578
C	9.41734	-2.636608	1.533843
H	9.699056	-3.382487	2.276948
H	10.321916	-2.22526	1.082566
C	4.998929	3.55559	-0.71427
H	4.342345	4.102679	-1.388164
H	5.85105	4.18178	-0.444965
H	8.982501	0.39061	-0.22553
H	5.336815	2.643434	-1.205663
H	8.848469	-1.843544	2.019604
H	-6.538453	3.296681	1.786174
H	-8.066265	-2.213036	-1.530489
C	-0.414657	-1.162211	-1.591313
C	0.933356	-1.055583	-1.536035
C	1.628589	0.255544	-1.64586
C	0.753568	1.453423	-1.80161

C	-0.599718	1.34709	-1.837452
C	-1.288859	0.027509	-1.738116
O	2.835403	0.358857	-1.63524
O	-2.498635	-0.048442	-1.802629
C	1.407384	2.709059	-1.925988
C	-1.446326	2.478772	-1.986416
N	1.920994	3.735782	-2.0408
N	-2.148019	3.387644	-2.105569
Cl	1.969675	-2.422409	-1.392741
Cl	-1.234124	-2.675111	-1.53505

LPL-DDQ-edge-CO parallel (offset)

Electronic Energy: -4239.838964 Hartrees
Free Energy: -4239.361888 Hartrees
Thermal Energy: 391.940 kcal/mol
Entropy: 312.468 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-6.726604	-1.162039	2.369148
S	-2.756189	4.430632	-1.6609
C	-6.467904	0.659441	2.485335
H	-7.443773	1.133674	2.594079
H	-5.916047	0.811721	3.413089
C	-5.704174	1.202108	1.313597
C	-6.34981	1.74646	0.201083
C	-5.612042	2.224731	-0.879506
H	-6.127753	2.629358	-1.742488
C	-4.218803	2.190457	-0.88267
C	-3.558646	1.636063	0.241235
C	-4.312116	1.14119	1.313602
H	-3.788454	0.711214	2.15942
C	-3.434531	2.757324	-2.025631
H	-4.041851	2.810618	-2.928721
H	-2.558897	2.144403	-2.239478
C	-2.144022	1.549543	0.279497
C	-0.945784	1.391148	0.27578
C	0.451021	1.141593	0.234801
C	0.960337	0.195956	-0.673471

H	0.271794	-0.325547	-1.32516
C	2.318257	-0.067837	-0.718847
H	2.708196	-0.797489	-1.417282
C	3.208002	0.603789	0.138695
C	2.695105	1.551012	1.044322
H	3.37854	2.078357	1.697899
C	1.33734	1.814716	1.092411
H	0.947714	2.547541	1.787587
C	-8.285319	-1.217844	1.426881
H	-9.1252	-0.946846	2.06662
H	-8.243624	-0.559674	0.560269
C	-4.314108	5.371601	-1.568199
H	-4.040526	6.409589	-1.37824
H	-4.861337	5.316349	-2.51112
H	-7.431869	1.809448	0.181065
S	9.611073	-3.248717	-2.260515
S	6.799858	2.841675	2.082617
C	9.923607	-1.436073	-2.159014
H	11.001325	-1.265275	-2.126538
H	9.551294	-1.048823	-3.109183
C	9.242149	-0.770535	-0.996368
C	9.978154	-0.323872	0.101165
C	9.34034	0.269666	1.189046
H	9.92751	0.601672	2.038322
C	7.95964	0.438544	1.214808
C	7.205291	-0.009137	0.102063
C	7.856619	-0.614297	-0.978871
H	7.264336	-0.972861	-1.812007
C	7.290826	1.090496	2.387051
H	7.935679	1.061223	3.267045
H	6.353116	0.590096	2.630835
C	5.796674	0.161046	0.085075
C	4.601156	0.343328	0.099036
C	10.27179	-3.764898	-0.642336
H	10.134192	-4.844299	-0.57954
H	11.336258	-3.537102	-0.563281
C	8.448786	3.588394	1.874498
H	8.288893	4.649594	1.683478
H	9.048855	3.476955	2.779698

