

Supplementary Material: Exploring Basic Components Effect on the Catalytic Efficiency of Chevron-Phillips Catalyst in Ethylene Trimerization

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Table S1. Coordinate data sets and absolute energies (in a.u.) of all optimized complexes.

6			
Ethylene SCF Done: -78.531587 A.U.			
C	-0.792900000	0.663400000	0.000000000
H	-0.259700000	-0.264300000	0.000000000
H	-1.862900000	0.663400000	0.000000000
C	-0.117600000	1.838400000	0.000000000
H	-0.650800000	2.766100000	0.000000000
H	0.952400000	1.838400000	0.000000000
19			
1-hexene SCF Done: -235.677932 A.U.			
C	-3.025900000	0.048500000	0.000000000
H	-2.669200000	-0.960300000	0.000000000
H	-2.669200000	0.552900000	-0.873700000
H	-4.095900000	0.048600000	0.000000000
C	-2.512500000	0.774500000	1.257400000
H	-2.869000000	1.783400000	1.257300000
H	-2.869400000	0.270200000	2.131100000
C	-0.972500000	0.774200000	1.257500000
H	-0.615700000	1.278500000	0.383900000
H	-0.616100000	-0.234600000	1.257700000
C	-0.459200000	1.500200000	2.514900000
H	0.610800000	1.500100000	2.515000000
H	-0.815700000	2.509100000	2.514800000
C	-0.972800000	0.774500000	3.772400000
H	-1.792300000	0.090800000	3.696000000
C	-0.390300000	0.998800000	4.975300000
H	-0.923400000	0.465800000	5.734600000
H	0.624700000	0.661500000	4.948500000

H	-0.412400000	2.046300000	5.192500000
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A-0-s SCF Done: -1157.352454 A.U.

Cr	-1.365032000	-0.001391000	1.336381000
Al	1.683091000	0.000308000	-0.312619000
Cl	0.996272000	-0.002307000	1.979383000
N	-0.170700000	0.001093000	-1.020020000
C	-0.991736000	-1.123372000	-0.956065000
C	-2.321379000	-0.717022000	-0.801504000
C	-2.321289000	0.719138000	-0.800508000
C	-0.991610000	1.125545000	-0.954500000
C	-0.497423000	-2.531646000	-1.102207000
H	0.089635000	-2.653576000	-2.025949000
H	-1.356605000	-3.215826000	-1.151370000
H	0.142730000	-2.854302000	-0.268325000
H	-3.189750000	-1.374566000	-0.797261000
H	-3.189585000	1.376771000	-0.795311000
C	-0.497099000	2.533972000	-1.098544000
H	0.091614000	2.656754000	-2.021104000
H	0.141535000	2.855927000	-0.263216000
H	-1.356223000	3.218162000	-1.148617000
C	2.671202000	1.675438000	-0.627514000
H	2.640402000	1.983892000	-1.688019000
H	3.734132000	1.500438000	-0.382656000
H	2.344139000	2.537632000	-0.025185000
C	2.670943000	-1.674134000	-0.632245000
H	2.635966000	-1.982437000	-1.692644000
H	2.346436000	-2.536520000	-0.028766000
H	3.734771000	-1.498917000	-0.391518000

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A-1-q SCF Done: -1235.904776 A.U.

Cr	1.243427000	-0.411675000	-0.144775000
Al	-2.031337000	-0.268075000	0.154639000
Cl	-0.611247000	-1.976716000	-0.610652000
N	-0.504396000	1.037138000	0.153330000
C	0.344809000	1.340293000	1.222046000
C	1.532754000	1.870345000	0.707417000
C	1.380968000	1.978375000	-0.711678000
C	0.118037000	1.479354000	-1.030438000
C	-0.012149000	1.150642000	2.664899000
H	-0.906656000	1.737025000	2.929427000
H	0.820386000	1.499365000	3.291577000
H	-0.217947000	0.104164000	2.926194000

H	2.386486000	2.194236000	1.300042000
H	2.098360000	2.391508000	-1.417675000
C	-0.533600000	1.443912000	-2.379629000
H	-1.437803000	2.072201000	-2.402454000
H	-0.830400000	0.429390000	-2.683400000
H	0.170320000	1.829155000	-3.130562000
C	-3.391425000	0.159035000	-1.202222000
H	-3.668187000	1.228915000	-1.180727000
H	-4.312507000	-0.406236000	-0.974356000
H	-3.113396000	-0.086151000	-2.239147000
C	-2.653881000	-0.763692000	1.953010000
H	-3.014396000	0.101635000	2.536900000
H	-1.915246000	-1.299323000	2.570333000
H	-3.518413000	-1.441677000	1.834673000
C	2.749168000	-1.517918000	0.694597000
C	3.038580000	-1.234326000	-0.695224000
H	3.326963000	-1.007451000	1.476644000
H	3.830619000	-0.514930000	-0.942078000
H	2.420428000	-2.525560000	0.981267000
H	2.928918000	-2.033004000	-1.441278000

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A-2-q SCF Done: -1314.443621 A.U.

Cr	1.448404000	0.066493000	0.065228000
Al	-2.241119000	-0.018088000	-0.536664000
Cl	-0.580166000	-0.493616000	-2.006350000
N	-0.975435000	0.036462000	1.023855000
C	-0.296657000	-1.083287000	1.470792000
C	0.802719000	-0.685529000	2.253492000
C	0.797285000	0.733160000	2.279643000
C	-0.298996000	1.151441000	1.504530000
C	-0.752885000	-2.486206000	1.218160000
H	-1.731836000	-2.668554000	1.687463000
H	-0.030312000	-3.195405000	1.644913000
H	-0.860038000	-2.699275000	0.145037000
H	1.483047000	-1.355208000	2.775660000
H	1.472779000	1.388836000	2.826567000
C	-0.811489000	2.552270000	1.381553000
H	-1.770385000	2.655606000	1.914891000
H	-0.986412000	2.858895000	0.343360000
H	-0.095135000	3.251230000	1.835248000
C	-3.038844000	1.738861000	-0.961401000
H	-3.594223000	2.184074000	-0.116471000
H	-3.779508000	1.576230000	-1.765890000

H	-2.335892000	2.501159000	-1.336282000
C	-3.533435000	-1.500948000	-0.347224000
H	-3.966367000	-1.547272000	0.669249000
H	-3.140296000	-2.503296000	-0.581218000
H	-4.379533000	-1.323507000	-1.035356000
C	2.344042000	-1.901978000	-0.229320000
C	2.952382000	-1.172176000	-1.239261000
H	1.487245000	-2.541825000	-0.457173000
H	2.562574000	-1.211001000	-2.258194000
H	2.896196000	-2.146143000	0.684469000
H	3.988212000	-0.842313000	-1.140446000
C	2.626497000	1.378773000	-1.453062000
C	1.707489000	2.082733000	-0.684720000
H	2.381500000	1.090220000	-2.476577000
H	0.735876000	2.349349000	-1.110797000
H	3.692308000	1.419646000	-1.216198000
H	2.045268000	2.691418000	0.160790000

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A-3-q SCF Done: -1314.471436 A.U.

Cr	1.001221000	0.101352000	-0.097085000
Al	-2.284546000	-0.660594000	-0.258335000
Cl	-0.445403000	-1.183257000	-1.636354000
N	-1.194675000	0.723875000	0.699301000
C	-0.422275000	0.529647000	1.839866000
C	0.591815000	1.499477000	1.870429000
C	0.396274000	2.349185000	0.742054000
C	-0.709314000	1.862960000	0.042200000
C	-0.694992000	-0.520886000	2.872063000
H	-1.714083000	-0.417912000	3.276768000
H	0.015603000	-0.407943000	3.702164000
H	-0.598835000	-1.542291000	2.479860000
H	1.340846000	1.605054000	2.653000000
H	0.983821000	3.223439000	0.468962000
C	-1.335892000	2.454016000	-1.183869000
H	-2.375479000	2.761650000	-0.992059000
H	-1.349027000	1.754009000	-2.032062000
H	-0.765656000	3.342642000	-1.488245000
C	-3.742909000	0.126745000	-1.318171000
H	-4.301843000	0.883699000	-0.738083000
H	-4.467094000	-0.665635000	-1.577500000
H	-3.435208000	0.601346000	-2.262930000
C	-2.685574000	-2.252591000	0.823739000
H	-3.260648000	-2.018644000	1.737065000

H	-1.805485000	-2.843137000	1.123913000
H	-3.322953000	-2.920586000	0.216617000
C	2.215749000	-1.370456000	0.675757000
C	3.652783000	-1.059014000	0.236853000
H	2.115223000	-1.496998000	1.768494000
H	4.091856000	-0.297751000	0.909887000
H	1.849110000	-2.297413000	0.194785000
H	4.317041000	-1.942359000	0.305787000
C	3.614623000	-0.491838000	-1.188098000
C	2.622157000	0.675737000	-1.211325000
H	4.623799000	-0.197896000	-1.537268000
H	3.046742000	1.559748000	-0.695727000
H	3.272813000	-1.283787000	-1.880425000
H	2.329154000	0.986376000	-2.230697000

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A-4-q SCF Done: -1392.997334 A.U.

Cr	-1.295613000	0.204095000	-0.028744000
Al	2.750238000	-0.154537000	0.225707000
Cl	1.883333000	-1.489878000	1.765520000
N	1.055711000	0.246399000	-0.856478000
C	0.339194000	-0.724005000	-1.539182000
C	-0.708979000	-0.107092000	-2.249121000
C	-0.585038000	1.298395000	-2.037844000
C	0.500318000	1.486438000	-1.176842000
C	0.706187000	-2.173595000	-1.564193000
H	1.576418000	-2.328789000	-2.221831000
H	-0.131169000	-2.762654000	-1.962381000
H	0.967767000	-2.549941000	-0.565824000
H	-1.425643000	-0.619201000	-2.887879000
H	-1.214010000	2.084008000	-2.451558000
C	1.065086000	2.798487000	-0.726957000
H	2.041016000	2.987281000	-1.201650000
H	1.231810000	2.844861000	0.357069000
H	0.385643000	3.612055000	-1.018595000
C	3.442527000	1.474831000	1.111405000
H	3.836756000	2.238608000	0.418481000
H	4.301118000	1.144130000	1.725207000
H	2.751115000	1.980904000	1.807462000
C	3.999882000	-1.063061000	-1.006616000
H	4.083565000	-0.545437000	-1.980168000
H	3.755674000	-2.117913000	-1.213890000
H	5.012057000	-1.057140000	-0.563190000
C	-2.054428000	-1.621152000	0.594761000

C	-3.540542000	-1.683921000	0.220904000
H	-1.473346000	-2.469761000	0.198159000
H	-3.648597000	-1.983866000	-0.838412000
H	-1.929700000	-1.640844000	1.692800000
H	-4.092757000	-2.442333000	0.808236000
C	-4.145071000	-0.285935000	0.393362000
C	-3.275308000	0.693942000	-0.397558000
H	-5.206745000	-0.254134000	0.079703000
H	-3.416597000	0.529677000	-1.481612000
H	-4.143707000	-0.021560000	1.468972000
H	-3.505741000	1.756498000	-0.198721000
C	-1.510865000	1.862887000	1.866138000
C	-0.775959000	0.851511000	2.371234000
H	-1.052207000	2.698875000	1.328971000
H	0.310400000	0.787301000	2.259428000
H	-2.585306000	1.932879000	2.048608000
H	-1.234853000	0.063952000	2.972847000

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A-5-q SCF Done: -1393.038232 A.U.

Cr	-0.638154000	0.128320000	-0.011369000
Al	2.693914000	-0.506156000	-0.545160000
Cl	0.764622000	-0.582918000	-1.906464000
N	1.679519000	0.441707000	0.890331000
C	1.166280000	1.727922000	0.708082000
C	0.088730000	1.914124000	1.578401000
C	-0.059503000	0.712866000	2.329668000
C	0.946716000	-0.166898000	1.903928000
C	1.731676000	2.728354000	-0.253344000
H	2.791713000	2.934543000	-0.040642000
H	1.174999000	3.671577000	-0.163915000
H	1.663646000	2.395153000	-1.299819000
H	-0.503474000	2.822807000	1.668235000
H	-0.770438000	0.519572000	3.130819000
C	1.258020000	-1.516042000	2.476206000
H	2.309552000	-1.575800000	2.795886000
H	1.084312000	-2.336469000	1.765942000
H	0.622617000	-1.693327000	3.354871000
C	3.178838000	-2.360794000	-0.106379000
H	3.837252000	-2.431589000	0.777674000
H	3.754734000	-2.768008000	-0.956980000
H	2.329064000	-3.042434000	0.055934000
C	4.070320000	0.617338000	-1.390797000
H	4.686592000	1.141466000	-0.637554000

H	3.693011000	1.378540000	-2.091302000
H	4.758946000	-0.030824000	-1.961339000
C	-2.003588000	1.292621000	-0.958375000
C	-3.374423000	1.417640000	-0.283064000
H	-1.519057000	2.283399000	-1.050224000
H	-3.267915000	1.474577000	0.820052000
H	-2.101171000	0.890985000	-1.983717000
H	-3.829983000	2.385687000	-0.568089000
C	-4.389773000	0.319372000	-0.634527000
C	-4.195706000	-1.079104000	-0.029195000
H	-5.389722000	0.671784000	-0.324403000
H	-4.219624000	-1.004349000	1.075104000
H	-4.436745000	0.228551000	-1.736276000
H	-5.089560000	-1.667686000	-0.300770000
C	-2.951375000	-1.885517000	-0.444813000
C	-1.675626000	-1.590027000	0.349747000
H	-3.198387000	-2.957553000	-0.319294000
H	-1.893949000	-1.631508000	1.434865000
H	-2.773043000	-1.759892000	-1.528976000
H	-0.917303000	-2.372336000	0.148207000

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A-6-q SCF Done: -1393.041261 A.U.

Cr	-0.397072000	-0.569798000	-0.273643000
Al	2.697013000	0.607096000	-0.403569000
Cl	0.908245000	0.744721000	-1.921263000
N	1.476098000	-0.111582000	1.018250000
C	0.465630000	0.666485000	1.614300000
C	-0.478577000	-0.185976000	2.185356000
C	-0.038463000	-1.524808000	1.947146000
C	1.189619000	-1.452504000	1.275748000
C	0.489510000	2.163487000	1.668498000
H	1.359941000	2.526130000	2.237383000
H	-0.420723000	2.521273000	2.169036000
H	0.530996000	2.627040000	0.672638000
H	-1.372056000	0.124488000	2.722910000
H	-0.519956000	-2.442010000	2.281138000
C	2.091781000	-2.593999000	0.918429000
H	3.062914000	-2.502871000	1.431110000
H	2.294009000	-2.662265000	-0.158358000
H	1.625644000	-3.536560000	1.237010000
C	3.978287000	-0.714552000	-1.097958000
H	4.641920000	-1.121718000	-0.314546000
H	4.632963000	-0.198564000	-1.823407000

H	3.528093000	-1.567349000	-1.630575000
C	3.382283000	2.404900000	0.014211000
H	3.764125000	2.468553000	1.049494000
H	2.661246000	3.226483000	-0.119172000
H	4.239441000	2.619600000	-0.648442000
C	-2.919742000	2.267268000	-0.264341000
C	-3.906678000	1.363332000	0.478513000
H	-2.642892000	3.143777000	0.344398000
H	-3.461393000	1.024879000	1.432719000
H	-3.358775000	2.643206000	-1.203509000
H	-4.781461000	1.973555000	0.765037000
C	-4.411332000	0.138575000	-0.304437000
C	-3.500900000	-1.099844000	-0.367409000
H	-5.365765000	-0.183395000	0.147553000
H	-3.275979000	-1.437197000	0.663385000
H	-4.664846000	0.450729000	-1.335172000
H	-4.106897000	-1.919127000	-0.804248000
C	-2.212848000	-0.980281000	-1.174704000
C	-1.301287000	-2.104339000	-1.268682000
H	-2.322394000	-0.374006000	-2.087825000
H	-1.513664000	-3.001699000	-0.669814000
H	-0.810638000	-2.323980000	-2.226358000
H	-1.991848000	1.738284000	-0.532839000

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A-7-q SCF Done: -1471.561956 A.U.

Al	3.125062000	-0.340106000	0.150640000
Cl	2.254793000	-1.678277000	1.685415000
N	1.432304000	0.244732000	-0.845135000
C	0.599801000	-0.632472000	-1.519079000
C	-0.389031000	0.101506000	-2.202482000
C	-0.099005000	1.483727000	-1.988481000
C	1.014038000	1.542101000	-1.148380000
C	0.803499000	-2.113624000	-1.559657000
H	1.597283000	-2.362524000	-2.282453000
H	-0.120580000	-2.610283000	-1.885516000
H	1.103745000	-2.515581000	-0.582518000
H	-1.163244000	-0.319783000	-2.840465000
H	-0.640469000	2.338940000	-2.387469000
C	1.714711000	2.783850000	-0.688695000
H	2.724765000	2.850848000	-1.121537000
H	1.837909000	2.831741000	0.401961000
H	1.146945000	3.666374000	-1.016378000
C	3.984912000	1.194208000	1.062440000

H	4.423979000	1.941118000	0.378365000
H	4.828952000	0.768452000	1.636520000
H	3.367810000	1.740205000	1.797013000
C	4.238279000	-1.283939000	-1.181974000
H	4.355585000	-0.703986000	-2.116118000
H	3.871031000	-2.285522000	-1.460639000
H	5.255083000	-1.425738000	-0.773078000
C	-0.956916000	1.923642000	2.111143000
C	-0.030330000	0.981355000	2.372031000
H	-0.688095000	2.879484000	1.650796000
H	1.025581000	1.120422000	2.126402000
H	-1.998995000	1.805070000	2.417809000
H	-0.274435000	0.050703000	2.888784000
Cr	-0.947691000	0.465005000	0.022183000
C	-1.668230000	-1.288824000	0.770540000
C	-2.718818000	-2.079182000	-0.020117000
H	-0.751875000	-1.888537000	0.923122000
H	-2.542282000	-1.999651000	-1.110899000
H	-2.058466000	-1.061921000	1.780735000
H	-2.604260000	-3.156427000	0.205511000
C	-4.178416000	-1.708750000	0.278296000
C	-4.697799000	-0.357600000	-0.230388000
H	-4.826765000	-2.492789000	-0.151839000
H	-4.627077000	-0.330568000	-1.334537000
H	-4.335517000	-1.763361000	1.372403000
H	-5.778283000	-0.323319000	-0.005670000
C	-4.054546000	0.922660000	0.333366000
C	-2.760230000	1.369400000	-0.355783000
H	-4.798258000	1.735868000	0.227057000
H	-2.904937000	1.313508000	-1.450548000
H	-3.913821000	0.809600000	1.425423000
H	-2.561662000	2.438160000	-0.135728000

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A-8-q SCF Done: -1471.599376 A.U.

C	-4.624538000	0.533669000	-0.994166000
C	-4.881894000	-0.781438000	-0.235869000
H	-5.581887000	0.838111000	-1.452298000
H	-5.591649000	-0.583148000	0.588527000
H	-3.954359000	0.344322000	-1.850112000
H	-5.412063000	-1.465454000	-0.923981000
Cr	-0.243340000	-0.074867000	0.045898000
Al	3.163626000	-0.099426000	-0.713412000
Cl	1.174446000	-0.143785000	-1.978856000

N	2.122813000	0.212186000	0.960337000
C	1.456981000	1.408929000	1.215055000
C	0.404668000	1.166700000	2.105723000
C	0.425498000	-0.223114000	2.411928000
C	1.499855000	-0.784275000	1.703290000
C	1.858463000	2.733208000	0.641616000
H	2.901083000	2.980314000	0.893172000
H	1.210356000	3.518934000	1.053956000
H	1.768464000	2.763249000	-0.454309000
H	-0.275346000	1.918585000	2.500715000
H	-0.221179000	-0.756605000	3.106016000
C	1.972680000	-2.204336000	1.774859000
H	3.035139000	-2.255458000	2.057288000
H	1.860716000	-2.741757000	0.822443000
H	1.389639000	-2.743366000	2.534241000
C	4.010216000	-1.872172000	-0.822752000
H	4.705204000	-2.058074000	0.015802000
H	4.621003000	-1.899042000	-1.743151000
H	3.319109000	-2.727708000	-0.875629000
C	4.258843000	1.440945000	-1.262944000
H	4.898614000	1.803638000	-0.437719000
H	3.700972000	2.307628000	-1.650077000
H	4.943268000	1.114838000	-2.066285000
C	-1.551376000	1.350779000	-0.599344000
C	-2.678523000	1.669925000	0.394983000
H	-0.969877000	2.249245000	-0.871685000
H	-2.687353000	0.942003000	1.226983000
H	-1.925742000	0.921323000	-1.544055000
H	-2.469271000	2.637741000	0.884329000
C	-4.105666000	1.742956000	-0.194811000
C	-3.660251000	-1.520044000	0.338745000
H	-4.811563000	1.954649000	0.629955000
H	-3.196849000	-0.900662000	1.121732000
H	-4.150739000	2.622469000	-0.862276000
H	-4.018812000	-2.419462000	0.869845000
C	-2.583218000	-1.940274000	-0.683412000
C	-1.158752000	-1.917106000	-0.115960000
H	-2.826866000	-2.953973000	-1.056253000
H	-1.131516000	-2.421226000	0.868983000
H	-2.631584000	-1.297494000	-1.578201000
H	-0.467078000	-2.471331000	-0.778619000

Cr	0.791739000	0.274088000	-0.336002000
Al	-2.462022000	-0.292459000	-0.345737000
Cl	-0.806224000	-0.670914000	-1.969013000
N	-1.057456000	0.114837000	1.031474000
C	-0.179100000	-0.863025000	1.535842000
C	0.933707000	-0.225275000	2.083239000
C	0.730613000	1.183233000	1.933970000
C	-0.520683000	1.368395000	1.333806000
C	-0.466166000	-2.333852000	1.517776000
H	-1.364768000	-2.571701000	2.108469000
H	0.384490000	-2.872636000	1.958025000
H	-0.626613000	-2.726753000	0.503232000
H	1.782173000	-0.718673000	2.552659000
H	1.386781000	1.979441000	2.280597000
C	-1.218286000	2.670013000	1.079583000
H	-2.176555000	2.715140000	1.621388000
H	-1.434430000	2.843877000	0.017108000
H	-0.585751000	3.494478000	1.436617000
C	-3.507453000	1.276515000	-0.905366000
H	-4.044246000	1.757222000	-0.068345000
H	-4.281672000	0.929842000	-1.613564000
H	-2.931044000	2.058300000	-1.425285000
C	-3.443700000	-1.954419000	0.036050000
H	-3.790727000	-1.992607000	1.084760000
H	-2.889209000	-2.885413000	-0.159543000
H	-4.350829000	-1.983085000	-0.593455000
C	4.192191000	-1.439356000	0.028990000
C	3.911393000	0.014048000	-0.360643000
H	5.126957000	-1.533645000	0.605532000
H	3.848767000	0.640312000	0.549296000
H	4.289857000	-2.076165000	-0.866301000
H	4.788353000	0.403564000	-0.916566000
C	2.661273000	0.208562000	-1.202629000
C	2.052244000	1.514458000	-1.362588000
H	2.620724000	-0.456130000	-2.081024000
H	2.464663000	2.357055000	-0.789520000
H	1.644594000	1.807618000	-2.339087000
H	3.374834000	-1.860292000	0.638348000

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A-2-3-q SCF Done: -1314.433819 A.U.

Cr	1.404762000	0.029563000	0.169610000
Al	-2.265362000	-0.030905000	-0.606955000
Cl	-0.460114000	-0.393467000	-1.951816000

N	-1.096883000	0.104503000	1.016470000
C	-0.437210000	-0.985530000	1.558985000
C	0.651215000	-0.539738000	2.330025000
C	0.666174000	0.878811000	2.238794000
C	-0.410388000	1.243839000	1.410347000
C	-0.884743000	-2.403930000	1.391517000
H	-1.891392000	-2.553366000	1.811152000
H	-0.189526000	-3.074138000	1.915569000
H	-0.923680000	-2.705220000	0.335201000
H	1.314237000	-1.174646000	2.914163000
H	1.340361000	1.569599000	2.741637000
C	-0.856856000	2.638464000	1.100342000
H	-1.857886000	2.828820000	1.518320000
H	-0.913694000	2.835814000	0.022253000
H	-0.156321000	3.357956000	1.546248000
C	-3.157565000	1.667471000	-1.075359000
H	-3.725004000	2.101192000	-0.232127000
H	-3.898437000	1.449786000	-1.866112000
H	-2.499028000	2.457088000	-1.471546000
C	-3.463172000	-1.599518000	-0.529003000
H	-3.985333000	-1.675127000	0.442620000
H	-2.988037000	-2.574401000	-0.722018000
H	-4.251388000	-1.474075000	-1.293212000
C	2.365118000	-1.757819000	-0.112830000
C	2.873415000	-1.079468000	-1.292007000
H	1.599089000	-2.527560000	-0.265392000
H	2.330715000	-1.288740000	-2.218745000
H	3.087767000	-2.011019000	0.674829000
H	3.955749000	-1.101000000	-1.440185000
C	2.951970000	0.917333000	-1.385779000
C	2.079742000	1.790147000	-0.622656000
H	2.807951000	0.904309000	-2.470442000
H	1.256240000	2.277279000	-1.157855000
H	4.009488000	0.981726000	-1.114071000
H	2.547464000	2.425026000	0.140812000

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A-3-9-q SCF Done: -1314.423669 A.U.