H	11.056294	-0.44086	0.106979
H	8.969783	3.148612	1.023619
H	9.726068	-3.285766	0.170698
H	-4.941647	5.015486	-0.750261
H	-8.406676	-2.243507	1.080381
C	-4.184346	-2.733299	0.657363
C	-3.134069	-2.031964	0.176105
C	-3.229595	-1.257006	-1.091678
C	-4.599514	-1.080416	-1.663225
C	-5.665896	-1.735094	-1.143575
C	-5.494216	-2.752454	-0.054295
O	-2.261267	-0.79958	-1.655161
O	-6.350663	-3.579739	0.153265
C	-4.709249	-0.272302	-2.827797
C	-6.970674	-1.598733	-1.688758
N	-4.807065	0.35832	-3.788991
N	-8.036878	-1.460713	-2.108252
Cl	-1.58653	-2.032702	0.922141
Cl	-4.079413	-3.739559	2.04358

LPL-DDQ-edge-CO parallel (offset)

Electronic Energy: -4239.841078 Hartrees
Free Energy: -4239.365914 Hartrees
Thermal Energy: 391.871 kcal/mol
Entropy: 316.262 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	-6.918909	-2.005409	3.667071
S	-2.512644	3.358433	1.518567
C	-6.135134	-2.311276	2.030445
H	-5.500966	-3.195273	2.093792
H	-6.967103	-2.543755	1.362434
C	-5.367761	-1.122454	1.532922
C	-6.049664	0.024794	1.091967
C	-5.350082	1.140098	0.656643
H	-5.893222	2.011946	0.310014
C	-3.955432	1.153062	0.616788
C	-3.255756	0.0013	1.070482

C	-3.977159	-1.11334	1.529476
H	-3.429196	-1.988598	1.855766
C	-3.215362	2.361958	0.138347
H	-3.861502	3.003533	-0.461623
H	-2.355352	2.080535	-0.469746
C	-1.844817	-0.028945	1.026299
C	-0.640975	-0.050613	0.906233
C	0.765979	-0.074132	0.752234
C	1.412721	-1.242828	0.310577
H	0.817771	-2.114688	0.072529
C	2.786909	-1.261889	0.154196
H	3.283545	-2.159522	-0.19152
C	3.556343	-0.118284	0.437259
C	2.905273	1.051982	0.872751
H	3.494202	1.936943	1.078181
C	1.531101	1.074987	1.024595
H	1.031125	1.975826	1.35786
C	-5.422976	-1.737399	4.674182
H	-5.763009	-1.554279	5.693362
H	-4.786424	-2.623536	4.665904
C	-4.058201	3.930947	2.296566
H	-3.76763	4.565968	3.133507
H	-4.654608	4.518984	1.59658
H	-7.133099	0.034539	1.106979
S	10.475567	-3.536394	-0.939729
S	6.666445	3.348705	0.447215
C	10.384531	-1.884886	-1.750249
H	11.397142	-1.547999	-1.980104
H	9.87389	-2.08045	-2.694947
C	9.650474	-0.854189	-0.938978
C	10.338664	0.19166	-0.323826
C	9.658764	1.131839	0.448526
H	10.211976	1.93218	0.927722
C	8.280988	1.061446	0.627446
C	7.574231	0.003784	0.003049
C	8.270321	-0.940725	-0.760169
H	7.719474	-1.756999	-1.211503
C	7.563241	2.088081	1.450441
H	8.256699	2.605909	2.115276

H	6.783547	1.627687	2.058068
C	6.166484	-0.09212	0.149748
C	4.964772	-0.128172	0.283038
C	11.33751	-3.075918	0.598656
H	11.446064	-3.990996	1.180728
H	12.328207	-2.670221	0.386181
C	8.083549	4.15476	-0.366434
H	7.673188	4.93896	-1.002696
H	8.753786	4.607112	0.367066
H	11.413014	0.272285	-0.447845
H	8.631501	3.444527	-0.98626
H	10.753233	-2.354541	1.170224
H	-4.643319	3.092268	2.675231
H	-4.861548	-0.870898	4.32371
C	-5.363867	0.782016	-2.534731
C	-6.469299	0.081301	-2.20795
C	-6.392182	-1.311016	-1.67709
C	-5.023689	-1.874663	-1.50093
C	-3.909336	-1.168104	-1.824012
C	-3.994134	0.212691	-2.382295
O	-7.377323	-1.960313	-1.406015
O	-2.997174	0.82502	-2.691519
C	-4.946247	-3.1926	-0.97496
C	-2.605555	-1.712426	-1.673662
N	-4.874895	-4.253359	-0.526284
N	-1.552458	-2.16462	-1.540837
Cl	-8.055857	0.732203	-2.327872
Cl	-5.423946	2.4008	-3.115081

LPL-DDQ-center-CO perpendicular

Electronic Energy: -4239.843858 Hartrees
Free Energy: -4239.364508 Hartrees
Thermal Energy: 391.900 kcal/mol
Entropy: 307.550 cal mol^{-1} $kelvin^{-1}$
Imaginary Frequencies: 0

S	6.733048	-3.676969	-0.229737

S	4.932591	3.970266	-1.237855
C	7.616738	-2.294629	-1.072628
H	8.664045	-2.303467	-0.766263
H	7.573486	-2.558586	-2.131234
C	6.994645	-0.950698	-0.813256
C	7.679043	0.032672	-0.099561
C	7.065705	1.248492	0.20146
H	7.611177	1.998016	0.764211
C	5.753314	1.51143	-0.177801
C	5.055265	0.51629	-0.90301
C	5.687684	-0.689771	-1.219108
H	5.126631	-1.451179	-1.745456
C	5.09337	2.807872	0.181775
H	5.636924	3.309945	0.983935
H	4.068122	2.644687	0.516051
C	3.683584	0.679995	-1.218318
C	2.488551	0.756121	-1.384586
C	1.07757	0.778933	-1.481914
C	0.387319	-0.292308	-2.076885
H	0.950914	-1.105238	-2.51684
C	-0.998291	-0.326795	-2.075421
H	-1.52232	-1.170259	-2.506177
C	-1.738827	0.710942	-1.480982
C	-1.049823	1.802031	-0.918695
H	-1.620369	2.594051	-0.450443
C	0.334244	1.832228	-0.914446
H	0.858269	2.659915	-0.453473
C	6.744994	-3.058038	1.485152
H	6.254623	-3.819392	2.091601
H	7.765663	-2.919375	1.844427
C	6.697097	4.279847	-1.572034
H	6.738396	4.972076	-2.413006
H	7.185763	4.739003	-0.710535
H	8.694236	-0.154192	0.232759
S	-8.653692	-3.076474	-1.191699
S	-4.419763	3.448587	0.726468
C	-8.122174	-2.263663	0.374084
H	-8.978676	-2.206026	1.048607
H	-7.400053	-2.960119	0.803368

C	-7.507977	-0.908204	0.16885
C	-8.215298	0.253841	0.479696
C	-7.647757	1.509633	0.272541
H	-8.213385	2.400692	0.521832
C	-6.365394	1.648139	-0.249265
C	-5.642907	0.472072	-0.562509
C	-6.223317	-0.78537	-0.357697
H	-5.64739	-1.669999	-0.599131
C	-5.77289	3.012033	-0.451412
H	-6.552162	3.772917	-0.388206
H	-5.296231	3.090569	-1.430291
C	-4.308146	0.555089	-1.030131
C	-3.143036	0.625887	-1.340725
C	-9.858481	-1.844556	-1.784794
H	-10.247999	-2.220246	-2.730961
H	-10.684581	-1.732725	-1.080104
C	-5.218499	3.067171	2.316389
H	-4.475541	3.275248	3.08462
H	-6.09904	3.691354	2.476795
H	-9.214962	0.177773	0.89343
H	-5.483001	2.011773	2.368593
H	-9.378382	-0.880282	-1.95295
H	7.210195	3.357358	-1.845516
H	6.188272	-2.124324	1.564315
C	2.014654	-0.596904	1.592231
C	1.860337	-1.719829	0.861878
C	0.508063	-2.206406	0.454819
C	-0.670106	-1.396855	0.909466
C	-0.509283	-0.246088	1.604551
C	0.854341	0.264153	1.963488
O	0.350164	-3.219595	-0.181954
O	0.98845	1.314902	2.543047
C	-1.954353	-1.926582	0.603692
C	-1.610636	0.52021	2.07373
N	-2.999116	-2.360152	0.377165
N	-2.504479	1.121941	2.486302
Cl	3.183305	-2.686731	0.349662

Cl	3.545682	-0.044552	2.142483