Cr	1.470606000	0.311631000	-0.086616000
Al	-2.268403000	-0.486472000	0.326058000
Cl	-1.326415000	-2.303068000	-0.530484000
N	-0.784069000	0.879321000	-0.078139000
C	-0.122123000	1.729833000	0.813610000
C	0.752193000	2.557071000	0.089291000

C	0.606183000	2.222713000	-1.288003000
C	-0.355018000	1.203946000	-1.366151000
C	-0.407994000	1.800348000	2.281378000
H	-1.403244000	2.238330000	2.460720000
H	0.338642000	2.443134000	2.768582000
H	-0.391380000	0.816056000	2.763592000
H	1.400716000	3.319528000	0.516724000
H	1.123541000	2.673291000	-2.133105000
C	-0.912645000	0.583276000	-2.609548000
H	-1.909238000	0.999514000	-2.826585000
H	-1.023097000	-0.505699000	-2.511743000
H	-0.258028000	0.805860000	-3.464030000
C	-3.848261000	0.124979000	-0.695151000
H	-4.051844000	1.202170000	-0.549432000
H	-4.742764000	-0.412043000	-0.330724000
H	-3.796164000	-0.056273000	-1.781482000
C	-2.519303000	-0.734956000	2.269445000
H	-2.922107000	0.146450000	2.797700000
H	-1.621780000	-1.075868000	2.812831000
H	-3.272430000	-1.536458000	2.385926000
H	3.072461000	0.635439000	-0.149824000
C	1.944307000	-0.799631000	1.574801000
C	3.249680000	-1.397740000	1.004250000
H	2.111322000	-0.211273000	2.490271000
H	4.139165000	-0.989969000	1.507466000
H	1.160730000	-1.551144000	1.763014000
H	3.298162000	-2.498358000	1.087449000
C	3.279253000	-1.017701000	-0.474172000
C	2.184205000	-1.369180000	-1.269180000
H	4.229419000	-0.729870000	-0.937189000
H	2.217806000	-1.218002000	-2.352283000
H	1.429473000	-2.070665000	-0.896082000

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A-4-5-q SCF Done: -1392.980028 A.U.

Cr	1.153728000	0.191020000	-0.027907000
Al	-2.703116000	-0.144190000	-0.331733000
Cl	-1.831585000	-1.720876000	-1.614227000
N	-1.061041000	0.349799000	0.805417000
C	-0.384797000	-0.553629000	1.623452000
C	0.607326000	0.136505000	2.342787000
C	0.497561000	1.510082000	1.992769000
C	-0.532689000	1.618053000	1.050745000
C	-0.778626000	-1.988254000	1.783987000

H	-1.648650000	-2.064033000	2.456218000
H	0.048221000	-2.555707000	2.233274000
H	-1.052829000	-2.449386000	0.825807000
H	1.287021000	-0.311244000	3.065801000
H	1.095362000	2.337558000	2.371992000
C	-1.079885000	2.886968000	0.473217000
H	-2.081271000	3.100906000	0.879633000
H	-1.182622000	2.853821000	-0.618635000
H	-0.421479000	3.726063000	0.740409000
C	-3.281337000	1.373285000	-1.462450000
H	-3.698241000	2.231077000	-0.906816000
H	-4.103185000	0.986558000	-2.093587000
H	-2.520052000	1.760306000	-2.161330000
C	-4.045560000	-0.823857000	0.951753000
H	-4.219464000	-0.120593000	1.787385000
H	-3.809081000	-1.806378000	1.392866000
H	-5.015672000	-0.938465000	0.434780000
C	1.949610000	-1.678888000	-0.385775000
C	3.369503000	-1.695078000	0.180896000
H	1.317964000	-2.481170000	0.025678000
H	3.336483000	-1.686642000	1.287485000
H	1.963467000	-1.809816000	-1.482827000
H	3.925985000	-2.612160000	-0.091914000
C	4.126753000	-0.453710000	-0.301341000
C	3.293015000	0.806467000	-0.095884000
H	5.099606000	-0.349390000	0.215405000
H	3.007933000	0.923917000	0.970919000
H	4.371362000	-0.562432000	-1.374137000
H	3.841263000	1.722637000	-0.343110000
C	2.172756000	1.284500000	-1.858062000
C	0.838383000	0.839177000	-1.992448000
H	2.344049000	2.357031000	-1.734107000
H	0.034212000	1.580583000	-1.971014000
H	2.970526000	0.768035000	-2.396956000
H	0.612273000	-0.074512000	-2.548867000

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A-5-6-q SCF Done: -1393.002662 A.U.

Cr	0.890945000	0.259144000	0.362196000
Al	-2.654783000	-0.276028000	-0.788289000
Cl	-0.763518000	-0.500547000	-2.008732000
N	-1.627370000	0.075811000	0.905636000
C	-0.926467000	-0.903366000	1.594458000
C	-0.018248000	-0.294057000	2.477965000

C	-0.151208000	1.110070000	2.302287000
C	-1.139405000	1.305604000	1.320062000
C	-1.181887000	-2.371878000	1.450859000
H	-2.208926000	-2.625855000	1.753622000
H	-0.487792000	-2.932564000	2.092600000
H	-1.051767000	-2.716647000	0.415144000
H	0.631607000	-0.815860000	3.178562000
H	0.370452000	1.899793000	2.839541000
C	-1.689439000	2.622180000	0.866663000
H	-2.744936000	2.727595000	1.162782000
H	-1.645422000	2.746822000	-0.222962000
H	-1.118709000	3.438367000	1.330835000
C	-3.711499000	1.282763000	-1.384527000
H	-4.388818000	1.670519000	-0.602168000
H	-4.360426000	0.945814000	-2.213554000
H	-3.128118000	2.134307000	-1.770088000
C	-3.678383000	-1.962905000	-0.667500000
H	-4.249402000	-2.040275000	0.276188000
H	-3.085389000	-2.885745000	-0.769395000
H	-4.425954000	-1.974800000	-1.481198000
C	2.161872000	-1.575559000	0.065445000
C	3.691797000	-1.467527000	0.196098000
H	1.732896000	-2.080232000	0.944125000
H	3.948230000	-1.056364000	1.190337000
H	1.877108000	-2.172381000	-0.817217000
H	4.145002000	-2.474733000	0.162332000
C	4.342359000	-0.579852000	-0.879960000
C	3.839535000	0.873259000	-0.841309000
H	5.437515000	-0.590342000	-0.752246000
H	4.062099000	1.303825000	0.152139000
H	4.145845000	-1.009837000	-1.880057000
H	4.399291000	1.484462000	-1.571030000
C	2.341138000	1.023539000	-1.125435000
C	1.568381000	2.043459000	-0.457655000
H	2.065095000	0.818442000	-2.169538000
H	2.075389000	2.689570000	0.270964000
H	0.767584000	2.540442000	-1.015652000
H	2.047194000	-0.311171000	-0.644724000

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A-7-8-q SCF Done: -1471.538584 A.U.

C	4.708740000	-0.237115000	0.240249000
C	4.145254000	1.047560000	-0.385486000
H	4.609930000	-0.171714000	1.340646000

H	4.770358000	1.885104000	-0.027031000
H	5.795274000	-0.232486000	0.045556000
H	4.307699000	1.025565000	-1.478505000
Cr	0.766507000	0.320645000	-0.015370000
Al	-3.107501000	-0.236203000	-0.339740000
Cl	-2.189829000	-1.820676000	-1.583356000
N	-1.494486000	0.349277000	0.789275000
C	-0.787608000	-0.501171000	1.636488000
C	0.150715000	0.251808000	2.362867000
C	-0.028651000	1.612182000	1.988693000
C	-1.042890000	1.649380000	1.025836000
C	-1.104502000	-1.952824000	1.814600000
H	-1.963023000	-2.067106000	2.496305000
H	-0.245620000	-2.473349000	2.260923000
H	-1.365879000	-2.438074000	0.864877000
H	0.834815000	-0.146140000	3.110586000
H	0.515828000	2.476651000	2.365594000
C	-1.647793000	2.878728000	0.420644000
H	-2.670805000	3.038132000	0.797180000
H	-1.716718000	2.832128000	-0.673416000
H	-1.047076000	3.756922000	0.698194000
C	-3.730214000	1.222040000	-1.523241000
H	-4.190530000	2.079245000	-1.002295000
H	-4.523572000	0.783632000	-2.156997000
H	-2.970113000	1.616542000	-2.219124000
C	-4.429062000	-0.929546000	0.957937000
H	-4.650286000	-0.199692000	1.758842000
H	-4.146054000	-1.876848000	1.446278000
H	-5.385113000	-1.119527000	0.436998000
C	1.544165000	-1.539165000	-0.425809000
C	2.790042000	-2.060149000	0.304168000
H	0.688519000	-2.207289000	-0.230690000
H	2.736152000	-1.847412000	1.390418000
H	1.709387000	-1.592897000	-1.517458000
H	2.785950000	-3.164897000	0.238984000
C	4.161635000	-1.596639000	-0.226129000
C	2.690819000	1.379198000	-0.046626000
H	4.903764000	-2.351272000	0.086395000
H	2.495344000	0.963048000	0.967082000
H	4.156744000	-1.635769000	-1.331925000
H	2.524646000	2.462225000	0.035628000
C	1.767820000	1.210807000	-1.940080000
C	0.386812000	0.910761000	-1.983101000

H	2.098237000	2.240903000	-2.093619000
H	-0.330580000	1.736146000	-2.020262000
H	2.470596000	0.464526000	-2.313808000
H	0.040265000	-0.029722000	-2.423800000

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B-0-s SCF Done: -1078.777161 A.U.

Cr	1.434892000	1.120963000	-0.000166000
Al	-1.642032000	-0.413771000	0.000103000
Cl	-0.894124000	1.857340000	-0.000505000
N	0.168101000	-1.187258000	0.000336000
C	0.985469000	-1.155283000	-1.109203000
C	2.326408000	-1.079022000	-0.718275000
C	2.326505000	-1.078660000	0.718581000
C	0.985607000	-1.154375000	1.109735000
H	3.194611000	-1.103130000	-1.375436000
H	3.194782000	-1.102389000	1.375660000
C	-2.509323000	-0.722712000	1.735291000
H	-2.730405000	-1.794233000	1.890494000
H	-3.473568000	-0.188019000	1.793436000
H	-1.907317000	-0.382654000	2.595263000
C	-2.509150000	-0.723872000	-1.734965000
H	-2.728481000	-1.795741000	-1.890272000
H	-1.907837000	-0.382718000	-2.594989000
H	-3.474293000	-0.190780000	-1.792873000
H	0.565761000	-1.183317000	-2.113396000
H	0.566038000	-1.181533000	2.114010000

26

B-1-q SCF Done: -1157.327998 A.U.

Cr	1.184439000	-0.291182000	-0.000602000
Al	-2.101448000	-0.065243000	0.000711000
Cl	-0.656930000	-1.917097000	-0.002808000
N	-0.567232000	1.200977000	0.000782000
C	0.167718000	1.566038000	1.118261000
C	1.395712000	2.094145000	0.716693000
C	1.394956000	2.094239000	-0.717349000
C	0.166578000	1.566005000	-1.117561000
H	2.184588000	2.460747000	1.370506000
H	2.183089000	2.461006000	-1.371956000
C	-3.008859000	0.020981000	-1.736951000
H	-3.532346000	0.984218000	-1.874898000
H	-3.775160000	-0.769913000	-1.816759000
H	-2.328981000	-0.112235000	-2.595780000
C	-3.006275000	0.017906000	1.739845000

H	-3.529487000	0.980955000	1.880138000
H	-2.325301000	-0.116873000	2.597558000
H	-3.772579000	-0.773030000	1.819251000
C	2.859871000	-1.221088000	0.724252000
C	2.863186000	-1.217963000	-0.721790000
H	3.559435000	-0.568992000	1.263937000
H	3.564928000	-0.563065000	-1.255226000
H	2.623867000	-2.148945000	1.261653000
H	2.630311000	-2.143533000	-1.264480000
H	-0.223346000	1.404160000	2.120876000
H	-0.225619000	1.404256000	-2.119753000

32

B-2-q SCF Done: -1235.866560 A.U.

Cr	-1.300557000	0.129118000	0.000034000
Al	2.329819000	-0.300199000	-0.000124000
Cl	0.767521000	-1.936418000	0.000313000
N	0.987923000	1.171112000	0.000120000
C	0.306823000	1.624549000	-1.103571000
C	-0.777259000	2.428346000	-0.708509000
C	-0.777021000	2.428492000	0.709069000
C	0.307201000	1.624787000	1.103903000
H	-1.468968000	2.947526000	-1.369300000
H	-1.468476000	2.947827000	1.370000000
C	3.284333000	-0.230853000	1.722453000
H	3.875410000	0.697164000	1.827206000
H	3.997562000	-1.069773000	1.808490000
H	2.618453000	-0.298313000	2.600713000
C	3.283433000	-0.230668000	-1.723205000
H	3.872988000	0.698205000	-1.828960000
H	2.617290000	-0.299921000	-2.601123000
H	3.997993000	-1.068497000	-1.808877000
C	-1.842469000	-0.416477000	-2.044708000
C	-2.636565000	-1.277573000	-1.303041000
H	-0.904759000	-0.773582000	-2.481158000
H	-2.328356000	-2.312561000	-1.146068000
H	-2.274210000	0.481053000	-2.500127000
H	-3.700363000	-1.072500000	-1.163843000
C	-2.635767000	-1.278823000	1.302646000
C	-1.843282000	-0.416453000	2.044544000
H	-2.325672000	-2.313265000	1.145718000
H	-0.905350000	-0.772111000	2.481691000
H	-3.699855000	-1.075570000	1.163114000
H	-2.276528000	0.480655000	2.499380000

H	0.659025000	1.398189000	-2.107812000
H	0.659670000	1.398578000	2.108089000

32

B-3-q SCF Done: -1235.894062 A.U.

Cr	0.887159000	0.093747000	-0.016522000
Al	-2.466879000	-0.434651000	0.036869000
Cl	-0.590033000	-1.858096000	-0.018515000
N	-1.311032000	1.177685000	-0.019522000
C	-0.642485000	1.699420000	1.067764000
C	0.435510000	2.478988000	0.630578000
C	0.409855000	2.443708000	-0.794901000
C	-0.679045000	1.641923000	-1.154817000
H	1.136833000	3.020364000	1.262468000
H	1.089745000	2.950406000	-1.476932000
C	-3.428537000	-0.611477000	-1.663729000
H	-4.202143000	0.170036000	-1.772165000
H	-3.949841000	-1.583081000	-1.719873000
H	-2.774079000	-0.553579000	-2.550157000
C	-3.292389000	-0.581219000	1.810531000
H	-4.045054000	0.210605000	1.975978000
H	-2.565826000	-0.525965000	2.639159000
H	-3.818990000	-1.545711000	1.917613000
C	2.273896000	-0.378248000	1.421483000
C	3.625823000	-0.544909000	0.715787000
H	2.301475000	0.348864000	2.252296000
H	4.088128000	0.447915000	0.555029000
H	1.915321000	-1.342539000	1.828661000
H	4.350212000	-1.119512000	1.324908000
C	3.388291000	-1.203937000	-0.649699000
C	2.321656000	-0.394015000	-1.394699000
H	4.329186000	-1.294604000	-1.226680000
H	2.737867000	0.570048000	-1.748882000
H	3.027506000	-2.237649000	-0.493781000
H	1.893280000	-0.919848000	-2.266294000
H	-0.966464000	1.478492000	2.083130000
H	-1.037220000	1.368728000	-2.145619000

38

B-4-q SCF Done: -1314.420321 A.U.

Cr	-1.103514000	0.084793000	0.225029000
Al	2.794948000	-0.042243000	-0.262215000
Cl	1.712681000	-1.946582000	-0.658579000
N	1.195295000	1.097644000	0.171852000
C	0.379527000	1.730707000	-0.727994000

C	-0.657515000	2.397202000	-0.052784000
C	-0.435182000	2.177572000	1.340157000
C	0.700164000	1.369152000	1.431104000
H	-1.441343000	2.997415000	-0.509721000
H	-1.033374000	2.552247000	2.168275000
C	3.826852000	-0.136635000	1.419505000
H	4.192265000	0.854720000	1.744447000
H	4.720983000	-0.771404000	1.286223000
H	3.265142000	-0.573459000	2.264880000
C	3.573129000	0.712176000	-1.908650000
H	3.928398000	1.749236000	-1.768348000
H	2.869471000	0.715703000	-2.759880000
H	4.447054000	0.119742000	-2.233089000
C	-1.797533000	-0.511283000	-1.627263000
C	-3.245256000	-0.026939000	-1.756570000
H	-1.146584000	-0.165101000	-2.447535000
H	-3.262302000	1.055993000	-1.984390000
H	-1.748252000	-1.615311000	-1.625752000
H	-3.781164000	-0.517615000	-2.592005000
C	-3.952363000	-0.261868000	-0.416807000
C	-3.100523000	0.369422000	0.692050000
H	-4.987187000	0.130631000	-0.423782000
H	-3.259785000	1.462105000	0.721175000
H	-4.048448000	-1.351525000	-0.252712000
H	-3.336706000	-0.019032000	1.700399000
C	-0.699741000	-1.666492000	1.970821000
C	-1.335026000	-2.353748000	1.000476000
H	0.393515000	-1.643854000	1.999489000
H	-0.761589000	-2.865076000	0.223427000
H	-1.244534000	-1.198114000	2.796593000
H	-2.422233000	-2.460302000	0.988135000
H	1.206295000	0.991119000	2.317373000
H	0.578554000	1.678819000	-1.796490000

38

B-5-q SCF Done: -1314.461105 A.U.

Cr	-0.489878000	0.113914000	0.050898000
Al	2.904679000	-0.465369000	-0.179096000
Cl	0.959770000	-1.724002000	-0.648768000
N	1.833006000	1.092160000	0.393202000
C	1.200318000	1.952557000	-0.476406000
C	0.138506000	2.591843000	0.172740000
C	0.128981000	2.099652000	1.510840000
C	1.184606000	1.185105000	1.605113000

H	-0.527693000	3.335855000	-0.260120000
H	-0.544826000	2.390343000	2.314512000
C	3.793949000	-1.273877000	1.372328000
H	4.610308000	-0.631285000	1.748713000
H	4.252301000	-2.240827000	1.100351000
H	3.115285000	-1.473858000	2.218999000
C	3.789784000	-0.071284000	-1.885689000
H	4.588129000	0.682676000	-1.762524000
H	3.100692000	0.300900000	-2.662958000
H	4.269865000	-0.976527000	-2.296821000
C	-1.701292000	0.232640000	-1.568641000
C	-3.096477000	0.819337000	-1.320847000
H	-1.139958000	0.846703000	-2.298357000
H	-3.052264000	1.661328000	-0.599067000
H	-1.766167000	-0.785199000	-1.993375000
H	-3.463470000	1.279610000	-2.258461000
C	-4.165633000	-0.182735000	-0.859324000
C	-4.107369000	-0.703282000	0.584879000
H	-5.153773000	0.292320000	-0.993466000
H	-4.194236000	0.151018000	1.283738000
H	-4.156194000	-1.045672000	-1.551605000
H	-5.021594000	-1.301898000	0.742046000
C	-2.899336000	-1.563293000	1.001147000
C	-1.658198000	-0.787457000	1.450544000
H	-3.227145000	-2.206230000	1.840774000
H	-1.944324000	-0.014555000	2.190652000
H	-2.645293000	-2.266740000	0.186581000
H	-0.944422000	-1.464472000	1.959316000
H	1.537906000	2.054994000	-1.506086000
H	1.508967000	0.595064000	2.460397000

38

B-6-q SCF Done: -1314.464675 A.U.

Cr	-0.278845000	-0.741614000	-0.374458000
Al	2.676562000	0.703855000	-0.023644000
Cl	1.130140000	0.698521000	-1.792072000
N	1.521494000	-0.493849000	1.061712000
C	0.452671000	-0.086608000	1.845638000
C	-0.371020000	-1.178878000	2.115408000
C	0.239782000	-2.318941000	1.496700000
C	1.411642000	-1.863853000	0.889336000
H	-1.286645000	-1.166223000	2.703293000
H	-0.114971000	-3.347180000	1.523373000
C	4.277910000	-0.277430000	-0.592239000

H	4.953301000	-0.475913000	0.259438000
H	4.857306000	0.309276000	-1.326432000
H	4.054823000	-1.246898000	-1.069675000
C	2.691058000	2.491420000	0.785791000
H	3.230116000	2.497724000	1.750327000
H	1.681941000	2.898905000	0.967595000
H	3.208445000	3.212850000	0.129360000
C	-2.117319000	2.512913000	0.310469000
C	-3.246768000	1.695556000	0.942592000
H	-1.623929000	3.159084000	1.055494000
H	-2.849216000	1.083187000	1.773666000
H	-2.503801000	3.168049000	-0.487990000
H	-3.957063000	2.398255000	1.412797000
C	-4.032557000	0.789197000	-0.021727000
C	-3.429431000	-0.582528000	-0.369848000
H	-5.026361000	0.601262000	0.420619000
H	-3.269541000	-1.155875000	0.564042000
H	-4.228148000	1.344591000	-0.958295000
H	-4.213232000	-1.147204000	-0.913814000
C	-2.163958000	-0.601820000	-1.220042000
C	-1.523202000	-1.859522000	-1.542421000
H	-2.152964000	0.163481000	-2.011460000
H	-1.908944000	-2.777846000	-1.076633000
H	-1.108493000	-2.018583000	-2.546680000
H	-1.344345000	1.875058000	-0.145638000
H	2.159980000	-2.417182000	0.325140000
H	0.343017000	0.954845000	2.141134000

44

B-7-q SCF Done: -1392.983345 A.U.

Al	-3.233186000	0.290314000	-0.145582000
Cl	-2.358990000	1.769687000	1.257637000
N	-1.557044000	-0.592174000	-0.844143000
C	-0.664836000	-0.051807000	-1.731654000
C	0.300794000	-1.007740000	-2.089441000
C	-0.053694000	-2.209396000	-1.397968000
C	-1.188488000	-1.906392000	-0.647350000
H	1.110882000	-0.870482000	-2.802731000
H	0.457964000	-3.168720000	-1.443295000
C	-4.175323000	-1.159752000	0.815233000
H	-4.496202000	-1.977128000	0.143798000
H	-5.093167000	-0.768311000	1.289141000
H	-3.581500000	-1.613070000	1.629744000
C	-4.056501000	1.165349000	-1.709611000

H	-4.334026000	0.438420000	-2.494498000
H	-3.404035000	1.922772000	-2.179064000
H	-4.984315000	1.690695000	-1.420902000
C	1.165611000	-0.598062000	2.767425000
C	-0.126881000	-0.799748000	2.445801000
H	1.852634000	-1.429438000	2.944594000
H	-0.532567000	-1.813932000	2.371021000
H	1.561767000	0.408304000	2.920932000
H	-0.833795000	0.032239000	2.330958000
Cr	0.832902000	-0.474963000	0.148187000
C	1.368790000	1.488451000	0.171816000
C	2.374774000	1.981330000	-0.872939000
H	0.397720000	2.006693000	0.072460000
H	2.190729000	1.507008000	-1.856956000
H	1.735808000	1.720204000	1.187775000
H	2.205790000	3.061415000	-1.046297000
C	3.854527000	1.810084000	-0.501166000
C	4.453590000	0.396263000	-0.522830000
H	4.452620000	2.427547000	-1.194470000
H	4.350930000	-0.030036000	-1.539040000
H	4.017417000	2.251381000	0.500565000
H	5.539949000	0.509489000	-0.362740000
C	3.932562000	-0.630992000	0.500097000
C	2.665530000	-1.389983000	0.091874000
H	4.739019000	-1.373099000	0.658448000
H	2.798343000	-1.788409000	-0.930381000
H	3.805587000	-0.138192000	1.482533000
H	2.516753000	-2.274743000	0.744390000
H	-0.761170000	0.980162000	-2.063820000
H	-1.771964000	-2.550834000	0.007364000

44

B-8-q SCF Done: -1393.021921 A.U.

C	-4.374225000	0.191090000	-1.191232000
C	-4.704237000	-0.729682000	-0.002066000
H	-5.303865000	0.317360000	-1.773271000
H	-5.435174000	-0.218859000	0.651533000
H	-3.683309000	-0.324840000	-1.879870000
H	-5.232837000	-1.614773000	-0.401464000
Cr	-0.052953000	-0.063122000	0.173220000
Al	3.356131000	-0.167759000	-0.505920000
Cl	1.407704000	-0.925867000	-1.601923000
N	2.293421000	0.630412000	0.955842000
C	1.580712000	1.801103000	0.829473000

C	0.540690000	1.832453000	1.765486000
C	0.621238000	0.612834000	2.497892000
C	1.709493000	-0.095273000	1.969056000
H	-0.172509000	2.641579000	1.908766000
H	-0.010818000	0.297973000	3.326022000
C	4.332257000	-1.734423000	0.161147000
H	5.143301000	-1.441002000	0.851932000
H	4.808176000	-2.283326000	-0.670266000
H	3.692601000	-2.459788000	0.692429000
C	4.152098000	1.249736000	-1.605223000
H	4.931713000	1.802235000	-1.050361000
H	3.418349000	1.989137000	-1.968941000
H	4.640791000	0.824448000	-2.499302000
C	-1.288095000	1.046723000	-1.009184000
C	-2.436349000	1.735176000	-0.254347000
H	-0.661797000	1.770393000	-1.559416000
H	-2.496129000	1.378714000	0.790509000
H	-1.643135000	0.311663000	-1.750980000
H	-2.213882000	2.812809000	-0.159703000
C	-3.839946000	1.602856000	-0.889156000
C	-3.528574000	-1.214536000	0.863933000
H	-4.564839000	2.126889000	-0.238638000
H	-3.072240000	-0.351783000	1.373199000
H	-3.832018000	2.162432000	-1.841886000
H	-3.933338000	-1.838535000	1.680137000
C	-2.431822000	-2.009857000	0.124947000
C	-1.028408000	-1.798626000	0.703513000
H	-2.694310000	-3.085009000	0.153704000
H	-1.049838000	-1.873753000	1.807544000
H	-2.428791000	-1.754190000	-0.947825000
H	-0.332091000	-2.579087000	0.343234000
H	1.851320000	2.542830000	0.080237000
H	2.101931000	-1.068327000	2.258703000

32

B-9-q SCF Done: -1235.899545 A.U.

Cr	0.684498000	0.021532000	-0.544458000
Al	-2.483493000	-0.322078000	0.315493000
Cl	-0.970452000	-1.790953000	-0.716891000
N	-1.114942000	1.117486000	0.399845000
C	-0.137344000	1.243963000	1.374078000
C	0.884807000	2.068602000	0.904125000
C	0.496391000	2.504276000	-0.405517000
C	-0.746112000	1.922923000	-0.666847000

H	1.788794000	2.344660000	1.443431000
H	1.041331000	3.183564000	-1.057830000
C	-3.862044000	0.172789000	-0.990286000
H	-4.473001000	1.020860000	-0.631965000
H	-4.556793000	-0.667665000	-1.163317000
H	-3.454625000	0.452345000	-1.976925000
C	-2.844929000	-0.970345000	2.131916000
H	-3.340631000	-0.198787000	2.748314000
H	-1.937589000	-1.292680000	2.670723000
H	-3.523475000	-1.841011000	2.109195000
C	3.530340000	-0.894885000	1.779256000
C	3.650218000	-0.459796000	0.316610000
H	4.399802000	-0.569706000	2.373562000
H	3.735295000	0.641526000	0.259225000
H	3.464698000	-1.992735000	1.861296000
H	4.609508000	-0.842243000	-0.087320000
C	2.515138000	-0.932535000	-0.576095000
C	2.232395000	-0.298838000	-1.845748000
H	2.340841000	-2.018803000	-0.523373000
H	2.807154000	0.595258000	-2.126086000
H	1.929875000	-0.912117000	-2.704889000
H	2.623693000	-0.479742000	2.250923000
H	-0.224101000	0.719453000	2.323667000
H	-1.384204000	2.014943000	-1.543767000

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B-2-3-q SCF Done: -1235.855502 A.U.

Cr	-1.257606000	0.231033000	0.005767000
Al	2.377771000	-0.389353000	0.008983000
Cl	0.618038000	-1.840127000	-0.099796000
N	1.179917000	1.191938000	0.018762000
C	0.510964000	1.646504000	-1.088614000
C	-0.590921000	2.429419000	-0.706650000
C	-0.609381000	2.420345000	0.716240000
C	0.479203000	1.626937000	1.116808000
H	-1.271603000	2.953117000	-1.374647000
H	-1.306072000	2.938275000	1.372490000
C	3.266799000	-0.510719000	1.761642000
H	3.971206000	0.325522000	1.922769000
H	3.859351000	-1.439856000	1.835190000
H	2.565405000	-0.520076000	2.614073000
C	3.384888000	-0.406014000	-1.682712000
H	4.098369000	0.435786000	-1.743229000
H	2.744481000	-0.360569000	-2.580754000

H	3.981093000	-1.331483000	-1.771913000
C	-2.155093000	-0.239837000	-1.774852000
C	-2.692302000	-1.341628000	-0.998220000
H	-1.358060000	-0.467995000	-2.493012000
H	-2.147066000	-2.285574000	-1.091399000
H	-2.862793000	0.520250000	-2.132657000
H	-3.774123000	-1.488851000	-1.040498000
C	-2.836744000	-1.232487000	0.998086000
C	-1.993933000	-0.381224000	1.814346000
H	-2.690645000	-2.312204000	1.098790000
H	-1.182428000	-0.856309000	2.378275000
H	-3.895825000	-0.959628000	0.998278000
H	-2.479383000	0.445889000	2.348224000
H	0.863424000	1.409837000	-2.090855000
H	0.809256000	1.381479000	2.124455000

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B-3-9-q SCF Done: -1235.843843 A.U.

Cr	1.359657000	0.403674000	-0.020663000
Al	-2.409707000	-0.362208000	0.041086000
Cl	-1.220618000	-2.215268000	-0.188259000
N	-0.919982000	1.015162000	0.028712000
C	-0.295769000	1.557587000	1.134141000
C	0.611813000	2.550544000	0.731897000
C	0.526923000	2.623144000	-0.690427000
C	-0.419793000	1.667082000	-1.079302000
H	1.240444000	3.152755000	1.385100000
H	1.084413000	3.286666000	-1.348820000
C	-3.465311000	0.040976000	-1.578194000
H	-3.896968000	1.058345000	-1.558282000
H	-4.314825000	-0.659763000	-1.665616000
H	-2.889578000	-0.056541000	-2.516011000
C	-3.204654000	-0.210894000	1.841285000
H	-3.625271000	0.792504000	2.036542000
H	-2.492588000	-0.437087000	2.654875000
H	-4.037361000	-0.927942000	1.953989000
H	2.940274000	0.783335000	-0.165292000
C	1.996643000	-0.894805000	1.431466000
C	3.245972000	-1.388300000	0.668492000
H	2.245418000	-0.420855000	2.393405000
H	4.177397000	-1.051764000	1.147924000
H	1.233150000	-1.672303000	1.587694000
H	3.295085000	-2.488618000	0.585186000
C	3.153587000	-0.797100000	-0.737427000

C	2.008666000	-1.056376000	-1.496610000
H	4.060434000	-0.416194000	-1.219918000
H	1.960644000	-0.744336000	-2.544177000
H	1.292968000	-1.822955000	-1.178630000
H	-0.553770000	1.224022000	2.137286000
H	-0.783539000	1.423538000	-2.075976000

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B-4-5-q SCF Done: -1314.401008 A.U.

Cr	-1.031626000	0.148007000	0.183653000
Al	2.790660000	-0.196652000	-0.004783000
Cl	1.908263000	-2.124074000	-0.604535000
N	1.140253000	0.989564000	-0.089006000
C	0.443236000	1.333454000	-1.227746000
C	-0.498429000	2.329944000	-0.929380000
C	-0.353586000	2.619673000	0.457505000
C	0.654443000	1.776678000	0.935823000
H	-1.183344000	2.797556000	-1.634685000
H	-0.917845000	3.344962000	1.041601000
C	3.317485000	-0.144553000	1.901308000
H	3.626990000	0.863362000	2.234425000
H	4.187852000	-0.804415000	2.067667000
H	2.530427000	-0.496529000	2.592138000
C	3.994317000	0.537013000	-1.387010000
H	4.282946000	1.583230000	-1.177355000
H	3.552180000	0.514905000	-2.398931000
H	4.931339000	-0.045285000	-1.443561000
C	-1.697332000	-1.092037000	-1.318436000
C	-3.110162000	-0.651128000	-1.699683000
H	-1.004412000	-1.109900000	-2.174153000
H	-3.074547000	0.314194000	-2.240385000
H	-1.701206000	-2.109260000	-0.887094000
H	-3.602215000	-1.360180000	-2.392325000
C	-3.950813000	-0.478975000	-0.430110000
C	-3.199153000	0.338990000	0.614705000
H	-4.924109000	-0.002061000	-0.652217000
H	-2.906320000	1.331783000	0.209609000
H	-4.196507000	-1.472122000	-0.010878000
H	-3.809199000	0.564570000	1.496568000
C	-2.128213000	-0.930541000	1.979384000
C	-0.761884000	-1.207026000	1.755987000
H	-2.390973000	-0.300102000	2.832656000
H	-0.020589000	-0.777825000	2.437141000
H	-2.880132000	-1.684500000	1.734745000

H	-0.455979000	-2.129338000	1.253902000
H	0.676814000	0.870237000	-2.183967000
H	1.077587000	1.704363000	1.935657000

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B-5-6-q SCF Done: -1314.424552 A.U.

Cr	-0.707779000	0.402204000	0.178239000
Al	2.826833000	-0.595846000	-0.145992000
Cl	0.983598000	-1.916229000	-0.085042000
N	1.763045000	1.081438000	-0.053391000
C	1.058437000	1.610046000	-1.106625000
C	0.107400000	2.532335000	-0.641521000
C	0.216701000	2.534867000	0.777150000
C	1.230559000	1.614744000	1.094063000
H	-0.563562000	3.132785000	-1.253458000
H	-0.349725000	3.138358000	1.483778000
C	3.860899000	-0.750816000	1.523951000
H	4.627832000	0.040567000	1.608214000
H	4.398019000	-1.715136000	1.562287000
H	3.238063000	-0.705268000	2.434484000
C	3.683042000	-0.677417000	-1.918402000
H	4.443573000	0.114194000	-2.046198000
H	2.969611000	-0.588281000	-2.756396000
H	4.204676000	-1.641258000	-2.055725000
C	-1.948728000	-0.163056000	-1.608253000
C	-3.475068000	0.019261000	-1.542209000
H	-1.488820000	0.613289000	-2.238390000
H	-3.709794000	1.069407000	-1.286136000
H	-1.680390000	-1.135005000	-2.055099000
H	-3.918410000	-0.152570000	-2.539651000
C	-4.161599000	-0.898422000	-0.514618000
C	-3.675739000	-0.657029000	0.924388000
H	-5.253119000	-0.749501000	-0.560299000
H	-3.883776000	0.392355000	1.202305000
H	-3.984488000	-1.955115000	-0.789536000
H	-4.257718000	-1.279338000	1.626791000
C	-2.185385000	-0.942449000	1.138553000
C	-1.412776000	-0.140934000	2.056306000
H	-1.925724000	-2.009958000	1.096292000
H	-1.913299000	0.683299000	2.580879000
H	-0.617749000	-0.625207000	2.633774000
H	-1.859450000	-0.680266000	-0.245499000
H	1.622076000	1.340199000	2.071681000
H	1.291105000	1.324604000	-2.131194000

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B-7-8-q SCF Done: -1392.960263 A.U.

C	4.343557000	-0.675187000	0.700758000
C	4.110145000	0.485930000	-0.277211000
H	4.183362000	-0.311406000	1.733650000
H	4.865077000	1.260062000	-0.049553000
H	5.417540000	-0.923388000	0.643771000
H	4.350925000	0.154725000	-1.303804000
Cr	0.644432000	0.514328000	-0.186243000
Al	-3.084209000	-0.538760000	0.200566000
Cl	-2.521514000	-1.197275000	-1.825862000
N	-1.531423000	0.693303000	0.667502000
C	-0.730689000	0.595728000	1.790534000
C	0.010617000	1.771168000	1.951623000
C	-0.351297000	2.631111000	0.874725000
C	-1.305312000	1.939134000	0.120118000
H	0.722321000	1.977658000	2.749402000
H	0.022069000	3.634766000	0.678118000
C	-4.648018000	0.667564000	0.173609000
H	-4.561613000	1.473788000	-0.576539000
H	-4.820955000	1.148375000	1.153852000
H	-5.569283000	0.110154000	-0.073272000
C	-2.976037000	-1.989554000	1.538567000
H	-3.147892000	-1.635264000	2.571768000
H	-2.015373000	-2.534297000	1.529148000
H	-3.758452000	-2.742728000	1.335429000
C	1.020277000	-1.491558000	0.022576000
C	2.088758000	-2.030351000	0.981391000
H	0.028588000	-1.878273000	0.316437000
H	2.016616000	-1.542555000	1.973450000
H	1.199752000	-1.885077000	-0.994684000
H	1.856641000	-3.094053000	1.179995000
C	3.554921000	-1.981666000	0.507882000
C	2.734909000	1.151529000	-0.221008000
H	4.102837000	-2.759073000	1.067379000
H	2.380705000	1.074834000	0.832162000
H	3.608747000	-2.296287000	-0.551585000
H	2.786557000	2.226682000	-0.442999000
C	1.950464000	0.639141000	-2.126642000
C	0.546304000	0.659878000	-2.273643000
H	2.543499000	1.484434000	-2.483108000
H	0.064090000	1.587082000	-2.599600000
H	2.466844000	-0.320126000	-2.193645000

H	-0.002289000	-0.259312000	-2.503687000
H	-0.763053000	-0.291650000	2.419025000
H	-1.854800000	2.264305000	-0.761163000

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C-0-s SCF Done: -1314.489063 A.U.

Cr	-0.000032000	-0.785573000	1.900080000
Al	0.000052000	1.829103000	-0.325001000
Cl	0.000302000	1.648112000	2.056035000
N	-0.000046000	-0.145043000	-0.659567000
C	1.127445000	-0.933467000	-0.409864000
C	0.717442000	-2.190723000	0.048284000
C	-0.717626000	-2.190678000	0.048324000
C	-1.127576000	-0.933395000	-0.409809000
C	2.536629000	-0.499189000	-0.746868000
H	2.672012000	0.535611000	-0.403339000
H	1.364819000	-3.037789000	0.264994000
H	-1.365043000	-3.037709000	0.265049000
C	-2.536747000	-0.499038000	-0.746767000
H	-2.672122000	0.535708000	-0.403067000
C	-1.660675000	2.782648000	-0.802644000
H	-2.012693000	2.567624000	-1.826927000
H	-1.438068000	3.864487000	-0.769009000
H	-2.509588000	2.616380000	-0.119505000
C	1.660720000	2.782494000	-0.803172000
H	2.012782000	2.566944000	-1.827327000
H	2.509616000	2.616587000	-0.119920000
H	1.438097000	3.864346000	-0.770102000
C	-3.596156000	-1.359461000	-0.046846000
H	-4.603719000	-0.974691000	-0.268275000
H	-3.564259000	-2.406125000	-0.391424000
H	-3.467141000	-1.356986000	1.047148000
C	-2.746800000	-0.506314000	-2.274655000
H	-2.653612000	-1.528704000	-2.676826000
H	-3.749651000	-0.127760000	-2.530270000
H	-2.005116000	0.125376000	-2.785369000
C	3.596016000	-1.359510000	-0.046789000
H	3.564112000	-2.406232000	-0.391192000
H	4.603589000	-0.974793000	-0.268266000
H	3.466981000	-1.356851000	1.047201000
C	2.746695000	-0.506719000	-2.274753000
H	3.749551000	-0.128216000	-2.530426000
H	2.653499000	-1.529174000	-2.676757000
H	2.005017000	0.124893000	-2.785574000

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C-1-q SCF Done: -1393.041939 A.U.

Cr	0.309623000	-1.388651000	0.486501000
Al	-0.497888000	1.702926000	1.079355000
Cl	-0.818010000	-0.239765000	2.355934000
N	-0.074362000	0.601188000	-0.565537000
C	1.202506000	0.248972000	-1.022230000
C	1.092147000	-0.927015000	-1.775210000
C	-0.295594000	-1.257213000	-1.869724000
C	-1.000769000	-0.301817000	-1.135787000
C	2.433533000	1.099627000	-0.806852000
H	2.452938000	1.418097000	0.244009000
H	1.913849000	-1.457885000	-2.249619000
H	-0.724454000	-2.091332000	-2.418894000
C	-2.500257000	-0.132934000	-1.034986000
H	-2.737467000	0.222113000	-0.020958000
C	-2.153585000	2.759396000	0.960689000
H	-2.076630000	3.528840000	0.170791000
H	-2.270871000	3.307137000	1.913270000
H	-3.091960000	2.210198000	0.790938000
C	1.038974000	2.624790000	1.895234000
H	1.474929000	3.417074000	1.262263000
H	1.857639000	1.964921000	2.225133000
H	0.658229000	3.127924000	2.803067000
C	1.706092000	-2.629926000	1.332901000
C	0.543904000	-3.381298000	0.908352000
H	2.645009000	-2.738324000	0.774069000
H	0.622544000	-4.043313000	0.036000000
H	1.854861000	-2.426136000	2.401434000
H	-0.169674000	-3.739194000	1.662934000
C	-3.245186000	-1.458811000	-1.240578000
H	-4.326869000	-1.308925000	-1.101093000
H	-3.100561000	-1.853061000	-2.259753000
H	-2.913934000	-2.227924000	-0.525898000
C	-2.986333000	0.934883000	-2.035004000
H	-2.807797000	0.606033000	-3.071893000
H	-4.066809000	1.113471000	-1.914580000
H	-2.467399000	1.892974000	-1.887731000
C	3.727094000	0.323447000	-1.081835000
H	3.805450000	0.024230000	-2.139903000
H	4.599739000	0.955558000	-0.856810000
H	3.795374000	-0.582722000	-0.461191000
C	2.356879000	2.372026000	-1.675191000

H	3.226693000	3.020292000	-1.483743000
H	2.350323000	2.116353000	-2.747549000
H	1.448723000	2.956108000	-1.462709000

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C-2-q SCF Done: -1471.574345 A.U.

Cr	-1.666700000	0.123523000	-0.171304000
Al	1.606947000	-0.032938000	1.505323000
Cl	-0.424065000	-0.763731000	2.224267000
N	1.034699000	0.010988000	-0.430182000
C	0.509200000	-1.105988000	-1.056054000
C	-0.387906000	-0.703527000	-2.059144000
C	-0.372149000	0.720314000	-2.081932000
C	0.511503000	1.135801000	-1.073436000
C	1.013016000	-2.507119000	-0.785929000
H	0.995416000	-2.676546000	0.302822000
H	-0.907919000	-1.359246000	-2.752313000
H	-0.879298000	1.364621000	-2.796214000
C	1.082734000	2.525902000	-0.881135000
H	0.951655000	2.825613000	0.169062000
C	1.918970000	1.743733000	2.316841000
H	2.781648000	2.290695000	1.898614000
H	2.161773000	1.552121000	3.378656000
H	1.057614000	2.431613000	2.320788000
C	3.027525000	-1.340630000	1.914704000
H	3.981427000	-1.087180000	1.417030000
H	2.811690000	-2.397062000	1.690979000
H	3.223344000	-1.280770000	3.001098000
C	-2.825926000	-1.717171000	-0.315011000
C	-3.649468000	-0.956592000	0.501065000
H	-2.162906000	-2.463705000	0.129634000
H	-3.636620000	-1.095803000	1.583379000
H	-3.070880000	-1.858308000	-1.372820000
H	-4.546329000	-0.483887000	0.095628000
C	-3.068468000	1.458221000	1.137544000
C	-1.948127000	2.110700000	0.638054000
H	-3.069983000	1.071615000	2.158320000
H	-1.070472000	2.258420000	1.273196000
H	-4.051674000	1.635978000	0.697444000
H	-2.051192000	2.797810000	-0.206756000
C	0.390110000	3.571319000	-1.765380000
H	0.794582000	4.572190000	-1.550162000
H	0.562992000	3.368501000	-2.834924000
H	-0.696072000	3.611012000	-1.600817000

C	2.597171000	2.518061000	-1.175497000
H	2.788887000	2.250809000	-2.227719000
H	3.025559000	3.516459000	-0.993849000
H	3.136726000	1.800388000	-0.542263000
C	2.473570000	-2.628569000	-1.270864000
H	2.880658000	-3.618620000	-1.011125000
H	2.526000000	-2.515495000	-2.366351000
H	3.120354000	-1.866600000	-0.817551000
C	0.157626000	-3.593916000	-1.449483000
H	0.180240000	-3.507956000	-2.548326000
H	0.555026000	-4.587979000	-1.193210000
H	-0.891860000	-3.561787000	-1.127464000

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C-3-q SCF Done: -1471.607708 A.U.

Cr	1.186808000	-0.383011000	0.044989000
Al	-1.709035000	0.384920000	1.462175000
Cl	0.052880000	-1.020025000	2.141390000
N	-1.059803000	0.333745000	-0.450186000
C	-0.243295000	1.282592000	-1.065440000
C	0.504449000	0.648516000	-2.070226000
C	0.076308000	-0.710998000	-2.123604000
C	-0.892791000	-0.883663000	-1.134862000
C	-0.301904000	2.760940000	-0.751229000
H	-0.147419000	2.892238000	0.329494000
H	1.226834000	1.126124000	-2.727034000
H	0.432657000	-1.473543000	-2.811484000
C	-1.744841000	-2.106389000	-0.880021000
H	-1.897158000	-2.195907000	0.205727000
C	-3.454629000	-0.472122000	1.761029000
H	-4.252554000	0.045213000	1.197417000
H	-3.710274000	-0.360860000	2.830201000
H	-3.531507000	-1.544128000	1.523625000
C	-1.397838000	2.084849000	2.404539000
H	-2.008438000	2.924954000	2.031188000
H	-0.346561000	2.413891000	2.431875000
H	-1.702236000	1.922701000	3.454928000
C	2.670473000	0.848298000	0.774386000
C	4.019338000	0.214066000	0.411786000
H	2.584650000	1.898087000	0.444716000
H	4.272599000	0.447288000	-0.640458000
H	2.511466000	0.830306000	1.869284000
H	4.853527000	0.616051000	1.019351000
C	3.893467000	-1.306653000	0.563018000

C	2.673805000	-1.766656000	-0.243414000
H	4.823350000	-1.826276000	0.259764000
H	2.894261000	-1.748351000	-1.329097000
H	3.744582000	-1.548866000	1.631748000
H	2.334662000	-2.786607000	0.014503000
C	-1.061621000	-3.395900000	-1.353528000
H	-1.681080000	-4.267703000	-1.092930000
H	-0.927780000	-3.407684000	-2.447628000
H	-0.074165000	-3.528504000	-0.886131000
C	-3.128189000	-1.938269000	-1.539314000
H	-3.031887000	-1.879278000	-2.635822000
H	-3.776009000	-2.796361000	-1.299134000
H	-3.633621000	-1.025688000	-1.192025000
C	0.791637000	3.549310000	-1.482091000
H	0.657082000	3.507431000	-2.575356000
H	0.751087000	4.608723000	-1.186474000
H	1.797666000	3.173263000	-1.244682000
C	-1.696891000	3.320355000	-1.096709000
H	-1.759293000	4.385931000	-0.825367000
H	-1.898839000	3.230825000	-2.176727000
H	-2.496739000	2.789596000	-0.559736000

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C-4-q SCF Done: -1550.127833 A.U.

Cr	1.504849000	-0.184060000	0.103363000
Al	-2.299317000	0.189811000	1.257243000
Cl	-0.168869000	0.347443000	2.151019000
N	-1.529996000	0.179438000	-0.577941000
C	-0.704393000	1.209456000	-0.969039000
C	0.349722000	0.696766000	-1.745133000
C	0.094914000	-0.710914000	-1.898405000
C	-1.056553000	-0.993194000	-1.176106000
C	-0.979668000	2.662498000	-0.658505000
H	1.072413000	1.287440000	-2.302032000
H	0.654105000	-1.402314000	-2.522916000
C	-1.818833000	-2.298263000	-1.134624000
C	-3.073791000	-1.511087000	1.903687000
H	-3.930743000	-1.868851000	1.305991000
H	-3.466939000	-1.314324000	2.918118000
H	-2.365043000	-2.350061000	2.003044000
C	-3.388965000	1.762029000	1.738162000
H	-4.340107000	1.772082000	1.174490000
H	-2.930947000	2.755915000	1.620477000
H	-3.666095000	1.662779000	2.803582000

C	2.760720000	1.228953000	0.918643000
C	4.002827000	1.403872000	0.045439000
H	2.222320000	2.165307000	1.139069000
H	3.771546000	2.074120000	-0.803820000
H	3.016948000	0.763483000	1.891571000
H	4.840843000	1.882264000	0.588919000
C	4.392722000	0.027430000	-0.503454000
C	3.142888000	-0.591475000	-1.138082000
H	5.239459000	0.093531000	-1.214146000
H	2.920323000	-0.071921000	-2.087233000
H	4.755561000	-0.600158000	0.333647000
H	3.258294000	-1.662322000	-1.384748000
C	2.463045000	-2.594536000	1.096891000
C	1.813793000	-2.137985000	2.179420000
H	1.969423000	-3.236756000	0.361037000
H	0.763961000	-2.371427000	2.367458000
H	3.525090000	-2.397837000	0.939514000
H	2.316833000	-1.531717000	2.937905000
C	-2.282195000	3.112886000	-1.351124000
H	-2.520928000	4.152842000	-1.077472000
H	-2.175807000	3.064675000	-2.447401000
H	-3.134178000	2.481760000	-1.063837000
C	0.184934000	3.578919000	-1.052493000
H	1.124963000	3.280911000	-0.565998000
H	0.347838000	3.580208000	-2.142745000
H	-0.035480000	4.615124000	-0.753513000
C	-3.174920000	-2.150867000	-1.853589000
H	-3.029150000	-1.928512000	-2.923476000
H	-3.756943000	-3.082900000	-1.773349000
H	-3.776178000	-1.338210000	-1.420283000
C	-1.013610000	-3.460867000	-1.726705000
H	-1.575960000	-4.401979000	-1.626830000
H	-0.810768000	-3.310563000	-2.799560000
H	-0.046419000	-3.592639000	-1.216451000
H	-2.034698000	-2.543366000	-0.085059000
H	-1.123858000	2.758988000	0.429539000

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C-5-q SCF Done: -1550.173203 A.U.

Cr	-0.920838000	-0.257918000	-0.130412000
Al	1.928816000	0.371281000	1.565350000
Cl	-0.079815000	-0.719857000	2.141227000
N	1.523554000	0.175713000	-0.394423000
C	1.294166000	-1.082110000	-0.973992000

C	0.475633000	-0.918009000	-2.091794000
C	0.205383000	0.476146000	-2.223282000
C	0.899017000	1.130914000	-1.194155000
C	1.970023000	-2.349392000	-0.498807000
H	1.950904000	-2.356428000	0.601523000
H	0.122890000	-1.708492000	-2.749261000
H	-0.362647000	0.954144000	-3.017162000
C	1.109689000	2.619388000	-1.027414000
H	0.877994000	2.891790000	0.012299000
C	1.753718000	2.194552000	2.288618000
H	2.502453000	2.904310000	1.896232000
H	1.935563000	2.120970000	3.376558000
H	0.758305000	2.651535000	2.169021000
C	3.484051000	-0.647137000	2.208946000
H	4.417567000	-0.258007000	1.762441000
H	3.477290000	-1.736077000	2.050898000
H	3.571158000	-0.480824000	3.297855000
C	-2.322432000	-1.713315000	-0.412131000
C	-3.745107000	-1.356661000	-0.857036000
H	-1.864177000	-2.397042000	-1.150733000
H	-3.724222000	-0.650933000	-1.710516000
H	-2.348567000	-2.263651000	0.548590000
H	-4.221341000	-2.271819000	-1.259641000
C	-4.675409000	-0.807040000	0.237555000
C	-4.574352000	0.682615000	0.593827000
H	-5.717197000	-0.990251000	-0.080001000
H	-4.783667000	1.283453000	-0.312286000
H	-4.536508000	-1.410464000	1.154622000
H	-5.402175000	0.905136000	1.290444000
C	-3.273966000	1.192808000	1.232109000
C	-2.084657000	1.361114000	0.279953000
H	-3.502191000	2.175892000	1.687607000
H	-2.421135000	1.786237000	-0.685742000
H	-3.000708000	0.543222000	2.085022000
H	-1.360798000	2.081206000	0.709126000
C	3.445384000	-2.363153000	-0.946787000
H	3.963735000	-3.246839000	-0.541462000
H	3.516785000	-2.399761000	-2.046238000
H	3.982367000	-1.468462000	-0.600737000
C	1.242306000	-3.613634000	-0.973758000
H	1.255808000	-3.703338000	-2.072365000
H	1.741136000	-4.507608000	-0.569135000
H	0.193701000	-3.632880000	-0.640836000

C	0.192746000	3.441019000	-1.941914000
H	0.346815000	4.515387000	-1.758510000
H	0.412056000	3.255225000	-3.006151000
H	-0.869801000	3.220293000	-1.764326000
C	2.588665000	2.976140000	-1.281424000
H	2.876323000	2.742609000	-2.319697000
H	2.754919000	4.052269000	-1.115638000
H	3.265701000	2.424668000	-0.612474000

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C-6-q SCF Done: -1550.176944 A.U.

Cr	0.600305000	-0.529009000	0.389276000
Al	-2.269296000	0.746766000	1.199386000
Cl	-0.179657000	0.871371000	2.270606000
N	-1.397474000	0.206239000	-0.543548000
C	-0.410314000	1.004985000	-1.161336000
C	0.386448000	0.188325000	-1.965432000
C	-0.119679000	-1.141271000	-1.852898000
C	-1.251895000	-1.097846000	-1.022403000
C	-0.396350000	2.514313000	-1.069492000
H	-0.615573000	2.798172000	-0.028971000
H	1.230910000	0.509609000	-2.569834000
H	0.255481000	-2.020664000	-2.370450000
C	-2.261264000	-2.195264000	-0.769521000
H	-2.466760000	-2.233641000	0.308961000
C	-3.232259000	-0.696001000	2.130388000
H	-4.145229000	-1.038551000	1.613215000
H	-3.561358000	-0.282008000	3.101236000
H	-2.618140000	-1.581772000	2.360368000
C	-3.151620000	2.504607000	1.167396000
H	-4.002385000	2.507600000	0.461712000
H	-2.522718000	3.374370000	0.923925000
H	-3.580595000	2.688279000	2.168963000
C	4.061893000	1.561564000	0.589179000
C	4.537676000	0.584902000	-0.490525000
H	4.049753000	2.596995000	0.211298000
H	3.852762000	0.622481000	-1.358318000
H	4.734880000	1.540395000	1.462802000
H	5.510670000	0.943744000	-0.870054000
C	4.709223000	-0.876984000	-0.040060000
C	3.459031000	-1.771246000	-0.005590000
H	5.434292000	-1.360798000	-0.717706000
H	3.033478000	-1.830943000	-1.026657000
H	5.186365000	-0.889265000	0.957946000

H	3.808852000	-2.800172000	0.212520000
C	2.372922000	-1.407334000	1.003935000
C	1.238435000	-2.289143000	1.203552000
H	2.756556000	-0.911912000	1.908890000
H	1.149772000	-3.178936000	0.564422000
H	0.849979000	-2.442483000	2.219190000
H	3.050255000	1.324730000	0.952263000
C	-1.500708000	3.109925000	-1.966006000
H	-1.541318000	4.204829000	-1.850439000
H	-1.302095000	2.885954000	-3.026925000
H	-2.491595000	2.707066000	-1.712842000
C	0.973062000	3.104228000	-1.427370000
H	1.239619000	2.904435000	-2.478197000
H	0.957187000	4.197379000	-1.298755000
H	1.770872000	2.700268000	-0.787645000
C	-3.587842000	-1.866883000	-1.484646000
H	-3.447053000	-1.830226000	-2.577470000
H	-4.343093000	-2.637745000	-1.263791000
H	-3.994849000	-0.895749000	-1.165180000
C	-1.738150000	-3.571835000	-1.195813000
H	-2.477026000	-4.348343000	-0.945436000
H	-1.566454000	-3.621861000	-2.283656000
H	-0.797086000	-3.824212000	-0.685634000

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C-7-q SCF Done: -1628.69403 A.U.

Al	2.727049000	-0.402494000	1.012576000
Cl	1.280129000	-1.384119000	2.396528000
N	1.446320000	-0.054259000	-0.544879000
C	0.653063000	-1.024626000	-1.129683000
C	-0.302818000	-0.402794000	-1.958055000
C	-0.003088000	0.994539000	-1.952893000
C	1.068298000	1.182973000	-1.078953000
C	0.969615000	-2.501683000	-1.053895000
H	1.352308000	-2.718696000	-0.045196000
H	-1.031815000	-0.909296000	-2.586390000
H	-0.504340000	1.765400000	-2.530983000
C	1.861723000	2.454118000	-0.871884000
H	2.100412000	2.546056000	0.196815000
C	3.363187000	1.255999000	1.895081000
H	4.063965000	1.859220000	1.292415000
H	3.937407000	0.906723000	2.773858000
H	2.593265000	1.937112000	2.295685000
C	4.191724000	-1.615584000	0.477064000

H	4.759764000	-1.249520000	-0.397737000
H	3.892731000	-2.654245000	0.264006000
H	4.911311000	-1.659963000	1.315146000
C	-0.636520000	2.171277000	1.830072000
C	-1.229154000	1.209814000	2.565101000
H	0.449079000	2.187591000	1.701680000
H	-0.642523000	0.400288000	3.010541000
H	-1.200346000	3.017636000	1.429031000
H	-2.301558000	1.235970000	2.772394000
Cr	-1.121564000	0.386130000	0.095363000
C	-2.190296000	-1.186983000	0.857622000
C	-3.354164000	-1.770336000	0.044277000
H	-1.393391000	-1.935414000	1.015293000
H	-3.140639000	-1.749384000	-1.041639000
H	-2.551602000	-0.924959000	1.867319000
H	-3.456138000	-2.844664000	0.291305000
C	-4.721144000	-1.117597000	0.303341000
C	-4.992089000	0.254992000	-0.325533000
H	-5.506565000	-1.803095000	-0.061528000
H	-4.972872000	0.158577000	-1.427753000
H	-4.874198000	-1.050189000	1.397276000
H	-6.031496000	0.529761000	-0.072884000
C	-4.078521000	1.425932000	0.072393000
C	-2.713757000	1.461407000	-0.626569000
H	-4.619287000	2.358776000	-0.178078000
H	-2.838222000	1.164061000	-1.683705000
H	-3.972511000	1.450077000	1.173934000
H	-2.321691000	2.497226000	-0.643207000
C	3.203307000	2.368483000	-1.628918000
H	3.034434000	2.296115000	-2.715759000
H	3.810725000	3.266895000	-1.435579000
H	3.792303000	1.492717000	-1.319438000
C	1.083661000	3.705905000	-1.296957000
H	1.670842000	4.609460000	-1.072316000
H	0.881240000	3.709984000	-2.380276000
H	0.118464000	3.792932000	-0.774480000
C	2.083222000	-2.811337000	-2.080214000
H	2.411983000	-3.857712000	-1.978381000
H	1.711514000	-2.669741000	-3.108474000
H	2.960358000	-2.166324000	-1.940518000
C	-0.238145000	-3.410592000	-1.312491000
H	-1.040670000	-3.260200000	-0.579960000
H	-0.657191000	-3.253312000	-2.320072000

H 0.075770000 -4.464186000 -1.254819000
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C-8-q SCF Done: -1628.733556 A.U.

C -5.088379000 -0.767933000 0.493462000
C -5.196344000 0.727164000 0.140197000
H -6.113512000 -1.134580000 0.677426000
H -5.760783000 0.830440000 -0.805002000
H -4.573530000 -0.882231000 1.462143000
H -5.824847000 1.206413000 0.913339000
Cr -0.536349000 -0.137970000 0.260962000
Al 2.618768000 0.373862000 1.305305000
Cl 0.741756000 -0.650733000 2.305994000
N 1.836244000 0.116107000 -0.529541000
C 1.434338000 -1.151230000 -0.971280000
C 0.395099000 -1.001257000 -1.890601000
C 0.164119000 0.397225000 -2.047810000
C 1.089208000 1.063755000 -1.228954000
C 2.152213000 -2.425519000 -0.587270000
H 2.338620000 -2.402114000 0.497462000
H -0.121981000 -1.803691000 -2.409713000
H -0.535732000 0.865171000 -2.735267000
C 1.389919000 2.546619000 -1.198171000
H 1.313915000 2.897891000 -0.158180000
C 2.611556000 2.227423000 1.969970000
H 3.313141000 2.893432000 1.438471000
H 2.957315000 2.186985000 3.019303000
H 1.625329000 2.718238000 1.985115000
C 4.244371000 -0.668386000 1.680860000
H 5.081560000 -0.340574000 1.037781000
H 4.169359000 -1.762210000 1.586069000
H 4.552379000 -0.455491000 2.720462000
C -1.986357000 -1.573869000 0.337278000
C -2.949248000 -1.537839000 -0.859564000
H -1.497405000 -2.557812000 0.444270000
H -2.829705000 -0.597812000 -1.428342000
H -2.489229000 -1.366314000 1.295995000
H -2.665120000 -2.328124000 -1.576954000
C -4.451224000 -1.714877000 -0.539212000
C -3.885146000 1.524707000 0.016056000
H -5.017039000 -1.641899000 -1.486873000
H -3.315112000 1.152805000 -0.848570000
H -4.603134000 -2.747988000 -0.177432000
H -4.139902000 2.567524000 -0.243581000

C	-2.976906000	1.525077000	1.264033000
C	-1.477790000	1.577305000	0.942684000
H	-3.255724000	2.387046000	1.900832000
H	-1.275466000	2.400591000	0.232454000
H	-3.185145000	0.641413000	1.888464000
H	-0.902845000	1.804849000	1.859331000
C	2.831602000	2.808783000	-1.678457000
H	2.959030000	2.491161000	-2.726369000
H	3.064321000	3.883551000	-1.617471000
H	3.573749000	2.270243000	-1.071557000
C	0.393157000	3.353151000	-2.039987000
H	0.610591000	4.428423000	-1.950664000
H	0.462802000	3.089385000	-3.107975000
H	-0.645607000	3.194374000	-1.715049000
C	3.516408000	-2.498135000	-1.302852000
H	4.078916000	-3.385541000	-0.971401000
H	3.378562000	-2.569334000	-2.394281000
H	4.131008000	-1.611010000	-1.095129000
C	1.317902000	-3.678077000	-0.882370000
H	1.139875000	-3.801249000	-1.963253000
H	1.852613000	-4.575854000	-0.536279000
H	0.342578000	-3.649851000	-0.374815000

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C-9-q SCF Done: -1471.613196 A.U.

Cr	0.978522000	-0.297715000	0.526566000
Al	-2.146206000	0.418937000	1.046419000
Cl	-0.243607000	0.814807000	2.363823000
N	-0.999293000	0.076242000	-0.583799000
C	-0.110136000	1.047320000	-1.096683000
C	0.886586000	0.397561000	-1.826558000
C	0.605410000	-1.001959000	-1.776443000
C	-0.588103000	-1.173356000	-1.059833000
C	-0.342816000	2.535964000	-0.966758000
H	-0.745018000	2.733332000	0.038031000
H	1.717207000	0.871121000	-2.343284000
H	1.175099000	-1.791304000	-2.260454000
C	-1.399389000	-2.439108000	-0.899707000
H	-1.728737000	-2.505830000	0.146001000
C	4.604438000	0.698739000	-0.237492000
C	4.073285000	-0.674673000	0.179732000
H	5.463863000	0.613125000	-0.922400000
H	3.778454000	-1.249658000	-0.718274000
H	4.937608000	1.276390000	0.641110000

H	4.907000000	-1.251693000	0.628841000
C	2.913624000	-0.627483000	1.161177000
C	2.077737000	-1.787940000	1.399387000
H	3.111090000	0.013903000	2.035926000
H	2.245529000	-2.684837000	0.786647000
H	1.737550000	-2.012387000	2.418888000
H	3.826858000	1.295607000	-0.742337000
C	-3.283021000	2.020707000	0.925634000
H	-4.021816000	1.919359000	0.109590000
H	-3.865997000	2.093484000	1.861504000
H	-2.777240000	2.988483000	0.788428000
C	-2.999991000	-1.174849000	1.825883000
H	-3.521303000	-0.836445000	2.740254000
H	-3.770934000	-1.631427000	1.181207000
H	-2.304562000	-1.970060000	2.139746000
C	-1.392584000	3.001839000	-1.995290000
H	-1.623753000	4.069836000	-1.854736000
H	-1.017055000	2.865853000	-3.022748000
H	-2.331244000	2.437404000	-1.898549000
C	0.956493000	3.340523000	-1.103479000
H	1.400662000	3.231594000	-2.106476000
H	0.753537000	4.412065000	-0.953340000
H	1.707855000	3.031408000	-0.360662000
C	-2.662720000	-2.374741000	-1.782011000
H	-2.394115000	-2.320861000	-2.849887000
H	-3.282091000	-3.272992000	-1.630635000
H	-3.281172000	-1.495800000	-1.545441000
C	-0.576373000	-3.695170000	-1.210091000
H	-1.180845000	-4.596025000	-1.023665000
H	-0.262925000	-3.725401000	-2.266581000
H	0.324368000	-3.754923000	-0.580942000

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C-2-3-q SCF Done: -1471.566632 A.U.

Cr	-1.599886000	-0.050935000	-0.215729000
Al	1.649112000	0.116195000	1.497714000
Cl	-0.333176000	-0.791135000	2.174024000
N	1.084962000	0.120981000	-0.439115000
C	0.668440000	-1.038791000	-1.071321000
C	-0.260009000	-0.716782000	-2.075112000
C	-0.389871000	0.702158000	-2.081502000
C	0.444998000	1.192356000	-1.063367000
C	1.275147000	-2.394409000	-0.787977000
H	1.298357000	-2.536157000	0.303961000

H	-0.723523000	-1.416698000	-2.765003000
H	-0.966095000	1.301488000	-2.782099000
C	0.835043000	2.634881000	-0.821316000
H	0.726404000	2.852491000	0.250841000
C	1.792909000	1.900631000	2.334747000
H	2.574215000	2.548961000	1.901566000
H	2.087074000	1.723766000	3.385970000
H	0.855711000	2.480225000	2.371119000
C	3.170688000	-1.073912000	1.901630000
H	4.095840000	-0.742057000	1.395650000
H	3.041794000	-2.144201000	1.677380000
H	3.370652000	-0.998731000	2.986245000
C	-2.705293000	-1.781510000	-0.316395000
C	-3.624355000	-1.050933000	0.523922000
H	-2.125170000	-2.586183000	0.148504000
H	-3.771404000	-1.419851000	1.543257000
H	-3.016760000	-1.994889000	-1.346845000
H	-4.564949000	-0.765875000	0.044838000
C	-3.247450000	0.821525000	1.219019000
C	-2.354530000	1.716664000	0.515497000
H	-2.956005000	0.574280000	2.243896000
H	-1.560528000	2.201292000	1.095493000
H	-4.317886000	1.018575000	1.128316000
H	-2.797925000	2.365056000	-0.251354000
C	2.727095000	-2.431455000	-1.309316000
H	3.205735000	-3.386664000	-1.040930000
H	2.746159000	-2.337750000	-2.407742000
H	3.332822000	-1.618715000	-0.886861000
C	0.466892000	-3.548731000	-1.393269000
H	0.928401000	-4.510356000	-1.121023000
H	-0.571908000	-3.561400000	-1.035473000
H	0.449599000	-3.496610000	-2.494406000
C	-0.049112000	3.619495000	-1.596600000
H	0.230162000	4.653640000	-1.342998000
H	0.078272000	3.503610000	-2.685566000
H	-1.115437000	3.493784000	-1.361112000
C	2.317605000	2.847239000	-1.190307000
H	2.483719000	2.659106000	-2.263846000
H	2.619887000	3.884489000	-0.975356000
H	2.981668000	2.179146000	-0.623810000

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C-3-9-q SCF Done: -1471.558575 A.U.

Cr	1.467315000	-0.425476000	-0.312222000
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Al	-1.701549000	0.549722000	1.390995000
Cl	-0.901716000	-1.271290000	2.384604000
N	-0.732002000	0.363766000	-0.424168000
C	0.107048000	1.297602000	-1.052502000
C	0.639131000	0.713987000	-2.214607000
C	0.099726000	-0.598925000	-2.315705000
C	-0.763849000	-0.780173000	-1.223891000
C	0.214172000	2.744558000	-0.626898000
H	0.308422000	2.772164000	0.466836000
H	1.324336000	1.188482000	-2.912423000
H	0.290840000	-1.319515000	-3.107966000
C	-1.723627000	-1.929654000	-1.009392000
H	-1.996003000	-1.946132000	0.054788000
C	-3.647516000	0.450364000	1.055474000
H	-3.986641000	1.165440000	0.283361000
H	-4.173011000	0.729907000	1.986932000
H	-4.025307000	-0.544554000	0.769051000
C	-1.097854000	2.120639000	2.428077000
H	-1.429764000	3.096698000	2.034273000
H	-0.010691000	2.174777000	2.604838000
H	-1.565573000	2.015436000	3.425004000
H	2.943978000	-0.569286000	-0.994464000
C	2.467352000	0.517394000	1.223588000
C	3.704074000	-0.406567000	1.213205000
H	2.723401000	1.572565000	1.047292000
H	4.591838000	0.105709000	0.812857000
H	1.871245000	0.440699000	2.146439000
H	3.970536000	-0.795166000	2.212832000
C	3.341182000	-1.580909000	0.310379000
C	2.173405000	-2.294910000	0.588899000
H	4.102468000	-2.006965000	-0.352328000
H	1.950736000	-3.213638000	0.039733000
H	1.644927000	-2.148114000	1.536554000
C	-1.075792000	3.500036000	-1.007164000
H	-1.028099000	4.540565000	-0.649084000
H	-1.210052000	3.521364000	-2.101295000
H	-1.969201000	3.035060000	-0.565308000
C	1.442488000	3.437535000	-1.230300000
H	1.371831000	3.507892000	-2.328231000
H	1.520203000	4.465362000	-0.844170000
H	2.376315000	2.911529000	-0.980377000
C	-3.000569000	-1.684089000	-1.840258000
H	-2.780580000	-1.720816000	-2.920156000

H	-3.752359000	-2.458506000	-1.619790000
H	-3.448018000	-0.705939000	-1.614601000
C	-1.108746000	-3.294471000	-1.347408000
H	-1.850316000	-4.091130000	-1.181580000
H	-0.794668000	-3.356103000	-2.402515000
H	-0.236780000	-3.511713000	-0.714173000

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C-4-5-q SCF Done: -1550.11225 A.U.

Cr	-1.301796000	0.305637000	0.096693000
Al	2.314437000	-0.309911000	1.085451000
Cl	1.066751000	-1.599852000	2.373088000
N	0.995114000	0.013897000	-0.483504000
C	0.300811000	-0.981524000	-1.181473000
C	-0.538124000	-0.369034000	-2.127629000
C	-0.304273000	1.031854000	-2.056869000
C	0.648527000	1.245009000	-1.053441000
C	0.633432000	-2.455516000	-1.095768000
H	0.935877000	-2.677419000	-0.061432000
H	-1.194166000	-0.886789000	-2.823947000
H	-0.770131000	1.800743000	-2.669134000
C	1.352243000	2.543501000	-0.731574000
H	1.517718000	2.583055000	0.353013000
C	2.718630000	1.343772000	2.101181000
H	3.377918000	2.063895000	1.586538000
H	3.281127000	0.994754000	2.987743000
H	1.849519000	1.896113000	2.495309000
C	3.921840000	-1.236568000	0.397014000
H	4.348072000	-0.778769000	-0.514356000
H	3.782062000	-2.310463000	0.192952000
H	4.704860000	-1.164021000	1.174155000
C	-2.289619000	-1.264811000	0.998080000
C	-3.639177000	-1.455011000	0.305299000
H	-1.670467000	-2.173597000	1.015280000
H	-3.493284000	-1.866266000	-0.711871000
H	-2.432797000	-0.965797000	2.052129000
H	-4.287812000	-2.183140000	0.829042000
C	-4.345596000	-0.099630000	0.194367000
C	-3.386310000	0.965391000	-0.325136000
H	-5.234570000	-0.158568000	-0.461842000
H	-2.976222000	0.675624000	-1.315067000
H	-4.730062000	0.201617000	1.186231000
H	-3.871463000	1.934255000	-0.491161000
C	-2.441773000	1.974719000	1.324761000

C	-1.155525000	1.582653000	1.756537000
H	-2.543503000	2.948214000	0.838461000
H	-0.320782000	2.268075000	1.588163000
H	-3.321103000	1.670260000	1.896695000
H	-1.043593000	0.906019000	2.608430000
C	2.738854000	2.574074000	-1.406720000
H	2.641365000	2.557872000	-2.504611000
H	3.282719000	3.489534000	-1.124598000
H	3.355108000	1.713128000	-1.108921000
C	0.525062000	3.770806000	-1.135383000
H	1.039009000	4.692776000	-0.823454000
H	0.387361000	3.828982000	-2.227432000
H	-0.472600000	3.768249000	-0.668385000
C	1.822976000	-2.751836000	-2.035954000
H	2.150956000	-3.796299000	-1.913354000
H	1.528824000	-2.609140000	-3.089070000
H	2.683331000	-2.102961000	-1.828879000
C	-0.548251000	-3.365228000	-1.458346000
H	-0.244073000	-4.419327000	-1.367110000
H	-1.413756000	-3.208983000	-0.801372000
H	-0.872940000	-3.213595000	-2.501285000

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C-5-6-q SCF Done: -1550.135859 A.U.

Cr	-1.129308000	0.162735000	-0.268290000
Al	2.065271000	-0.062651000	1.517255000
Cl	0.079677000	-0.868810000	2.247353000
N	1.462996000	-0.005443000	-0.413586000
C	0.933992000	-1.119524000	-1.045657000
C	0.115422000	-0.703616000	-2.110101000
C	0.173530000	0.718561000	-2.150666000
C	1.004213000	1.124472000	-1.092715000
C	1.358860000	-2.532476000	-0.711441000
H	1.482833000	-2.599219000	0.378921000
H	-0.402039000	-1.352356000	-2.813095000
H	-0.293205000	1.369755000	-2.885725000
C	1.565710000	2.509191000	-0.853661000
H	1.463843000	2.746945000	0.214075000
C	2.330480000	1.710749000	2.351315000
H	3.177198000	2.288100000	1.940923000
H	2.576689000	1.515296000	3.411751000
H	1.445094000	2.368084000	2.358520000
C	3.565635000	-1.315464000	1.799698000
H	4.448107000	-1.030484000	1.197446000

H	3.366739000	-2.380444000	1.600726000
H	3.879358000	-1.243900000	2.857082000
C	-2.718536000	-1.444437000	-0.296552000
C	-4.192196000	-1.086826000	-0.562086000
H	-2.278467000	-1.928624000	-1.179702000
H	-4.273165000	-0.566356000	-1.534517000
H	-2.625261000	-2.154640000	0.542349000
H	-4.788832000	-2.011020000	-0.665772000
C	-4.819272000	-0.191739000	0.520350000
C	-4.104769000	1.162656000	0.652096000
H	-5.883901000	-0.023187000	0.288090000
H	-4.151714000	1.688716000	-0.318903000
H	-4.795810000	-0.716451000	1.493825000
H	-4.641104000	1.804056000	1.373373000
C	-2.640896000	1.056278000	1.092061000
C	-1.660959000	1.985928000	0.583355000
H	-2.513251000	0.749913000	2.139753000
H	-1.995638000	2.736959000	-0.143277000
H	-0.871259000	2.336207000	1.256396000
H	-2.496766000	-0.267156000	0.531919000
C	3.070611000	2.529203000	-1.191882000
H	3.235285000	2.314528000	-2.260703000
H	3.498291000	3.520476000	-0.973290000
H	3.631383000	1.785027000	-0.608134000
C	0.824946000	3.587136000	-1.653853000
H	1.225605000	4.581737000	-1.404875000
H	0.954585000	3.444660000	-2.739348000
H	-0.252893000	3.595231000	-1.436246000
C	2.724675000	-2.824483000	-1.366899000
H	3.085582000	-3.822561000	-1.071149000
H	2.643092000	-2.803554000	-2.466307000
H	3.482948000	-2.088105000	-1.065783000
C	0.323811000	-3.587005000	-1.120353000
H	0.685461000	-4.590168000	-0.846692000
H	-0.640055000	-3.430479000	-0.615904000
H	0.149134000	-3.591913000	-2.209047000

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C-7-8-q SCF Done: -1628.670687 A.U.

C	-4.953000000	-0.057689000	-0.327054000
C	-4.318527000	1.325324000	-0.123321000
H	-4.793866000	-0.372381000	-1.376094000
H	-4.830444000	2.022833000	-0.810931000
H	-6.043906000	0.077342000	-0.226122000

H	-4.565734000	1.698539000	0.887153000
Cr	-0.978100000	0.323730000	0.080984000
Al	2.694538000	-0.348711000	1.065110000
Cl	1.480161000	-1.723912000	2.300435000
N	1.373174000	0.035795000	-0.482563000
C	0.693491000	-0.928435000	-1.230978000
C	-0.140718000	-0.279989000	-2.157534000
C	0.090240000	1.117406000	-2.024219000
C	1.027331000	1.290423000	-1.000124000
C	1.036251000	-2.402384000	-1.204014000
H	1.349551000	-2.660551000	-0.181292000
H	-0.781967000	-0.769604000	-2.887397000
H	-0.372167000	1.910001000	-2.608127000
C	1.721139000	2.575386000	-0.609090000
H	1.883145000	2.557932000	0.476524000
C	3.081298000	1.252394000	2.168984000
H	3.740274000	2.000448000	1.695416000
H	3.639756000	0.861439000	3.040430000
H	2.207341000	1.780935000	2.584188000
C	4.313769000	-1.216622000	0.328590000
H	4.731106000	-0.705814000	-0.558507000
H	4.188579000	-2.280160000	0.068490000
H	5.097664000	-1.173998000	1.107055000
C	-1.926045000	-1.298917000	0.922700000
C	-3.195307000	-1.920373000	0.323270000
H	-1.115989000	-2.047170000	0.956254000
H	-3.095139000	-2.063215000	-0.770062000
H	-2.114051000	-1.040725000	1.980963000
H	-3.292101000	-2.946122000	0.727988000
C	-4.535961000	-1.210537000	0.601754000
C	-2.818263000	1.427070000	-0.398520000
H	-5.329954000	-1.972805000	0.523535000
H	-2.589762000	0.707582000	-1.216014000
H	-4.563432000	-0.872198000	1.654939000
H	-2.541325000	2.420895000	-0.776430000
C	-2.090080000	1.757577000	1.567871000
C	-0.743599000	1.432799000	1.843399000
H	-2.363670000	2.799489000	1.384701000
H	0.017875000	2.208194000	1.725314000
H	-2.875292000	1.175344000	2.052556000
H	-0.505746000	0.644827000	2.564965000
C	3.109323000	2.653398000	-1.277152000
H	3.014871000	2.701277000	-2.374411000

H	3.647814000	3.553326000	-0.939895000
H	3.729237000	1.779368000	-1.029248000
C	0.886576000	3.817192000	-0.948374000
H	-0.108962000	3.787776000	-0.477571000
H	1.397862000	4.725107000	-0.593405000
H	0.744136000	3.929001000	-2.035670000
C	2.220913000	-2.652922000	-2.163652000
H	2.561336000	-3.697350000	-2.080503000
H	1.916138000	-2.476585000	-3.208605000
H	3.075776000	-2.001715000	-1.941061000
C	-0.139899000	-3.309534000	-1.588871000
H	-0.483165000	-3.116109000	-2.618904000
H	0.177535000	-4.362918000	-1.548533000
H	-0.996443000	-3.191980000	-0.913180000

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D-0-s SCF Done: -1393.030504 A.U.

Cr	-0.000143000	-0.755363000	1.974043000
Al	0.000192000	1.806526000	-0.361226000
Cl	-0.000665000	1.686636000	2.016760000
N	0.000037000	-0.216918000	-0.627973000
C	1.133611000	-1.008688000	-0.348959000
C	0.713667000	-2.229569000	0.190034000
C	-0.713903000	-2.229511000	0.189928000
C	-1.133663000	-1.008575000	-0.349120000
C	2.590700000	-0.691348000	-0.713346000
H	1.348508000	-3.077143000	0.432338000
H	-1.348852000	-3.077063000	0.432040000
C	-2.590648000	-0.691174000	-0.713843000
C	-1.549775000	2.924684000	-0.875850000
H	-1.486841000	3.156923000	-1.955161000
H	-1.375141000	3.884042000	-0.353696000
H	-2.584936000	2.630257000	-0.664980000
C	1.550951000	2.924404000	-0.874088000
H	1.489574000	3.156754000	-1.953461000
H	2.585748000	2.629710000	-0.661799000
H	1.375807000	3.883744000	-0.352066000
C	-3.387405000	-2.013235000	-0.816814000
H	-4.417815000	-1.790637000	-1.134892000
H	-2.945433000	-2.700609000	-1.554287000
H	-3.454372000	-2.536586000	0.149016000
C	-2.654280000	-0.028149000	-2.107546000
H	-2.230726000	-0.700649000	-2.870314000
H	-3.702322000	0.175865000	-2.379945000

H	-2.110493000	0.920517000	-2.154379000
C	3.387273000	-2.013475000	-0.816929000
H	2.945268000	-2.700399000	-1.554803000
H	4.417748000	-1.790864000	-1.134794000
H	3.454077000	-2.537338000	0.148632000
C	2.654613000	-0.027590000	-2.106685000
H	3.702727000	0.176363000	-2.378856000
H	2.231011000	-0.699600000	-2.869858000
H	2.111023000	0.921214000	-2.153078000
C	3.287535000	0.159649000	0.375976000
H	3.379047000	-0.422124000	1.307542000
H	4.304341000	0.439096000	0.054115000
H	2.744425000	1.080120000	0.614099000
C	-3.287470000	0.160516000	0.374939000
H	-4.304213000	0.439913000	0.052830000
H	-3.379142000	-0.420712000	1.306830000
H	-2.744265000	1.081062000	0.612561000

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D-1-q SCF Done: -1471.582989 A.U.

Cr	0.009977000	-1.356631000	0.786180000
Al	-0.021261000	1.970054000	0.684890000
Cl	-0.040928000	0.452637000	2.461321000
N	-0.005439000	0.406471000	-0.684691000
C	1.144557000	-0.337567000	-1.065618000
C	0.724362000	-1.589294000	-1.518297000
C	-0.699050000	-1.606529000	-1.511922000
C	-1.143840000	-0.366003000	-1.051489000
C	2.600059000	0.145331000	-1.090750000
H	1.365235000	-2.388853000	-1.875341000
H	-1.323827000	-2.420446000	-1.864405000
C	-2.609837000	0.086138000	-1.072792000
C	-1.580566000	3.175784000	0.834304000
H	-1.512741000	3.968625000	0.066967000
H	-1.425124000	3.686043000	1.803717000
H	-2.611442000	2.802185000	0.831909000
C	1.533817000	3.170132000	0.905446000
H	1.484860000	3.985771000	0.161116000
H	2.564359000	2.795840000	0.917637000
H	1.354424000	3.650044000	1.886203000
C	0.808175000	-2.990275000	1.731878000
C	-0.634671000	-3.089095000	1.674539000
H	1.416466000	-3.651787000	1.100924000
H	-1.093953000	-3.823106000	0.999400000

H	1.291783000	-2.726889000	2.681810000
H	-1.222877000	-2.905720000	2.583626000
C	-3.441069000	-0.939720000	-1.877495000
H	-4.484587000	-0.593088000	-1.929855000
H	-3.072213000	-1.050596000	-2.908623000
H	-3.451056000	-1.931237000	-1.400401000
C	-2.719725000	1.434303000	-1.819882000
H	-2.374764000	1.323637000	-2.860335000
H	-3.769425000	1.767957000	-1.845031000
H	-2.130941000	2.228612000	-1.350164000
C	3.443751000	-0.843609000	-1.927997000
H	3.064278000	-0.939758000	-2.956819000
H	4.478908000	-0.473343000	-1.984539000
H	3.481229000	-1.845012000	-1.473625000
C	2.677189000	1.513620000	-1.803995000
H	3.721301000	1.863584000	-1.837146000
H	2.316658000	1.425351000	-2.841293000
H	2.085645000	2.286826000	-1.303428000
C	-3.230165000	0.137041000	0.343332000
H	-3.263083000	-0.874673000	0.777346000
H	-2.676082000	0.775105000	1.038754000
H	-4.263068000	0.517851000	0.290417000
C	3.229582000	0.173485000	0.322327000
H	3.295918000	-0.848726000	0.726368000
H	4.249728000	0.588044000	0.274819000
H	2.659780000	0.773610000	1.038941000

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D-2-q SCF Done: -1550.111764 A.U.

Cr	1.315645000	-1.363878000	-0.225722000
Al	-1.059832000	0.965332000	1.651897000
Cl	0.938165000	-0.067606000	2.136821000
N	-0.801736000	0.763716000	-0.355321000
C	0.395022000	1.145681000	-0.966325000
C	0.741269000	0.184700000	-1.928072000
C	-0.299798000	-0.789803000	-1.946445000
C	-1.262357000	-0.378285000	-1.015436000
C	1.044406000	2.537191000	-0.852191000
H	1.549183000	0.259450000	-2.648654000
H	-0.414727000	-1.583680000	-2.680219000
C	-2.732144000	-0.849834000	-1.014589000
C	-2.307289000	-0.188932000	2.675433000
H	-3.387576000	-0.056933000	2.500123000
H	-2.126219000	0.127502000	3.720480000

H	-2.087949000	-1.267651000	2.648757000
C	-1.269138000	2.825953000	2.289159000
H	-2.261637000	3.200171000	1.973587000
H	-0.535532000	3.597786000	2.018575000
H	-1.299869000	2.784517000	3.393336000
C	3.382361000	-0.761667000	-0.550126000
C	3.552465000	-1.821027000	0.330306000
H	3.385558000	0.267231000	-0.182572000
H	3.644279000	-1.639108000	1.403780000
H	3.611171000	-0.888017000	-1.614201000
H	3.941556000	-2.777136000	-0.021450000
C	1.596465000	-3.432422000	0.806806000
C	0.297728000	-3.156254000	0.394487000
H	1.890776000	-3.287263000	1.848386000
H	-0.445668000	-2.798756000	1.111517000
H	2.218393000	-4.122396000	0.232955000
H	-0.098799000	-3.619551000	-0.515190000
C	-3.113287000	-1.216586000	-2.472156000
H	-4.184468000	-1.469379000	-2.517828000
H	-2.929479000	-0.380683000	-3.164397000
H	-2.557260000	-2.093420000	-2.836362000
C	-3.658357000	0.309217000	-0.588750000
H	-3.508983000	1.192255000	-1.228461000
H	-4.709165000	-0.006911000	-0.683203000
H	-3.504978000	0.612334000	0.454036000
C	-0.078247000	3.590658000	-1.016592000
H	0.354482000	4.604037000	-1.002375000
H	-0.601785000	3.457818000	-1.976765000
H	-0.822675000	3.527669000	-0.214131000
C	2.035483000	2.731221000	-2.022413000
H	1.544285000	2.622062000	-3.001253000
H	2.460066000	3.745653000	-1.972784000
H	2.876635000	2.022992000	-1.975122000
C	-2.998050000	-2.099981000	-0.150837000
H	-2.750317000	-1.937855000	0.902931000
H	-4.065449000	-2.368400000	-0.208422000
H	-2.420731000	-2.962185000	-0.515455000
C	1.833568000	2.800736000	0.449048000
H	1.225303000	2.695262000	1.351777000
H	2.688523000	2.116775000	0.546376000
H	2.228147000	3.829457000	0.428328000

Cr	1.376064000	-0.068405000	0.100242000
Al	-1.747276000	0.059804000	1.459261000
Cl	0.379578000	-0.478439000	2.305116000
N	-1.025818000	0.076690000	-0.477784000
C	-0.440382000	1.195808000	-1.097228000
C	0.515729000	0.745280000	-2.019392000
C	0.451075000	-0.670922000	-2.047710000
C	-0.518670000	-1.077516000	-1.124662000
C	-0.917743000	2.653036000	-0.989507000
H	1.126241000	1.368655000	-2.665091000
H	1.020265000	-1.317658000	-2.707039000
C	-1.079325000	-2.506094000	-1.039878000
C	-3.133203000	-1.269323000	1.914153000
H	-4.114209000	-0.864592000	1.600631000
H	-3.159411000	-1.288721000	3.019614000
H	-3.085773000	-2.310879000	1.575515000
C	-2.190568000	1.701741000	2.476406000
H	-2.870253000	2.431840000	2.009966000
H	-1.319801000	2.253354000	2.862430000
H	-2.723239000	1.308610000	3.362221000
C	2.834889000	1.333813000	0.495268000
C	4.201278000	0.658064000	0.317063000
H	2.735178000	2.254769000	-0.104901000
H	4.485081000	0.670758000	-0.752662000
H	2.659800000	1.603706000	1.554541000
H	5.010347000	1.193535000	0.850656000
C	4.092178000	-0.801034000	0.775402000
C	2.905968000	-1.437051000	0.045115000
H	5.037910000	-1.352860000	0.607631000
H	3.145423000	-1.592213000	-1.024824000
H	3.916107000	-0.826613000	1.867134000
H	2.597736000	-2.409267000	0.468616000
C	-0.466030000	-3.352473000	-2.179067000
H	-0.899021000	-4.363944000	-2.147312000
H	-0.681758000	-2.928530000	-3.171526000
H	0.624096000	-3.460015000	-2.072993000
C	-2.604869000	-2.446503000	-1.292105000
H	-2.812019000	-2.031822000	-2.291662000
H	-3.034547000	-3.460264000	-1.251486000
H	-3.130972000	-1.828953000	-0.555989000
C	-0.467225000	3.417404000	-2.256810000
H	-0.838078000	2.942958000	-3.178332000
H	-0.866412000	4.442691000	-2.219358000

H	0.628006000	3.499047000	-2.323115000
C	-2.462542000	2.679653000	-0.972292000
H	-2.817186000	3.721982000	-0.942566000
H	-2.871674000	2.206704000	-1.879028000
H	-2.885970000	2.165731000	-0.101134000
C	-0.736063000	-3.238804000	0.276508000
H	0.352009000	-3.373317000	0.367181000
H	-1.078146000	-2.714223000	1.172903000
H	-1.201873000	-4.237244000	0.275512000
C	-0.321942000	3.404117000	0.220622000
H	0.772206000	3.470501000	0.133649000
H	-0.722077000	4.430231000	0.257587000
H	-0.556362000	2.921761000	1.173241000

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D-4-q SCF Done: -1628.672304 A.U.

Cr	1.674178000	-0.397884000	0.163725000
Al	-2.082860000	0.345294000	1.396156000
Cl	0.126909000	0.336939000	2.155740000
N	-1.467494000	0.315987000	-0.522329000
C	-0.500645000	1.229628000	-0.918033000
C	0.511637000	0.549928000	-1.621504000
C	0.076217000	-0.811383000	-1.758063000
C	-1.149910000	-0.916117000	-1.118889000
C	-0.630324000	2.759530000	-0.830672000
H	1.308457000	1.012886000	-2.196613000
H	0.546839000	-1.567991000	-2.380310000
C	-2.118263000	-2.096796000	-1.294053000
C	-2.772212000	-1.245421000	2.356812000
H	-3.853710000	-1.420001000	2.223128000
H	-2.637676000	-0.973130000	3.420915000
H	-2.260416000	-2.209076000	2.220673000
C	-3.190041000	1.882604000	1.956039000
H	-4.212529000	1.723851000	1.563279000
H	-2.906028000	2.912267000	1.702387000
H	-3.279641000	1.832090000	3.056639000
C	3.098165000	1.017840000	0.654373000
C	4.231366000	0.959700000	-0.371323000
H	2.632079000	2.012574000	0.745516000
H	3.929755000	1.496200000	-1.290795000
H	3.446603000	0.723949000	1.662373000
H	5.150252000	1.465686000	-0.015577000
C	4.489892000	-0.509729000	-0.720722000
C	3.149127000	-1.146884000	-1.110426000

H	5.254732000	-0.611978000	-1.514878000
H	2.880429000	-0.841815000	-2.138033000
H	4.915570000	-1.016315000	0.166081000
H	3.182352000	-2.252879000	-1.106637000
C	1.682933000	-2.642719000	1.488682000
C	2.673303000	-1.970935000	2.102900000
H	0.646547000	-2.552938000	1.825580000
H	2.467873000	-1.308127000	2.947665000
H	1.887719000	-3.343521000	0.674655000
H	3.717054000	-2.092499000	1.803332000
C	-2.079785000	3.143272000	-1.210535000
H	-2.192137000	4.239219000	-1.195205000
H	-2.323814000	2.790563000	-2.225178000
H	-2.816285000	2.716012000	-0.519924000
C	0.310881000	3.399738000	-1.877575000
H	1.370150000	3.202688000	-1.652910000
H	0.098366000	3.041104000	-2.896274000
H	0.173235000	4.492021000	-1.869605000
C	-3.569672000	-1.696545000	-0.970124000
H	-3.885847000	-0.835011000	-1.577963000
H	-4.243952000	-2.537254000	-1.197404000
H	-3.713338000	-1.444388000	0.086487000
C	-2.090485000	-2.509843000	-2.789212000
H	-2.819615000	-3.317135000	-2.965107000
H	-2.352773000	-1.663965000	-3.443231000
H	-1.103717000	-2.885476000	-3.097379000
C	-0.246990000	3.368920000	0.537614000
H	-0.861626000	2.998350000	1.363427000
H	0.802876000	3.156396000	0.782992000
H	-0.370613000	4.463114000	0.492079000
C	-1.682812000	-3.324035000	-0.463379000
H	-2.372111000	-4.167309000	-0.633373000
H	-0.672947000	-3.653959000	-0.755038000
H	-1.674500000	-3.108187000	0.612037000

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D-5-q SCF Done: -1628.711669 A.U.

Cr	-1.096141000	-0.068387000	0.200738000
Al	2.099286000	0.157035000	1.446671000
Cl	0.004547000	-0.459213000	2.350759000
N	1.400514000	0.030675000	-0.474960000
C	0.843481000	-1.154795000	-1.006123000
C	-0.157908000	-0.799066000	-1.916767000
C	-0.192858000	0.618151000	-1.993724000

C	0.816688000	1.110283000	-1.153975000
C	1.412381000	-2.576409000	-0.856934000
H	-0.757914000	-1.480090000	-2.511783000
H	-0.805575000	1.204384000	-2.672098000
C	1.373626000	2.544524000	-1.214843000
C	2.359548000	1.869911000	2.402920000
H	3.137663000	2.549277000	2.019310000
H	2.706567000	1.537673000	3.399712000
H	1.449307000	2.461221000	2.581731000
C	3.593093000	-1.037814000	1.928947000
H	4.525959000	-0.594463000	1.531535000
H	3.595172000	-2.099027000	1.650615000
H	3.683983000	-0.989823000	3.029568000
C	-2.481486000	-1.550704000	0.248046000
C	-3.696182000	-1.383495000	-0.673114000
H	-1.923046000	-2.470407000	-0.002581000
H	-3.406626000	-0.898824000	-1.628550000
H	-2.790143000	-1.644656000	1.304917000
H	-4.065538000	-2.383756000	-0.971072000
C	-4.885005000	-0.623422000	-0.067941000
C	-4.739526000	0.889079000	0.153551000
H	-5.758924000	-0.778077000	-0.725893000
H	-4.550840000	1.383711000	-0.818834000
H	-5.149745000	-1.101062000	0.894171000
H	-5.726606000	1.258843000	0.482227000
C	-3.684972000	1.370776000	1.168022000
C	-2.267075000	1.553250000	0.615409000
H	-4.029329000	2.346985000	1.561048000
H	-2.308694000	2.169618000	-0.303764000
H	-3.679825000	0.697751000	2.045229000
H	-1.651461000	2.114367000	1.344278000
C	2.920747000	-2.526110000	-1.199943000
H	3.355932000	-3.536589000	-1.137894000
H	3.071421000	-2.155277000	-2.226415000
H	3.482033000	-1.874534000	-0.520366000
C	0.737641000	-3.497170000	-1.899455000
H	0.895356000	-3.140911000	-2.928733000
H	1.173156000	-4.505356000	-1.824840000
H	-0.344934000	-3.595136000	-1.726124000
C	1.063118000	3.125626000	-2.616478000
H	1.528596000	4.119307000	-2.707943000
H	1.459461000	2.488143000	-3.421717000
H	-0.016679000	3.258808000	-2.779417000

C	2.910975000	2.511314000	-1.074478000
H	3.364464000	1.867740000	-1.844466000
H	3.316229000	3.527748000	-1.199267000
H	3.239052000	2.152686000	-0.091461000
C	0.740342000	3.499709000	-0.181044000
H	1.188533000	4.501966000	-0.276373000
H	-0.341860000	3.597490000	-0.350189000
H	0.892932000	3.161919000	0.848214000
C	1.174183000	-3.229924000	0.522367000
H	1.597583000	-2.659509000	1.353977000
H	0.099053000	-3.352710000	0.717941000
H	1.636198000	-4.229980000	0.536034000

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D-6-q SCF Done: -1628.716861 A.U.

Cr	-0.607282000	-0.709277000	-0.448844000
Al	2.055817000	0.976136000	-1.236118000
Cl	0.045302000	0.623311000	-2.403560000
N	1.207403000	0.365074000	0.545857000
C	0.056692000	0.992824000	1.115114000
C	-0.636293000	0.032083000	1.855539000
C	0.100537000	-1.182523000	1.795951000
C	1.273107000	-0.941924000	1.064715000
C	-0.206807000	2.506601000	1.204131000
H	-1.548833000	0.190326000	2.420462000
H	-0.146822000	-2.101085000	2.319599000
C	2.493483000	-1.876173000	1.035872000
C	3.268157000	-0.168629000	-2.299752000
H	4.240961000	-0.430675000	-1.853787000
H	3.493434000	0.469677000	-3.175173000
H	2.818995000	-1.088652000	-2.702435000
C	2.739898000	2.825046000	-1.285298000
H	3.708506000	2.854268000	-0.751203000
H	2.139935000	3.666079000	-0.915655000
H	2.974906000	3.034547000	-2.344963000
C	-4.181317000	1.103940000	-0.688352000
C	-4.603610000	0.117941000	0.404443000
H	-4.195298000	2.141981000	-0.317054000
H	-3.925292000	0.206898000	1.273540000
H	-4.869410000	1.054344000	-1.548899000
H	-5.597287000	0.423875000	0.776561000
C	-4.683305000	-1.356862000	-0.028517000
C	-3.381980000	-2.176410000	-0.032433000
H	-5.389049000	-1.874814000	0.644212000

H	-2.971135000	-2.203518000	0.995730000
H	-5.143601000	-1.409332000	-1.033146000
H	-3.669226000	-3.225596000	-0.245998000
C	-2.299744000	-1.766202000	-1.027690000
C	-1.093761000	-2.559328000	-1.159626000
H	-2.699193000	-1.347451000	-1.964242000
H	-0.939562000	-3.394033000	-0.461119000
H	-0.672575000	-2.741113000	-2.157318000
H	-3.169658000	0.895345000	-1.067891000
C	1.055542000	3.173599000	1.801891000
H	0.889868000	4.256778000	1.917658000
H	1.278312000	2.756913000	2.797165000
H	1.940515000	3.033505000	1.170499000
C	-1.366597000	2.752902000	2.195991000
H	-1.138185000	2.371433000	3.202665000
H	-1.541228000	3.836152000	2.282769000
H	-2.307180000	2.295555000	1.853708000
C	3.786158000	-1.039444000	1.147157000
H	3.778659000	-0.420932000	2.058393000
H	4.659391000	-1.708540000	1.197755000
H	3.936961000	-0.377907000	0.285404000
C	2.436782000	-2.791336000	2.282998000
H	3.347209000	-3.409392000	2.319930000
H	2.381641000	-2.210348000	3.216548000
H	1.580018000	-3.480979000	2.251812000
C	2.523729000	-2.797871000	-0.202423000
H	3.428478000	-3.427050000	-0.180072000
H	1.646431000	-3.460886000	-0.211897000
H	2.527522000	-2.234836000	-1.140256000
C	-0.617234000	3.177660000	-0.123708000
H	0.129464000	3.070812000	-0.915692000
H	-1.562525000	2.758404000	-0.497444000
H	-0.768581000	4.255962000	0.045124000

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D-7-q SCF Done: -1707.226657 A.U.

Al	-2.678234000	0.522519000	1.052399000
Cl	-1.146947000	1.147918000	2.549771000
N	-1.407332000	0.159442000	-0.562121000
C	-0.474857000	1.071478000	-1.053741000
C	0.498464000	0.368888000	-1.796462000
C	0.068437000	-0.988494000	-1.870239000
C	-1.103340000	-1.095458000	-1.127235000
C	-0.630472000	2.603998000	-1.160989000

H	1.294408000	0.811869000	-2.386126000
H	0.534225000	-1.770523000	-2.460018000
C	-2.012879000	-2.333147000	-1.144373000
C	-3.572372000	-0.969657000	2.025212000
H	-4.304650000	-1.593067000	1.487482000
H	-4.147788000	-0.408107000	2.786349000
H	-2.913618000	-1.642304000	2.598651000
C	-4.070899000	1.845677000	0.565141000
H	-4.664499000	1.486192000	-0.296297000
H	-3.776335000	2.881528000	0.342837000
H	-4.771822000	1.892638000	1.418453000
C	1.603432000	-2.469807000	1.905779000
C	0.723677000	-1.626574000	2.474574000
H	1.274133000	-3.310203000	1.287993000
H	-0.354759000	-1.738772000	2.341261000
H	2.677157000	-2.389915000	2.089854000
H	1.035380000	-0.816253000	3.137004000
Cr	1.319617000	-0.519112000	0.163068000
C	2.378450000	0.937661000	1.104024000
C	3.521528000	1.662671000	0.386312000
H	1.575751000	1.640613000	1.391191000
H	3.270401000	1.844939000	-0.675605000
H	2.747655000	0.489095000	2.046055000
H	3.631901000	2.671619000	0.828173000
C	4.895716000	0.981523000	0.459617000
C	5.138468000	-0.240336000	-0.436417000
H	5.662655000	1.732417000	0.199790000
H	5.010478000	0.053403000	-1.495686000
H	5.099391000	0.704769000	1.511687000
H	6.203937000	-0.511427000	-0.333863000
C	4.304019000	-1.504247000	-0.171729000
C	2.883147000	-1.504625000	-0.747062000
H	4.851912000	-2.355913000	-0.619251000
H	2.914294000	-1.105261000	-1.777472000
H	4.303825000	-1.712157000	0.914720000
H	2.505395000	-2.542769000	-0.832669000
C	-3.470689000	-1.895708000	-1.409407000
H	-3.543317000	-1.340898000	-2.357934000
H	-4.120337000	-2.782260000	-1.483336000
H	-3.875314000	-1.262271000	-0.611711000
C	-1.597429000	-3.249496000	-2.318908000
H	-2.284567000	-4.108325000	-2.368248000
H	-1.642126000	-2.724599000	-3.285084000

H	-0.581919000	-3.654252000	-2.191002000
C	-1.865555000	2.840889000	-2.070286000
H	-1.989196000	3.920609000	-2.253609000
H	-1.736382000	2.344674000	-3.045456000
H	-2.788764000	2.465218000	-1.613910000
C	0.595681000	3.200794000	-1.890102000
H	1.531324000	3.015635000	-1.342779000
H	0.706000000	2.815630000	-2.914593000
H	0.468269000	4.290969000	-1.966325000
C	-1.900798000	-3.178542000	0.142099000
H	-2.598457000	-4.030496000	0.100389000
H	-0.883369000	-3.590214000	0.241367000
H	-2.137913000	-2.601288000	1.039862000
C	-0.784299000	3.395058000	0.151462000
H	-1.667806000	3.114516000	0.730399000
H	0.091337000	3.269981000	0.802816000
H	-0.875818000	4.464902000	-0.095062000

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D-8-q SCF Done: -1707.27209 A.U.

C	5.295096000	0.612966000	0.497808000
C	5.458598000	-0.878254000	0.151638000
H	6.302208000	1.008622000	0.717641000
H	6.085994000	-0.965012000	-0.754738000
H	4.742788000	0.714895000	1.447205000
H	6.045395000	-1.346802000	0.963203000
Cr	0.748560000	-0.046690000	0.219820000
Al	-2.479415000	-0.079720000	1.454364000
Cl	-0.350969000	0.432928000	2.354984000
N	-1.794709000	0.050427000	-0.464757000
C	-1.143787000	1.202418000	-0.955067000
C	-0.157941000	0.797818000	-1.863078000
C	-0.221872000	-0.616835000	-1.972419000
C	-1.279022000	-1.051753000	-1.158256000
C	-1.621931000	2.655162000	-0.784078000
H	0.495254000	1.447628000	-2.435804000
H	0.348976000	-1.229622000	-2.664151000
C	-1.955150000	-2.431146000	-1.271901000
C	-2.782169000	-1.799816000	2.383277000
H	-3.608148000	-2.430951000	2.017532000
H	-3.070823000	-1.476350000	3.401489000
H	-1.895127000	-2.438111000	2.509621000
C	-3.927361000	1.160265000	1.959541000
H	-4.877409000	0.739556000	1.578403000

H	-3.904561000	2.218704000	1.670921000
H	-4.004442000	1.124453000	3.061639000
C	2.197367000	1.390245000	0.283071000
C	3.171946000	1.346121000	-0.902200000
H	1.715264000	2.376977000	0.384696000
H	3.062955000	0.399435000	-1.461415000
H	2.688726000	1.177895000	1.247054000
H	2.894077000	2.128320000	-1.630845000
C	4.668430000	1.538363000	-0.560875000
C	4.176726000	-1.700537000	-0.065260000
H	5.251024000	1.456572000	-1.497541000
H	3.654910000	-1.325142000	-0.958159000
H	4.804549000	2.578144000	-0.212280000
H	4.469890000	-2.732684000	-0.326678000
C	3.188255000	-1.749427000	1.120518000
C	1.716869000	-1.811110000	0.685148000
H	3.433263000	-2.630104000	1.744517000
H	1.608172000	-2.502532000	-0.171196000
H	3.345570000	-0.886626000	1.788878000
H	1.087668000	-2.215492000	1.500252000
C	-3.480920000	-2.280388000	-1.091769000
H	-3.895468000	-1.560609000	-1.814618000
H	-3.970953000	-3.252193000	-1.259773000
H	-3.758647000	-1.951555000	-0.082874000
C	-1.722651000	-2.964262000	-2.708009000
H	-2.275996000	-3.907259000	-2.839122000
H	-2.074879000	-2.253312000	-3.471158000
H	-0.661884000	-3.182646000	-2.901672000
C	-3.122093000	2.708077000	-1.162608000
H	-3.493202000	3.742942000	-1.088711000
H	-3.272866000	2.367468000	-2.199471000
H	-3.738494000	2.080174000	-0.508292000
C	-0.861898000	3.552730000	-1.786887000
H	-1.016918000	3.232548000	-2.828357000
H	-1.230261000	4.586152000	-1.697334000
H	0.219978000	3.571751000	-1.584670000
C	-1.382948000	-3.485212000	-0.300822000
H	-1.913382000	-4.441793000	-0.435210000
H	-0.316225000	-3.662116000	-0.500231000
H	-1.485987000	-3.187971000	0.747145000
C	-1.385005000	3.264344000	0.615158000
H	-1.877088000	2.710984000	1.420231000
H	-0.311792000	3.307374000	0.849479000

H	-1.776956000	4.293844000	0.632968000
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D-9-q SCF Done: -1550.15306 A.U.

Cr	-0.889269000	-0.680301000	-0.591052000
Al	1.882150000	1.017761000	-1.036293000
Cl	0.086345000	0.565934000	-2.473336000
N	0.810542000	0.334985000	0.601676000
C	-0.389542000	0.952047000	1.072332000
C	-1.153509000	-0.024104000	1.715422000
C	-0.412290000	-1.238544000	1.705570000
C	0.821815000	-0.988316000	1.095015000
C	-0.700569000	2.457443000	1.118216000
H	-2.117205000	0.121777000	2.191103000
H	-0.714289000	-2.168423000	2.177399000
C	2.019076000	-1.949487000	1.130434000
C	-4.696444000	-0.442926000	-0.026181000
C	-3.860218000	-1.688505000	-0.328788000
H	-5.553618000	-0.674851000	0.626901000
H	-3.500455000	-2.137629000	0.616071000
H	-5.097259000	-0.001860000	-0.954275000
H	-4.525458000	-2.455646000	-0.774633000
C	-2.686324000	-1.446200000	-1.263535000
C	-1.616506000	-2.413966000	-1.399053000
H	-2.970392000	-0.908011000	-2.182600000
H	-1.617763000	-3.288585000	-0.733310000
H	-1.189915000	-2.618866000	-2.389720000
H	-4.094641000	0.337116000	0.468832000
C	2.446419000	2.909437000	-0.997893000
H	3.308857000	3.010906000	-0.312176000
H	2.842462000	3.117489000	-2.008853000
H	1.742681000	3.715260000	-0.756213000
C	3.336467000	-0.009649000	-1.902088000
H	3.691319000	0.688759000	-2.683234000
H	4.218541000	-0.254534000	-1.288947000
H	3.028390000	-0.924197000	-2.430054000
C	0.474586000	3.174552000	1.824395000
H	0.280367000	4.257897000	1.877195000
H	0.587973000	2.800795000	2.854541000
H	1.428470000	3.028408000	1.306128000
C	-1.957724000	2.682246000	1.989776000
H	-1.822677000	2.310520000	3.016642000
H	-2.163122000	3.761895000	2.050837000
H	-2.850029000	2.203486000	1.558491000

C	3.299282000	-1.162646000	1.485759000
H	3.186844000	-0.647568000	2.452879000
H	4.153307000	-1.853445000	1.566107000
H	3.557929000	-0.413461000	0.728261000
C	1.791819000	-2.981861000	2.259901000
H	2.677350000	-3.631166000	2.338653000
H	1.638473000	-2.496811000	3.236173000
H	0.929915000	-3.634399000	2.055576000
C	-1.013975000	3.083423000	-0.258522000
H	-0.201841000	2.981597000	-0.983729000
H	-1.910149000	2.619023000	-0.698162000
H	-1.216739000	4.159447000	-0.135437000
C	2.184396000	-2.746170000	-0.182057000
H	3.067520000	-3.402465000	-0.116818000
H	1.301434000	-3.377561000	-0.362901000
H	2.315993000	-2.094985000	-1.050912000

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D-2-3-q SCF Done: -1550.10441 A.U.

Cr	1.344023000	-1.158905000	-0.258477000
Al	-1.145162000	0.893849000	1.643602000
Cl	0.938329000	0.043983000	2.134655000
N	-0.870568000	0.678718000	-0.368890000
C	0.266879000	1.190626000	-1.002413000
C	0.688986000	0.279322000	-1.982824000
C	-0.238023000	-0.801468000	-1.986144000
C	-1.214310000	-0.508695000	-1.022219000
C	0.790454000	2.633255000	-0.884064000
H	1.491025000	0.430102000	-2.697595000
H	-0.274963000	-1.607893000	-2.713529000
C	-2.607220000	-1.169038000	-0.974312000
C	-2.287730000	-0.331878000	2.704611000
H	-3.372990000	-0.319881000	2.512378000
H	-2.155590000	0.049936000	3.735018000
H	-1.957630000	-1.381697000	2.730448000
C	-1.514071000	2.740720000	2.247881000
H	-2.540508000	3.013382000	1.936592000
H	-0.859722000	3.574511000	1.960407000
H	-1.533153000	2.712836000	3.352797000
C	3.314077000	-0.637510000	-0.534263000
C	3.521164000	-1.629833000	0.496774000
H	3.399423000	0.417470000	-0.251171000
H	3.593335000	-1.247424000	1.519720000
H	3.704189000	-0.855875000	-1.537622000

H	4.258203000	-2.410107000	0.296944000
C	2.157600000	-3.128764000	0.774414000
C	0.776779000	-3.029180000	0.364061000
H	2.359792000	-3.159780000	1.849230000
H	0.017195000	-2.900542000	1.142206000
H	2.756092000	-3.852511000	0.215594000
H	0.452793000	-3.652013000	-0.479025000
C	-0.420221000	3.585940000	-1.035739000
H	-0.080345000	4.633513000	-0.997476000
H	-0.922248000	3.427297000	-2.003575000
H	-1.162936000	3.440433000	-0.242665000
C	1.751987000	2.919428000	-2.060167000
H	2.086232000	3.966904000	-2.006954000
H	2.651847000	2.286598000	-2.022542000
H	1.265060000	2.773897000	-3.036392000
C	-2.958010000	-1.655835000	-2.403240000
H	-3.987387000	-2.047387000	-2.412333000
H	-2.897074000	-0.839942000	-3.139802000
H	-2.298895000	-2.471594000	-2.736148000
C	-3.670359000	-0.119614000	-0.585697000
H	-3.647071000	0.740940000	-1.271846000
H	-4.672554000	-0.573077000	-0.640187000
H	-3.540587000	0.255125000	0.436575000
C	1.570341000	2.948708000	0.410950000
H	2.468359000	2.320226000	0.496197000
H	1.894740000	4.001634000	0.388665000
H	0.979084000	2.802073000	1.319335000
C	-2.686583000	-2.399095000	-0.046738000
H	-2.002335000	-3.190383000	-0.385913000
H	-2.440298000	-2.153111000	0.990547000
H	-3.708638000	-2.811253000	-0.063399000

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D-3-9-q SCF Done: -1550.101394 A.U.

Cr	1.769113000	-0.480546000	-0.014517000
Al	-1.792583000	0.492367000	1.408539000
Cl	0.405461000	0.022850000	2.065455000
N	-1.247092000	0.286295000	-0.520958000
C	-0.290236000	1.147528000	-1.062883000
C	0.598559000	0.406947000	-1.854799000
C	0.121560000	-0.940788000	-1.870226000
C	-1.015590000	-0.985245000	-1.073421000
C	-0.305533000	2.683272000	-1.001518000
H	1.364636000	0.810727000	-2.510235000

H	0.505416000	-1.741730000	-2.494886000
C	-1.936932000	-2.207201000	-0.969689000
C	-2.905884000	-0.810344000	2.403377000
H	-3.978222000	-0.572840000	2.280032000
H	-2.672974000	-0.597612000	3.464036000
H	-2.791776000	-1.892990000	2.266300000
C	-2.426546000	2.241823000	2.085628000
H	-3.489195000	2.362798000	1.802253000
H	-1.918656000	3.184224000	1.847461000
H	-2.423782000	2.141621000	3.187054000
H	2.737328000	-1.108158000	-1.172832000
C	3.406489000	0.720711000	0.361728000
C	4.500220000	-0.361275000	0.248006000
H	3.521174000	1.519831000	-0.386194000
H	5.100324000	-0.236088000	-0.665385000
H	3.325991000	1.169969000	1.363997000
H	5.202225000	-0.365402000	1.101889000
C	3.769929000	-1.697833000	0.197402000
C	2.880622000	-2.017101000	1.208858000
H	4.088048000	-2.461392000	-0.519172000
H	2.396353000	-2.996987000	1.247250000
H	2.848856000	-1.418848000	2.123118000
C	-1.761894000	3.184681000	-1.126011000
H	-1.780510000	4.286223000	-1.111275000
H	-2.203402000	2.850645000	-2.078305000
H	-2.403562000	2.828704000	-0.313856000
C	0.465273000	3.245052000	-2.220223000
H	0.045587000	2.885625000	-3.172275000
H	0.399229000	4.344333000	-2.214466000
H	1.533993000	2.984800000	-2.191459000
C	-3.408848000	-1.777872000	-0.800136000
H	-3.723320000	-1.137424000	-1.639107000
H	-4.057361000	-2.668371000	-0.792280000
H	-3.592861000	-1.233917000	0.131669000
C	-1.862017000	-3.003942000	-2.295870000
H	-2.563959000	-3.851738000	-2.252945000
H	-2.135160000	-2.378512000	-3.159667000
H	-0.860848000	-3.422302000	-2.476825000
C	-1.472805000	-3.159912000	0.158901000
H	-0.491413000	-3.593052000	-0.092875000
H	-1.372668000	-2.651584000	1.124412000
H	-2.185624000	-3.991999000	0.281423000
C	0.394920000	3.246474000	0.258011000

H	1.468890000	3.008111000	0.236738000
H	0.292638000	4.343798000	0.281945000
H	-0.011433000	2.849505000	1.193018000

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D-4-5-q SCF Done: -1628.655396 A.U.

Cr	1.679390000	-0.294956000	0.366324000
Al	-2.196958000	0.253657000	1.321933000
Cl	0.014973000	0.344589000	2.109691000
N	-1.550922000	0.161690000	-0.573742000
C	-0.699910000	1.171983000	-1.028352000
C	0.402119000	0.591084000	-1.656747000
C	0.184356000	-0.824445000	-1.669233000
C	-1.039361000	-1.053693000	-1.047481000
C	-1.001881000	2.677493000	-1.025065000
H	1.159793000	1.125390000	-2.223327000
H	0.761272000	-1.552064000	-2.236410000
C	-1.806817000	-2.383668000	-1.123223000
C	-2.935218000	-1.286896000	2.325898000
H	-4.027017000	-1.380750000	2.186192000
H	-2.790480000	-0.999798000	3.384583000
H	-2.500883000	-2.289077000	2.212891000
C	-3.272466000	1.807500000	1.907137000
H	-4.300187000	1.695738000	1.512545000
H	-2.955669000	2.836558000	1.695106000
H	-3.362418000	1.715016000	3.005204000
C	3.003123000	1.108621000	1.100868000
C	4.081069000	1.430530000	0.069266000
H	2.418223000	1.991969000	1.405445000
H	3.654429000	2.055619000	-0.737952000
H	3.439634000	0.668330000	2.015996000
H	4.908558000	2.025868000	0.500679000
C	4.611398000	0.131469000	-0.543065000
C	3.445789000	-0.741454000	-0.990738000
H	5.286429000	0.338989000	-1.395485000
H	2.793348000	-0.177046000	-1.679087000
H	5.230081000	-0.405905000	0.200059000
H	3.760765000	-1.631634000	-1.548792000
C	3.048576000	-2.266257000	0.569509000
C	2.126745000	-1.990740000	1.585163000
H	2.793903000	-3.015573000	-0.184150000
H	1.169080000	-2.518591000	1.604751000
H	4.118061000	-2.152873000	0.754922000
H	2.464106000	-1.578378000	2.539444000

C	-3.321980000	-2.174412000	-0.936648000
H	-3.711025000	-1.455822000	-1.674274000
H	-3.848086000	-3.130929000	-1.083791000
H	-3.580590000	-1.812173000	0.063759000
C	-1.612730000	-2.971937000	-2.544934000
H	-2.202264000	-3.897414000	-2.646051000
H	-1.948454000	-2.266564000	-3.320593000
H	-0.562886000	-3.229479000	-2.749223000
C	-2.509527000	2.903775000	-1.273908000
H	-2.727202000	3.983692000	-1.299653000
H	-2.809222000	2.473383000	-2.242548000
H	-3.137940000	2.453608000	-0.498474000
C	-0.247490000	3.340263000	-2.203021000
H	-0.520380000	4.405892000	-2.256155000
H	0.844766000	3.293388000	-2.075648000
H	-0.505168000	2.875279000	-3.166954000
C	-1.255652000	-3.418128000	-0.115870000
H	-1.832261000	-4.356154000	-0.169778000
H	-0.205428000	-3.660221000	-0.345153000
H	-1.300712000	-3.050628000	0.916496000
C	-0.523473000	3.391875000	0.261275000
H	-0.963587000	2.979403000	1.174667000
H	0.570213000	3.314725000	0.358743000
H	-0.783818000	4.462015000	0.211596000

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D-5-6-q SCF Done: -1628.673105 A.U.

Cr	1.309384000	-0.330877000	-0.138625000
Al	-2.012363000	0.262559000	1.541572000
Cl	0.158266000	0.373126000	2.258223000
N	-1.452284000	0.188408000	-0.432061000
C	-0.664248000	1.191792000	-1.016427000
C	0.183438000	0.607021000	-1.969419000
C	-0.105475000	-0.783630000	-2.000329000
C	-1.140806000	-1.010716000	-1.081754000
C	-0.889639000	2.709147000	-0.890593000
H	0.849930000	1.131080000	-2.647479000
H	0.296950000	-1.504954000	-2.705094000
C	-2.001623000	-2.288229000	-1.061910000
C	-2.703381000	-1.311490000	2.536918000
H	-3.622381000	-1.795779000	2.168704000
H	-2.961913000	-0.876391000	3.520921000
H	-1.965559000	-2.101940000	2.743276000
C	-3.172181000	1.786431000	2.047572000

H	-4.195278000	1.593542000	1.671986000
H	-2.919283000	2.819894000	1.777787000
H	-3.248134000	1.752032000	3.150110000
C	2.927202000	1.252839000	-0.014271000
C	4.360192000	0.930769000	-0.470949000
H	2.415681000	1.887211000	-0.751683000
H	4.340995000	0.571457000	-1.516845000
H	2.926244000	1.804878000	0.940582000
H	4.968853000	1.853047000	-0.481562000
C	5.057726000	-0.131585000	0.396405000
C	4.323899000	-1.482541000	0.386146000
H	6.092339000	-0.274912000	0.043024000
H	4.276994000	-1.856461000	-0.652919000
H	5.136597000	0.236402000	1.436639000
H	4.905325000	-2.230995000	0.952982000
C	2.903750000	-1.430231000	0.960607000
C	1.862277000	-2.260982000	0.404353000
H	2.872766000	-1.287466000	2.050575000
H	2.107347000	-2.905324000	-0.449955000
H	1.116340000	-2.682869000	1.084250000
H	2.739976000	-0.035009000	0.622451000
C	-3.487718000	-1.901487000	-0.894056000
H	-3.803222000	-1.200996000	-1.682975000
H	-4.115195000	-2.803752000	-0.968882000
H	-3.697582000	-1.439200000	0.077350000
C	-1.875049000	-2.992311000	-2.435061000
H	-2.545475000	-3.865681000	-2.458009000
H	-2.155771000	-2.326304000	-3.265438000
H	-0.855427000	-3.363457000	-2.617494000
C	-2.394327000	2.985471000	-1.125056000
H	-2.590140000	4.068581000	-1.071308000
H	-2.699722000	2.634912000	-2.123941000
H	-3.029011000	2.488313000	-0.383764000
C	-0.118270000	3.435002000	-2.017189000
H	-0.319089000	4.515343000	-1.952581000
H	0.970992000	3.301966000	-1.929263000
H	-0.429902000	3.096329000	-3.016960000
C	-1.566963000	-3.311984000	0.007709000
H	-2.268570000	-4.161954000	0.019223000
H	-0.566005000	-3.706786000	-0.219211000
H	-1.545085000	-2.880754000	1.012670000
C	-0.406338000	3.325920000	0.440837000
H	-0.868396000	2.874347000	1.323011000

H	0.682957000	3.219957000	0.549071000
H	-0.642997000	4.402251000	0.450758000

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D-7-8-q SCF Done: -1707.202849 A.U.

C	-5.108125000	0.241895000	-0.389954000
C	-4.388574000	1.567167000	-0.101384000
H	-4.944092000	-0.029538000	-1.450245000
H	-4.815037000	2.323880000	-0.784678000
H	-6.190017000	0.444102000	-0.305714000
H	-4.658359000	1.921246000	0.909971000
Cr	-1.120708000	0.307710000	0.203826000
Al	2.622961000	-0.345033000	1.141927000
Cl	1.242629000	-1.331710000	2.576100000
N	1.339192000	-0.038846000	-0.499054000
C	0.547635000	-1.027236000	-1.116851000
C	-0.373291000	-0.388665000	-1.968986000
C	-0.077307000	0.995021000	-1.959792000
C	0.988200000	1.197661000	-1.079760000
C	0.854770000	-2.536178000	-1.266673000
H	-1.095906000	-0.879819000	-2.612657000
H	-0.566049000	1.753909000	-2.562332000
C	1.788406000	2.512170000	-1.013304000
C	3.253242000	1.202472000	2.220468000
H	3.915150000	1.950545000	1.755805000
H	3.862209000	0.688221000	2.989003000
H	2.468738000	1.737598000	2.780190000
C	4.180413000	-1.417141000	0.539227000
H	4.674164000	-0.970034000	-0.343364000
H	4.018806000	-2.481881000	0.312430000
H	4.923566000	-1.379590000	1.356729000
C	-2.209195000	-1.293914000	0.892234000
C	-3.491905000	-1.766300000	0.195192000
H	-1.458545000	-2.101564000	0.874847000
H	-3.351388000	-1.826920000	-0.901620000
H	-2.415221000	-1.107888000	1.961686000
H	-3.677174000	-2.812026000	0.506970000
C	-4.790454000	-0.984060000	0.484010000
C	-2.872550000	1.565792000	-0.304923000
H	-5.630499000	-1.686172000	0.347372000
H	-2.666448000	0.856411000	-1.133270000
H	-4.821560000	-0.702005000	1.553337000
H	-2.502382000	2.546181000	-0.634585000
C	-2.232450000	1.759328000	1.694793000

C	-0.937116000	1.313050000	2.035353000
H	-2.412919000	2.827285000	1.547905000
H	-0.106348000	2.021571000	2.001805000
H	-3.086647000	1.224399000	2.113471000
H	-0.808962000	0.476754000	2.727187000
C	3.289962000	2.200413000	-1.205353000
H	3.458965000	1.668633000	-2.154815000
H	3.865155000	3.139418000	-1.233920000
H	3.703648000	1.591060000	-0.393769000
C	1.366046000	3.416004000	-2.195924000
H	0.313029000	3.729132000	-2.123951000
H	1.976850000	4.331719000	-2.184858000
H	1.516415000	2.922286000	-3.167951000
C	2.110016000	-2.614506000	-2.175982000
H	2.351115000	-3.668625000	-2.388650000
H	1.933857000	-2.105157000	-3.136727000
H	2.984461000	-2.155879000	-1.697962000
C	-0.310755000	-3.223943000	-2.016286000
H	-0.439105000	-2.843179000	-3.040221000
H	-0.096526000	-4.299880000	-2.098652000
H	-1.265566000	-3.115365000	-1.480388000
C	1.101522000	-3.357721000	0.010747000
H	1.964402000	-3.015419000	0.586931000
H	0.234071000	-3.348765000	0.683579000
H	1.294408000	-4.402144000	-0.282144000
C	1.544513000	3.328029000	0.272312000
H	1.784059000	2.763931000	1.177260000
H	2.173130000	4.233031000	0.267129000
H	0.493996000	3.655878000	0.326682000

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E-0-s SCF Done: -1540.554896 A.U.

Cr	-0.000182000	2.339103000	-0.313205000
Al	-0.000001000	-0.921641000	-1.472114000
Cl	-0.001060000	1.268178000	-2.467957000
N	0.000126000	-0.318214000	0.457306000
C	1.121433000	0.319748000	0.984278000
C	0.716397000	1.406726000	1.779194000
C	-0.716048000	1.406652000	1.779329000
C	-1.121137000	0.319672000	0.984461000
H	1.371026000	2.010046000	2.406331000
H	-1.370637000	2.009929000	2.406547000
C	-1.678218000	-1.723577000	-2.102005000
H	-1.870794000	-2.713985000	-1.654254000

H	-1.574196000	-1.882138000	-3.191105000
H	-2.578631000	-1.110976000	-1.944361000
C	1.678711000	-1.722224000	-2.102408000
H	1.871891000	-2.712668000	-1.654988000
H	2.578825000	-1.109207000	-1.944662000
H	1.574664000	-1.880498000	-3.191547000
C	2.501417000	-0.183512000	0.846997000
C	3.581567000	0.700839000	0.667327000
C	2.775039000	-1.556099000	0.993914000
C	4.893619000	0.226026000	0.628049000
C	4.087028000	-2.029328000	0.951754000
C	5.151582000	-1.141390000	0.768144000
H	3.386301000	1.768655000	0.539173000
H	1.948325000	-2.250468000	1.156647000
H	5.718791000	0.926996000	0.478623000
H	4.279976000	-3.098767000	1.068495000
H	6.178587000	-1.513376000	0.733872000
C	-2.501128000	-0.183606000	0.847239000
C	-3.581290000	0.700693000	0.667437000
C	-2.774718000	-1.556186000	0.994343000
C	-4.893333000	0.225836000	0.628184000
C	-4.086692000	-2.029455000	0.952221000
C	-5.151263000	-1.141563000	0.768466000
H	-3.386048000	1.768495000	0.539138000
H	-1.947982000	-2.250511000	1.157147000
H	-5.718517000	0.926764000	0.478624000
H	-4.279614000	-3.098884000	1.069091000
H	-6.178259000	-1.513576000	0.734214000

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E-1-q SCF Done: -1619.103873 A.U.

Cr	0.020047000	1.733896000	0.209980000
Al	0.015078000	-1.232699000	1.466439000
Cl	0.788889000	0.819100000	2.328099000
N	-0.039992000	-0.500598000	-0.446962000
C	-1.180229000	0.046242000	-1.044765000
C	-0.780955000	1.038363000	-1.957365000
C	0.644571000	1.027265000	-2.006262000
C	1.081930000	0.061109000	-1.090213000
H	-1.450959000	1.619394000	-2.587689000
H	1.282710000	1.607546000	-2.668596000
C	1.360260000	-2.623696000	1.790080000
H	1.224704000	-3.501647000	1.133521000
H	1.229949000	-2.983220000	2.826923000

H	2.403028000	-2.289816000	1.684429000
C	-1.760762000	-1.439606000	2.275132000
H	-2.263992000	-2.377638000	1.987274000
H	-2.461994000	-0.613846000	2.078542000
H	-1.607390000	-1.481497000	3.369480000
C	-1.036504000	3.436188000	0.640839000
C	0.304316000	3.765515000	0.208273000
H	-1.881067000	3.652842000	-0.027076000
H	0.452774000	4.224272000	-0.778068000
H	-1.292280000	3.505310000	1.706159000
H	1.046866000	4.083251000	0.952459000
C	-2.554258000	-0.449492000	-0.834221000
C	-3.632973000	0.444826000	-0.708048000
C	-2.818651000	-1.830741000	-0.857254000
C	-4.939950000	-0.032353000	-0.599273000
C	-4.126781000	-2.304798000	-0.745419000
C	-5.191525000	-1.408197000	-0.615388000
H	-3.438246000	1.518927000	-0.671310000
H	-1.992973000	-2.535149000	-0.981846000
H	-5.766313000	0.674681000	-0.491876000
H	-4.315787000	-3.380990000	-0.766266000
H	-6.215175000	-1.780326000	-0.526853000
C	2.477136000	-0.394148000	-0.902235000
C	3.509765000	0.534308000	-0.676862000
C	2.807877000	-1.752554000	-1.050544000
C	4.837852000	0.112319000	-0.594397000
C	4.136648000	-2.172267000	-0.966461000
C	5.155055000	-1.242153000	-0.737341000
H	3.263391000	1.591510000	-0.551304000
H	2.017194000	-2.479825000	-1.244415000
H	5.627907000	0.844503000	-0.410302000
H	4.377743000	-3.231585000	-1.084626000
H	6.194677000	-1.572425000	-0.670391000

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E-2-q SCF Done: -1697.629740 A.U.

Cr	-0.172475000	2.070314000	0.086398000
Al	0.157644000	-2.351571000	0.465528000
Cl	0.142575000	-1.550166000	2.543597000
N	0.081391000	-0.529188000	-0.513722000
C	-1.063395000	0.027299000	-1.053885000
C	-0.715032000	1.072394000	-1.944867000
C	0.696057000	1.181311000	-1.908709000
C	1.162659000	0.195307000	-1.007121000

H	-1.412277000	1.650120000	-2.547016000
H	1.322106000	1.868038000	-2.474650000
C	1.816922000	-3.315333000	-0.027884000
H	2.171268000	-3.093783000	-1.050429000
H	1.577667000	-4.394445000	-0.006900000
H	2.672316000	-3.163077000	0.647766000
C	-1.435975000	-3.435916000	0.017589000
H	-1.698330000	-3.385960000	-1.054982000
H	-2.352982000	-3.223690000	0.586260000
H	-1.164754000	-4.488606000	0.220399000
C	-2.152612000	2.951501000	0.037861000
C	-1.774111000	3.087724000	1.371800000
H	-2.822275000	2.146364000	-0.271500000
H	-2.057357000	2.318652000	2.099745000
H	-2.125739000	3.825939000	-0.624539000
H	-1.554520000	4.064903000	1.800509000
C	0.777970000	3.282057000	1.807743000
C	1.700273000	2.614122000	1.015932000
H	0.493557000	2.888993000	2.786993000
H	2.157248000	1.685800000	1.363472000
H	0.588137000	4.347425000	1.655792000
H	2.251002000	3.143816000	0.229529000
C	-2.452354000	-0.387449000	-0.751613000
C	-2.897498000	-0.594906000	0.567263000
C	-3.382933000	-0.482387000	-1.802747000
C	-4.238327000	-0.888353000	0.821553000
C	-4.721617000	-0.784629000	-1.544967000
C	-5.154056000	-0.985037000	-0.230808000
H	-2.190105000	-0.536927000	1.397957000
H	-3.048394000	-0.336654000	-2.832518000
H	-4.567171000	-1.047521000	1.851393000
H	-5.427986000	-0.868122000	-2.374632000
H	-6.201898000	-1.219554000	-0.027351000
C	2.590992000	-0.089600000	-0.742351000
C	3.076800000	-0.454592000	0.526809000
C	3.515752000	0.063391000	-1.794356000
C	4.443155000	-0.652282000	0.733593000
C	4.881074000	-0.137869000	-1.585068000
C	5.350652000	-0.493732000	-0.317580000
H	2.385554000	-0.586977000	1.361671000
H	3.158545000	0.318948000	-2.794370000
H	4.798562000	-0.935535000	1.727338000
H	5.578876000	-0.023894000	-2.418424000

H	6.419088000	-0.652343000	-0.151130000
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E-3-q SCF Done: -1697.670251 A.U.

Cr	-0.009447000	1.575153000	-0.034061000
Al	-0.041319000	-1.368400000	1.568964000
Cl	-0.710366000	0.818431000	2.161446000
N	0.011794000	-0.912090000	-0.419582000
C	-1.102507000	-0.391582000	-1.089002000
C	-0.666644000	0.481450000	-2.096605000
C	0.756092000	0.478639000	-2.069920000
C	1.146990000	-0.424693000	-1.062161000
H	-1.309212000	1.005092000	-2.800764000
H	1.426041000	0.975484000	-2.768360000
C	1.730323000	-1.543127000	2.393634000
H	2.193368000	-2.529960000	2.227164000
H	1.584502000	-1.437415000	3.484644000
H	2.461521000	-0.778376000	2.089372000
C	-1.454166000	-2.622690000	2.096801000
H	-1.363321000	-3.596691000	1.583806000
H	-2.479226000	-2.258575000	1.933261000
H	-1.341541000	-2.823970000	3.177554000
C	-1.114593000	3.288703000	-0.306106000
C	-0.149720000	4.478964000	-0.223573000
H	-1.720410000	3.287483000	-1.229446000
H	0.326033000	4.640070000	-1.209707000
H	-1.809847000	3.280493000	0.555215000
H	-0.670590000	5.425241000	0.019403000
C	0.945455000	4.156157000	0.801515000
C	1.565753000	2.806519000	0.427129000
H	1.697502000	4.967230000	0.858930000
H	2.169406000	2.905673000	-0.496975000
H	0.492239000	4.090230000	1.808092000
H	2.209784000	2.379937000	1.215983000
C	-2.499380000	-0.815034000	-0.845994000
C	-2.837660000	-2.179536000	-0.881551000
C	-3.524023000	0.133889000	-0.680097000
C	-4.166861000	-2.584303000	-0.749235000
C	-4.852844000	-0.273914000	-0.547549000
C	-5.178156000	-1.633349000	-0.581448000
H	-2.052199000	-2.923994000	-1.026346000
H	-3.273239000	1.196051000	-0.640462000
H	-4.414290000	-3.648264000	-0.781352000
H	-5.637089000	0.474790000	-0.411261000

H	-6.218492000	-1.951517000	-0.477373000
C	2.510951000	-0.935651000	-0.825108000
C	2.725208000	-2.316507000	-0.660685000
C	3.625031000	-0.077542000	-0.861584000
C	4.018051000	-2.822640000	-0.520036000
C	4.916755000	-0.587119000	-0.720201000
C	5.118030000	-1.960115000	-0.546492000
H	1.871246000	-2.997542000	-0.661733000
H	3.474482000	0.997083000	-0.978329000
H	4.167418000	-3.897990000	-0.395053000
H	5.770945000	0.094229000	-0.738707000
H	6.129999000	-2.357079000	-0.434514000

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E-4-q SCF Done: -1776.191316 A.U.

Cr	-0.266736000	1.731163000	0.154743000
Al	0.429323000	-2.696381000	0.151485000
Cl	0.432787000	-2.324260000	2.346965000
N	0.149591000	-0.740618000	-0.526313000
C	-1.052334000	-0.271209000	-1.030210000
C	-0.800968000	0.816635000	-1.901517000
C	0.608313000	0.992750000	-1.943307000
C	1.169711000	0.047216000	-1.068251000
H	-1.554415000	1.377294000	-2.450000000
H	1.157688000	1.746090000	-2.501485000
C	2.157367000	-3.362251000	-0.541903000
H	2.344347000	-3.059831000	-1.588247000
H	2.091509000	-4.466022000	-0.545536000
H	3.052724000	-3.094615000	0.038364000
C	-1.078024000	-3.822109000	-0.450944000
H	-1.350112000	-3.639441000	-1.506380000
H	-2.003494000	-3.759843000	0.139750000
H	-0.728249000	-4.869906000	-0.398504000
C	-2.136228000	2.460751000	0.674161000
C	-2.241133000	3.901748000	0.158599000
H	-2.938703000	1.806546000	0.296579000
H	-2.514376000	3.896936000	-0.913270000
H	-2.191879000	2.441456000	1.778289000
H	-3.037916000	4.474064000	0.670903000
C	-0.874371000	4.579833000	0.310291000
C	0.166628000	3.688731000	-0.369830000
H	-0.878026000	5.607190000	-0.102851000
H	0.035156000	3.729354000	-1.466304000
H	-0.643758000	4.692429000	1.387267000

H	1.212661000	3.969097000	-0.152903000
C	1.231855000	2.221368000	2.097739000
C	0.307402000	1.359235000	2.571721000
H	2.147875000	1.871822000	1.610300000
H	0.421859000	0.269592000	2.498152000
H	1.141835000	3.298131000	2.258632000
H	-0.561033000	1.720785000	3.127956000
C	-2.391089000	-0.797994000	-0.690635000
C	-2.733601000	-1.185995000	0.617606000
C	-3.381133000	-0.842641000	-1.689494000
C	-4.030660000	-1.606401000	0.913381000
C	-4.677307000	-1.266426000	-1.390828000
C	-5.007055000	-1.647535000	-0.087077000
H	-1.982394000	-1.166510000	1.409631000
H	-3.127085000	-0.561723000	-2.714056000
H	-4.278659000	-1.904993000	1.934768000
H	-5.430458000	-1.304417000	-2.181732000
H	-6.021521000	-1.978774000	0.148372000
C	2.612782000	-0.074650000	-0.762100000
C	3.090919000	-0.419433000	0.516136000
C	3.551737000	0.232080000	-1.766467000
C	4.462226000	-0.446962000	0.778934000
C	4.921302000	0.203642000	-1.500710000
C	5.383088000	-0.132757000	-0.224610000
H	2.392960000	-0.688456000	1.310982000
H	3.205256000	0.474350000	-2.773404000
H	4.810699000	-0.723053000	1.777227000
H	5.631449000	0.436563000	-2.298045000
H	6.455441000	-0.158097000	-0.015911000

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E-5-q SCF Done: -1776.235808 A.U.

Cr	-0.384513000	1.284446000	0.090190000
Al	0.615043000	-1.498726000	-1.598552000
Cl	0.603810000	0.826758000	-2.074042000
N	0.476663000	-1.196343000	0.403534000
C	1.371615000	-0.352537000	1.066757000
C	0.697482000	0.317355000	2.096783000
C	-0.647837000	-0.148105000	2.091997000
C	-0.740531000	-1.116099000	1.072939000
H	1.151332000	1.000710000	2.811122000
H	-1.419870000	0.077229000	2.824747000
C	-1.046687000	-2.132380000	-2.431507000
H	-1.184644000	-3.223262000	-2.346326000

H	-0.968520000	-1.903566000	-3.510505000
H	-1.969300000	-1.655114000	-2.066257000
C	2.313495000	-2.246130000	-2.236419000
H	2.541160000	-3.224023000	-1.775953000
H	3.188800000	-1.598131000	-2.081509000
H	2.218741000	-2.423416000	-3.323036000
C	0.239780000	3.186774000	0.461533000
C	-0.773104000	4.190058000	1.027361000
H	1.091581000	3.079583000	1.158552000
H	-1.383458000	3.727971000	1.828784000
H	0.656996000	3.553198000	-0.495041000
H	-0.214030000	5.000664000	1.533246000
C	-1.701148000	4.855634000	-0.002802000
C	-2.929351000	4.074175000	-0.491067000
H	-2.075080000	5.797272000	0.436792000
H	-3.585593000	3.858275000	0.374107000
H	-1.093823000	5.159357000	-0.876310000
H	-3.509924000	4.758455000	-1.134815000
C	-2.703229000	2.769420000	-1.270701000
C	-2.329549000	1.549579000	-0.422267000
H	-3.643565000	2.546675000	-1.810745000
H	-2.919319000	1.537767000	0.515691000
H	-1.952881000	2.935400000	-2.066801000
H	-2.569314000	0.615424000	-0.965125000
C	2.825499000	-0.312627000	0.797573000
C	3.559244000	-1.511050000	0.730394000
C	3.517523000	0.908404000	0.703184000
C	4.945065000	-1.488551000	0.565884000
C	4.903796000	0.928354000	0.538178000
C	5.622177000	-0.269182000	0.468186000
H	3.036554000	-2.465070000	0.821595000
H	2.963858000	1.848266000	0.743988000
H	5.499294000	-2.429208000	0.517867000
H	5.424329000	1.885857000	0.457437000
H	6.707187000	-0.252134000	0.338451000
C	-1.853986000	-2.058338000	0.860281000
C	-3.190553000	-1.662388000	1.055146000
C	-1.589075000	-3.408866000	0.564302000
C	-4.229885000	-2.586364000	0.938158000
C	-2.630306000	-4.330155000	0.447168000
C	-3.955124000	-3.922550000	0.630502000
H	-3.418660000	-0.619735000	1.281507000
H	-0.555301000	-3.740823000	0.448233000

H	-5.262236000	-2.258502000	1.083312000
H	-2.404554000	-5.374963000	0.219591000
H	-4.770284000	-4.644510000	0.538615000

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E-6-q SCF Done: -1776.238808 A.U.

Cr	-0.290472000	1.077749000	0.422693000
Al	1.057176000	-1.658376000	1.408680000
Cl	-0.649448000	-0.340481000	2.372407000
N	0.713083000	-0.887367000	-0.456336000
C	-0.575627000	-0.844819000	-1.022650000
C	-0.672333000	0.278689000	-1.854461000
C	0.590756000	0.935618000	-1.820765000
C	1.446413000	0.161076000	-1.010465000
H	-1.537421000	0.550510000	-2.455447000
H	0.892591000	1.798602000	-2.410586000
C	2.695654000	-0.961795000	2.234963000
H	3.603377000	-1.506921000	1.927329000
H	2.589557000	-1.103734000	3.326387000
H	2.879117000	0.110711000	2.065140000
C	0.617745000	-3.558527000	1.623729000
H	1.161488000	-4.198885000	0.906329000
H	-0.452734000	-3.794206000	1.531737000
H	0.941362000	-3.871072000	2.632970000
C	-4.250030000	1.925296000	0.354356000
C	-3.884032000	2.910957000	-0.758625000
H	-4.916401000	1.131084000	-0.020762000
H	-3.367548000	2.376846000	-1.578032000
H	-4.781395000	2.436308000	1.174603000
H	-4.821294000	3.290787000	-1.202030000
C	-3.034647000	4.117472000	-0.322567000
C	-1.514809000	3.920205000	-0.199973000
H	-3.196712000	4.931523000	-1.050499000
H	-1.112036000	3.625743000	-1.188867000
H	-3.425613000	4.500947000	0.638681000
H	-1.079274000	4.921122000	-0.007911000
C	-1.015641000	2.968072000	0.884787000
C	0.405699000	2.851941000	1.145165000
H	-1.670858000	2.917570000	1.767820000
H	1.100637000	3.402909000	0.495728000
H	0.759864000	2.753339000	2.179474000
H	-3.362344000	1.444852000	0.792971000
C	-1.569948000	-1.932443000	-0.891049000
C	-2.921505000	-1.655879000	-0.619775000

C	-1.189499000	-3.262680000	-1.143728000
C	-3.865480000	-2.684073000	-0.595645000
C	-2.135109000	-4.289277000	-1.118504000
C	-3.475803000	-4.003898000	-0.843667000
H	-3.230889000	-0.631157000	-0.409160000
H	-0.146498000	-3.488288000	-1.373256000
H	-4.910314000	-2.452816000	-0.374026000
H	-1.822630000	-5.317117000	-1.318950000
H	-4.215378000	-4.808212000	-0.822656000
C	2.909629000	0.298276000	-0.884709000
C	3.729982000	-0.843215000	-0.945886000
C	3.518611000	1.564081000	-0.804824000
C	5.120136000	-0.722640000	-0.909800000
C	4.908506000	1.681540000	-0.772270000
C	5.714671000	0.539303000	-0.820991000
H	3.272750000	-1.830548000	-1.042651000
H	2.895302000	2.457989000	-0.744203000
H	5.742168000	-1.619866000	-0.958834000
H	5.365174000	2.671691000	-0.699158000
H	6.803012000	0.633266000	-0.792077000

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E-7-q SCF Done: -1854.755665 A.U.

Al	2.063773000	-2.283004000	0.097071000
Cl	1.908603000	-2.000587000	2.303172000
N	0.791521000	-0.759545000	-0.532638000
C	-0.488818000	-0.973079000	-1.011383000
C	-0.860964000	0.104014000	-1.852577000
C	0.252830000	0.986057000	-1.903305000
C	1.240598000	0.453287000	-1.059460000
H	-1.798693000	0.191795000	-2.395916000
H	0.325173000	1.919216000	-2.454894000
C	3.877777000	-1.936203000	-0.612197000
H	3.869011000	-1.557613000	-1.650389000
H	4.395972000	-2.912530000	-0.642925000
H	4.509609000	-1.254666000	-0.023627000
C	1.368012000	-4.027717000	-0.518041000
H	0.969790000	-3.992040000	-1.548182000
H	0.596528000	-4.492972000	0.112958000
H	2.229875000	-4.720099000	-0.541808000
C	0.220117000	2.325417000	2.176556000
C	-0.105106000	1.089590000	2.607818000
H	1.173641000	2.523426000	1.676365000
H	0.560682000	0.226023000	2.480121000

H	-0.419568000	3.188283000	2.378905000
H	-1.023988000	0.914764000	3.172939000
Cr	-0.897158000	1.223704000	0.192356000
C	-2.741758000	0.725040000	0.910720000
C	-3.977885000	1.000491000	0.043653000
H	-2.644579000	-0.356087000	1.121247000
H	-3.753246000	0.865730000	-1.032094000
H	-2.855300000	1.231625000	1.886259000
H	-4.746788000	0.236902000	0.265500000
C	-4.626920000	2.375232000	0.260322000
C	-3.895767000	3.612236000	-0.279474000
H	-5.630102000	2.360394000	-0.201439000
H	-3.835592000	3.547463000	-1.382488000
H	-4.803244000	2.508288000	1.344685000
H	-4.541077000	4.483835000	-0.072348000
C	-2.489512000	3.919035000	0.266337000
C	-1.346432000	3.140155000	-0.394415000
H	-2.305835000	4.998635000	0.105490000
H	-1.531309000	3.089337000	-1.482764000
H	-2.486967000	3.792780000	1.365868000
H	-0.384215000	3.675221000	-0.269418000
C	-1.346730000	-2.131013000	-0.685635000
C	-1.388060000	-2.696226000	0.602519000
C	-2.208312000	-2.644060000	-1.673928000
C	-2.265272000	-3.743219000	0.888625000
C	-3.082705000	-3.692842000	-1.385152000
C	-3.115955000	-4.244904000	-0.101243000
H	-0.726261000	-2.322731000	1.386466000
H	-2.176521000	-2.231356000	-2.684752000
H	-2.280918000	-4.170777000	1.894081000
H	-3.735634000	-4.084780000	-2.168938000
H	-3.799776000	-5.066508000	0.126113000
C	2.536822000	1.102013000	-0.760478000
C	3.144355000	1.033151000	0.507435000
C	3.157464000	1.881933000	-1.756375000
C	4.325998000	1.730092000	0.769356000
C	4.338821000	2.576114000	-1.492016000
C	4.926821000	2.506803000	-0.225362000
H	2.706203000	0.416927000	1.294500000
H	2.720736000	1.926826000	-2.756355000
H	4.782049000	1.657502000	1.759843000
H	4.806789000	3.167299000	-2.283142000
H	5.852901000	3.048452000	-0.017585000

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E-8-q SCF Done: -1854.796075 A.U.

C	5.399040000	1.363194000	0.227797000
C	5.617843000	-0.126311000	-0.097606000
H	6.396188000	1.827369000	0.323654000
H	6.099572000	-0.207856000	-1.089498000
H	4.948925000	1.460687000	1.230220000
H	6.357521000	-0.519989000	0.623591000
Cr	0.972443000	0.226061000	0.331529000
Al	-2.184852000	-0.388172000	1.482112000
Cl	-0.321367000	0.828400000	2.295364000
N	-1.558982000	-0.267398000	-0.444746000
C	-1.179771000	0.954790000	-1.000488000
C	-0.081629000	0.758329000	-1.849735000
C	0.203234000	-0.636312000	-1.851828000
C	-0.752986000	-1.247976000	-1.016911000
H	0.392483000	1.522654000	-2.460752000
H	0.908391000	-1.156722000	-2.496572000
C	-1.937733000	-2.163496000	2.286296000
H	-2.764417000	-2.859150000	2.065659000
H	-1.928533000	-2.015554000	3.382124000
H	-0.998597000	-2.674324000	2.021741000
C	-3.814217000	0.611103000	1.928532000
H	-4.683696000	0.279828000	1.332835000
H	-3.732749000	1.702195000	1.814315000
H	-4.060128000	0.404471000	2.985865000
C	2.224692000	1.836034000	0.250078000
C	3.112095000	1.880073000	-1.003505000
H	1.618227000	2.750219000	0.365970000
H	3.057374000	0.925040000	-1.557631000
H	2.804246000	1.726159000	1.181591000
H	2.706583000	2.626102000	-1.709790000
C	4.603890000	2.216176000	-0.777139000
C	4.382814000	-1.044885000	-0.074839000
H	5.115632000	2.181589000	-1.757020000
H	3.693262000	-0.747317000	-0.879536000
H	4.669148000	3.266938000	-0.441446000
H	4.706255000	-2.065768000	-0.344998000
C	3.611243000	-1.097974000	1.259986000
C	2.104328000	-1.321294000	1.096271000
H	4.045335000	-1.899662000	1.888668000
H	1.914674000	-2.215262000	0.474492000
H	3.780260000	-0.173279000	1.834807000

H	1.631970000	-1.511569000	2.077136000
C	-1.935833000	2.211883000	-0.829901000
C	-3.340658000	2.205514000	-0.906501000
C	-1.274448000	3.447771000	-0.704537000
C	-4.062631000	3.398549000	-0.845737000
C	-1.998401000	4.639396000	-0.644480000
C	-3.395077000	4.619551000	-0.712737000
H	-3.865787000	1.257118000	-1.030689000
H	-0.185432000	3.472480000	-0.639219000
H	-5.153389000	3.373621000	-0.908540000
H	-1.467980000	5.588892000	-0.537515000
H	-3.961045000	5.553188000	-0.664525000
C	-1.041176000	-2.690284000	-0.927600000
C	-2.371309000	-3.141028000	-0.827565000
C	-0.017824000	-3.648483000	-1.056854000
C	-2.664846000	-4.504984000	-0.829574000
C	-0.313791000	-5.012113000	-1.059607000
C	-1.637665000	-5.446779000	-0.940992000
H	-3.182919000	-2.412934000	-0.772190000
H	1.020185000	-3.323295000	-1.144425000
H	-3.704204000	-4.833827000	-0.752500000
H	0.496244000	-5.739976000	-1.150878000
H	-1.868167000	-6.514945000	-0.942004000

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E-9-q SCF Done: -1697.675149 A.U.

Cr	-0.119930000	1.356406000	0.469291000
Al	0.347896000	-1.712969000	1.340918000
Cl	-0.739847000	0.063703000	2.440093000
N	0.240946000	-0.764696000	-0.470875000
C	-0.971954000	-0.305658000	-1.021933000
C	-0.714072000	0.818348000	-1.817983000
C	0.693186000	1.045023000	-1.782155000
C	1.265246000	0.020022000	-1.005710000
H	-1.452030000	1.366718000	-2.398886000
H	1.248770000	1.790472000	-2.347124000
C	2.150329000	-1.706754000	2.117132000
H	2.795433000	-2.511332000	1.726701000
H	2.030376000	-1.889957000	3.201075000
H	2.700702000	-0.759204000	2.008902000
C	-0.740746000	-3.337886000	1.494461000
H	-0.483321000	-4.091911000	0.729355000
H	-1.826176000	-3.167857000	1.438854000
H	-0.526135000	-3.798297000	2.475799000

C	-2.488653000	4.185859000	-0.648613000
C	-1.020068000	4.289336000	-0.230802000
H	-2.748567000	4.935521000	-1.413615000
H	-0.368732000	4.153097000	-1.114573000
H	-3.156792000	4.347745000	0.213954000
H	-0.826077000	5.326633000	0.109752000
C	-0.606252000	3.324057000	0.867752000
C	0.789566000	3.057147000	1.150323000
H	-1.282389000	3.341537000	1.737974000
H	1.547868000	3.503129000	0.490709000
H	1.123437000	2.950751000	2.190669000
H	-2.723672000	3.190179000	-1.059903000
C	-2.271803000	-0.999341000	-0.881005000
C	-3.432374000	-0.291507000	-0.519808000
C	-2.384813000	-2.361785000	-1.209232000
C	-4.672218000	-0.932174000	-0.482863000
C	-3.625449000	-3.000708000	-1.170588000
C	-4.772449000	-2.288672000	-0.807073000
H	-3.357385000	0.765078000	-0.252633000
H	-1.494078000	-2.917951000	-1.507755000
H	-5.563047000	-0.369806000	-0.192440000
H	-3.696574000	-4.059895000	-1.430001000
H	-5.743007000	-2.790091000	-0.776450000
C	2.702600000	-0.289250000	-0.880943000
C	3.648842000	0.733953000	-0.688775000
C	3.157830000	-1.608894000	-1.054002000
C	5.013065000	0.441168000	-0.660836000
C	4.522922000	-1.898712000	-1.022615000
C	5.455030000	-0.875774000	-0.825174000
H	3.306450000	1.759782000	-0.536744000
H	2.435694000	-2.409070000	-1.231593000
H	5.735220000	1.245535000	-0.500312000
H	4.860415000	-2.929085000	-1.159632000
H	6.523476000	-1.103731000	-0.799810000

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E-2-3-q SCF Done: -1697.621487 A.U.

Cr	0.009857000	1.979245000	-0.108597000
Al	-0.013867000	-2.196837000	0.777056000
Cl	-0.021417000	-0.939245000	2.631500000
N	-0.000772000	-0.608183000	-0.533952000
C	-1.114764000	0.002307000	-1.095603000
C	-0.697589000	0.953000000	-2.057677000
C	0.718652000	0.943571000	-2.055458000

C	1.120246000	-0.015731000	-1.094433000
H	-1.360079000	1.560555000	-2.670341000
H	1.391194000	1.539344000	-2.668812000
C	1.614458000	-3.300469000	0.566201000
H	1.944381000	-3.388601000	-0.484714000
H	1.351742000	-4.322108000	0.896913000
H	2.490428000	-2.986949000	1.153033000
C	-1.646375000	-3.289228000	0.540789000
H	-1.964486000	-3.368440000	-0.514481000
H	-2.527255000	-2.973551000	1.119082000
H	-1.394428000	-4.314659000	0.868065000
C	-1.726902000	2.908587000	0.457384000
C	-0.961136000	2.857777000	1.695754000
H	-2.572014000	2.222484000	0.339101000
H	-1.021268000	1.913525000	2.258702000
H	-1.912332000	3.906172000	0.035220000
H	-0.998275000	3.710779000	2.376335000
C	1.006731000	3.313117000	1.506865000
C	1.761963000	2.935981000	0.332478000
H	1.289561000	2.850993000	2.459023000
H	2.566672000	2.201886000	0.443656000
H	0.796182000	4.381055000	1.604706000
H	1.980511000	3.722428000	-0.401875000
C	2.533061000	-0.359750000	-0.805184000
C	3.413760000	-0.546848000	-1.886763000
C	3.046660000	-0.426119000	0.502377000
C	4.769566000	-0.800408000	-1.668852000
C	4.403813000	-0.673494000	0.716681000
C	5.269389000	-0.861685000	-0.365142000
H	5.435916000	-0.954621000	-2.521225000
H	4.785809000	-0.721974000	1.739371000
C	-2.533014000	-0.327699000	-0.816500000
C	-3.409552000	-0.493559000	-1.905452000
C	-3.056354000	-0.402512000	0.486676000
C	-4.769240000	-0.734339000	-1.698931000
C	-4.417569000	-0.637115000	0.689777000
C	-5.278234000	-0.804202000	-0.399069000
H	-5.431627000	-0.872181000	-2.557172000
H	-4.806237000	-0.692028000	1.709605000
H	-3.015728000	-0.450964000	-2.923654000
H	-6.342422000	-0.991131000	-0.234778000
H	-2.396773000	-0.281497000	1.348131000
H	2.381368000	-0.287397000	1.357212000

H	6.330406000	-1.058446000	-0.192069000
H	3.026537000	-0.510323000	-2.907787000

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E-3-9-q SCF Done: -1697.612136 A.U.

Cr	-0.077738000	1.747612000	-0.424196000
Al	-0.047729000	-1.454526000	1.598455000
Cl	0.778603000	0.321869000	2.684763000
N	-0.035137000	-0.659008000	-0.319822000
C	-1.164732000	-0.266618000	-1.050001000
C	-0.756446000	0.366444000	-2.239663000
C	0.660011000	0.331062000	-2.261362000
C	1.084142000	-0.318439000	-1.086515000
H	-1.423233000	0.740938000	-3.013161000
H	1.317121000	0.714440000	-3.039186000
C	1.136297000	-3.031034000	1.560828000
H	0.801051000	-3.763455000	0.802978000
H	1.081688000	-3.545559000	2.537404000
H	2.198720000	-2.821929000	1.362243000
C	-1.857504000	-1.694564000	2.339943000
H	-2.373674000	-2.610791000	2.010783000
H	-2.540744000	-0.846480000	2.171113000
H	-1.721771000	-1.778363000	3.434687000
H	-0.224189000	3.064578000	-1.369954000
C	-1.391088000	2.751390000	0.801591000
C	-0.745403000	4.146323000	0.640558000
H	-2.444455000	2.739161000	0.486251000
H	-1.395252000	4.834302000	0.078956000
H	-1.314078000	2.339441000	1.819359000
H	-0.507972000	4.630468000	1.604756000
C	0.553360000	3.926114000	-0.130420000
C	1.490380000	3.032437000	0.391582000
H	0.841689000	4.633023000	-0.916282000
H	2.473490000	2.922251000	-0.075047000
H	1.385906000	2.666740000	1.417963000
C	-2.555430000	-0.716292000	-0.788726000
C	-3.629413000	0.188691000	-0.770643000
C	-2.829269000	-2.093399000	-0.715310000
C	-4.943747000	-0.271518000	-0.660256000
C	-4.143079000	-2.551061000	-0.606909000
C	-5.204639000	-1.641852000	-0.575566000
H	-5.767380000	0.446416000	-0.636771000
H	-4.337931000	-3.624790000	-0.549493000
C	2.501501000	-0.699352000	-0.836749000

C	3.170154000	-1.368701000	-1.881402000
C	3.220755000	-0.392054000	0.330615000
C	4.514739000	-1.724497000	-1.761719000
C	4.566755000	-0.748001000	0.445657000
C	5.219297000	-1.413445000	-0.595708000
H	5.010169000	-2.251353000	-2.581143000
H	5.107493000	-0.500674000	1.362575000
H	6.271933000	-1.690961000	-0.498167000
H	2.622349000	-1.626912000	-2.790734000
H	2.726622000	0.118298000	1.157140000
H	-3.432294000	1.260073000	-0.832371000
H	-2.006156000	-2.810171000	-0.756306000
H	-6.233029000	-2.001058000	-0.487978000

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E-4-5-q SCF Done: -1776.168154 A.U.

Cr	-0.108586000	1.604449000	0.080525000
Al	0.363408000	-2.017909000	1.295122000
Cl	-0.730119000	-0.834310000	2.834647000
N	0.169937000	-0.777938000	-0.372837000
C	-1.008488000	-0.388858000	-1.022958000
C	-0.683668000	0.531903000	-2.042284000
C	0.725122000	0.658406000	-2.068205000
C	1.229075000	-0.163902000	-1.049653000
H	-1.401401000	0.999167000	-2.713046000
H	1.328888000	1.237136000	-2.764556000
C	2.213619000	-2.114573000	1.980748000
H	2.853435000	-2.853015000	1.471748000
H	2.115743000	-2.445119000	3.031782000
H	2.766550000	-1.161143000	2.005007000
C	-0.494339000	-3.720271000	0.784269000
H	-1.573650000	-3.657485000	0.574721000
H	-0.363126000	-4.454772000	1.599519000
H	-0.013708000	-4.157220000	-0.111037000
C	-1.904364000	2.238675000	0.863567000
C	-2.364688000	3.460867000	0.070368000
H	-2.646380000	1.426216000	0.855589000
H	-2.688371000	3.153746000	-0.942351000
H	-1.709322000	2.498413000	1.919593000
H	-3.245172000	3.953032000	0.525823000
C	-1.207940000	4.456868000	-0.058267000
C	0.065101000	3.751263000	-0.512935000
H	-1.455687000	5.273662000	-0.762384000
H	-0.102134000	3.214521000	-1.469490000

H	-1.030352000	4.948960000	0.915871000
H	0.885395000	4.447569000	-0.720984000
C	1.274087000	3.199930000	1.161907000
C	1.173613000	1.902687000	1.710552000
H	2.196875000	3.468134000	0.640625000
H	2.014108000	1.211380000	1.591493000
H	0.796375000	4.038809000	1.673655000
H	0.541619000	1.721966000	2.583488000
C	2.667114000	-0.497431000	-0.903679000
C	3.633429000	0.510998000	-0.745335000
C	3.100948000	-1.822643000	-1.083175000
C	4.995593000	0.201354000	-0.742459000
C	4.462008000	-2.130775000	-1.082989000
C	5.413802000	-1.121622000	-0.908465000
H	5.732214000	0.997485000	-0.608399000
H	4.780746000	-3.166544000	-1.223214000
C	-2.362299000	-0.990555000	-0.885329000
C	-3.033259000	-1.218255000	0.328474000
C	-3.020188000	-1.335093000	-2.085494000
C	-4.316405000	-1.770918000	0.336362000
C	-4.301996000	-1.886419000	-2.073285000
C	-4.957627000	-2.105673000	-0.858870000
H	-4.817090000	-1.937973000	1.293258000
H	-4.784697000	-2.153006000	-3.016937000
H	-5.961128000	-2.538585000	-0.844623000
H	-2.509514000	-1.191736000	-3.040162000
H	-2.556240000	-0.963345000	1.274015000
H	3.316634000	1.549049000	-0.621472000
H	6.479018000	-1.365434000	-0.905756000
H	2.365113000	-2.614766000	-1.237298000

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E-5-6-q SCF Done: -1776.191459 A.U.

Cr	-0.196779000	1.465903000	-0.482264000
Al	0.491667000	-2.229532000	1.242939000
Cl	0.158414000	-0.517213000	2.658018000
N	0.284617000	-1.067757000	-0.434807000
C	-0.899694000	-0.801000000	-1.118519000
C	-0.617380000	-0.006975000	-2.253283000
C	0.773695000	0.253603000	-2.238656000
C	1.301396000	-0.403581000	-1.102251000
H	-1.349334000	0.328738000	-2.985567000
H	1.353624000	0.830029000	-2.955968000
C	2.300337000	-3.024877000	1.355293000

H	2.197695000	-3.979139000	1.903531000
H	3.053888000	-2.426242000	1.888474000
H	2.728079000	-3.275897000	0.368162000
C	-0.908865000	-3.627054000	1.324631000
H	-0.459324000	-4.506529000	1.820794000
H	-1.251970000	-3.968158000	0.331873000
H	-1.808686000	-3.359200000	1.899157000
C	-2.249996000	2.113847000	0.125297000
C	-2.697528000	3.586514000	0.077737000
H	-2.717859000	1.540920000	-0.689932000
H	-2.601856000	3.967476000	-0.955790000
H	-2.559911000	1.638380000	1.069853000
H	-3.771607000	3.654854000	0.325578000
C	-1.893591000	4.506976000	1.011658000
C	-0.403454000	4.558590000	0.638946000
H	-2.312504000	5.526159000	0.976565000
H	-0.309489000	4.927851000	-0.398043000
H	-2.005345000	4.164283000	2.057452000
H	0.121358000	5.292925000	1.274140000
C	0.332728000	3.215941000	0.750013000
C	1.327633000	2.849994000	-0.231386000
H	0.545885000	2.913608000	1.786279000
H	1.461673000	3.508480000	-1.100135000
H	2.247629000	2.356434000	0.094779000
H	-0.908798000	2.486866000	0.567095000
C	2.745672000	-0.425850000	-0.759984000
C	3.666287000	-0.720219000	-1.782935000
C	3.238111000	-0.089013000	0.513237000
C	5.041073000	-0.685021000	-1.540543000
C	4.613274000	-0.049024000	0.751036000
C	5.518944000	-0.346085000	-0.271815000
H	5.739805000	-0.926671000	-2.345395000
H	4.978292000	0.214990000	1.746658000
C	-2.244653000	-1.342804000	-0.803013000
C	-2.831581000	-1.246859000	0.470835000
C	-2.996211000	-1.911371000	-1.849658000
C	-4.130082000	-1.711018000	0.688159000
C	-4.293485000	-2.377759000	-1.628471000
C	-4.865383000	-2.277376000	-0.357055000
H	-4.569045000	-1.629681000	1.685641000
H	-4.856176000	-2.825828000	-2.451299000
H	2.543988000	0.141667000	1.323675000
H	3.297604000	-0.994265000	-2.774315000

H	6.594379000	-0.315913000	-0.079463000
H	-2.549173000	-2.004824000	-2.842210000
H	-5.880682000	-2.641487000	-0.180640000
H	-2.269940000	-0.808120000	1.296906000

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E-7-8-q SCF Done: -1854.727285 A.U.

C	3.927429000	-3.509064000	-0.345062000
C	2.512224000	-4.100583000	-0.281440000
H	4.098679000	-3.101429000	-1.359616000
H	2.451076000	-4.884805000	-1.057676000
H	4.628747000	-4.356010000	-0.249688000
H	2.381068000	-4.641483000	0.673071000
Cr	0.716840000	-1.114121000	0.089452000
Al	-1.660106000	1.727312000	1.218869000
Cl	0.193273000	2.001193000	2.375792000
N	-0.853882000	0.780468000	-0.463757000
C	0.355418000	1.041554000	-1.112783000
C	0.589362000	0.032833000	-2.072785000
C	-0.535633000	-0.828260000	-2.058117000
C	-1.413834000	-0.341517000	-1.078571000
H	1.422535000	0.012635000	-2.771864000
H	-0.730682000	-1.670222000	-2.719192000
C	-2.853055000	0.562162000	2.284027000
H	-2.948921000	1.080269000	3.257668000
H	-2.491187000	-0.451035000	2.514303000
H	-3.872350000	0.466666000	1.876897000
C	-2.550249000	3.401069000	0.608271000
H	-2.720251000	3.471390000	-0.481862000
H	-2.001523000	4.310897000	0.906903000
H	-3.545480000	3.465945000	1.084156000
C	2.480122000	-0.596458000	1.005689000
C	3.854201000	-0.993139000	0.451097000
H	2.391650000	0.502758000	1.046586000
H	3.929556000	-0.771916000	-0.631844000
H	2.397585000	-0.934592000	2.054796000
H	4.605445000	-0.329315000	0.919578000
C	4.333291000	-2.441031000	0.685365000
C	1.361927000	-3.122696000	-0.523757000
H	5.436368000	-2.422398000	0.692492000
H	1.727618000	-2.374256000	-1.260906000
H	4.044439000	-2.767710000	1.702281000
H	0.495922000	-3.618527000	-0.984557000
C	0.557346000	-3.030832000	1.432196000

C	-0.255374000	-1.921669000	1.752792000
H	0.088722000	-3.982325000	1.168881000
H	-1.331874000	-1.988142000	1.572856000
H	1.515005000	-3.138216000	1.944649000
H	0.051522000	-1.228302000	2.542387000
C	1.182751000	2.260733000	-0.978822000
C	2.574652000	2.190672000	-1.182603000
C	0.603236000	3.524108000	-0.775302000
C	3.360750000	3.342749000	-1.164056000
C	1.391159000	4.676073000	-0.756602000
C	2.772507000	4.592345000	-0.946765000
H	4.440354000	3.262025000	-1.313926000
H	0.916470000	5.646759000	-0.593702000
C	-2.798005000	-0.820768000	-0.873480000
C	-3.078171000	-2.197542000	-0.797960000
C	-3.874722000	0.084043000	-0.876808000
C	-4.394130000	-2.655988000	-0.712656000
C	-5.189947000	-0.375840000	-0.792234000
C	-5.455238000	-1.745762000	-0.707139000
H	-4.591288000	-3.728983000	-0.646863000
H	-6.012976000	0.342938000	-0.796997000
H	3.052015000	1.222975000	-1.342627000
H	3.387969000	5.495244000	-0.927739000
H	-0.472972000	3.611657000	-0.644735000
H	-3.681464000	1.154943000	-0.962718000
H	-2.255546000	-2.916960000	-0.801072000
H	-6.485593000	-2.103340000	-0.639199000

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F-0-s SCF Done: -1277.083129 A.U.

Cr	-1.426360000	-0.011232000	1.348412000
Al	1.749527000	0.002059000	-0.271005000
Cl	0.925171000	-0.017071000	1.977129000
N	-0.089209000	0.008862000	-1.094940000
C	-0.927677000	-1.075394000	-1.035826000
C	-2.256808000	-0.719127000	-0.858896000
C	-2.256274000	0.734772000	-0.848147000
C	-0.927005000	1.092730000	-1.019794000
H	-3.116069000	-1.386126000	-0.884214000
H	-3.115011000	1.402757000	-0.862834000
C	2.629362000	1.730774000	-0.542782000
H	2.810709000	1.917645000	-1.616558000
H	3.614723000	1.742466000	-0.044821000
H	2.051599000	2.584829000	-0.155814000

C	2.630188000	-1.720967000	-0.574641000
H	2.808150000	-1.888972000	-1.652107000
H	2.054989000	-2.582479000	-0.200607000
H	3.617267000	-1.739879000	-0.080316000
F	-0.428091000	-2.298335000	-1.128884000
F	-0.426546000	2.316555000	-1.094189000

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F-1-q SCF Done: -1355.628994 A.U.

Cr	-1.256667000	0.433535000	-0.048536000
Al	2.095093000	0.305504000	0.052667000
Cl	0.553722000	2.066908000	-0.190234000
N	0.572597000	-1.055182000	0.046503000
C	-0.214466000	-1.425171000	1.118606000
C	-1.434795000	-1.940183000	0.710725000
C	-1.379401000	-1.975199000	-0.735391000
C	-0.137178000	-1.464295000	-1.069114000
H	-2.228292000	-2.311770000	1.354344000
H	-2.124309000	-2.372586000	-1.420019000
C	3.134571000	0.138691000	-1.596336000
H	3.638662000	-0.842867000	-1.652901000
H	3.928256000	0.905783000	-1.624708000
H	2.531747000	0.252457000	-2.510741000
C	2.881744000	0.396359000	1.841946000
H	3.378482000	-0.552922000	2.111373000
H	2.152673000	0.622982000	2.635607000
H	3.657911000	1.181208000	1.872695000
C	-2.896745000	1.373972000	0.733976000
C	-3.003083000	1.276475000	-0.703294000
H	-3.535666000	0.742280000	1.365165000
H	-3.720722000	0.571091000	-1.142772000
H	-2.636042000	2.335479000	1.194894000
H	-2.826168000	2.165775000	-1.322322000
F	0.224019000	-1.241398000	2.351412000
F	0.396198000	-1.326197000	-2.271263000

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F-2-q SCF Done: -1434.175792 A.U.

Cr	1.507897000	0.000103000	0.093051000
Al	-2.313766000	-0.001173000	-0.629436000
Cl	-0.452768000	-0.003876000	-1.942845000
N	-1.155901000	0.001828000	1.045948000
C	-0.443017000	-1.073780000	1.492624000
C	0.692870000	-0.715741000	2.215336000
C	0.692660000	0.723534000	2.213114000

C	-0.443352000	1.079011000	1.489357000
H	1.354524000	-1.387650000	2.756104000
H	1.354157000	1.397329000	2.751717000
C	-3.271342000	1.709419000	-0.747203000
H	-3.963808000	1.844541000	0.103385000
H	-3.888423000	1.735264000	-1.663052000
H	-2.608822000	2.589194000	-0.774224000
C	-3.271712000	-1.711997000	-0.740486000
H	-3.962619000	-1.844501000	0.111781000
H	-2.609077000	-2.591742000	-0.765813000
H	-3.890378000	-1.740833000	-1.655157000
C	2.107978000	-2.028392000	-0.361831000
C	2.846616000	-1.309266000	-1.291072000
H	1.165223000	-2.504924000	-0.650264000
H	2.487635000	-1.196240000	-2.315895000
H	2.592451000	-2.430188000	0.535090000
H	3.915670000	-1.145242000	-1.141287000
C	2.846326000	1.305703000	-1.294890000
C	2.107158000	2.027396000	-0.368071000
H	2.487693000	1.189403000	-2.319460000
H	1.164322000	2.502696000	-0.658270000
H	3.915383000	1.142473000	-1.144260000
H	2.591237000	2.432244000	0.527677000
F	-0.866960000	-2.297970000	1.243253000
F	-0.867762000	2.302274000	1.236394000

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F-3-q SCF Done: -1434.197616 A.U.

Cr	1.059990000	-0.012188000	-0.057626000
Al	-2.361899000	-0.726921000	0.097031000
Cl	-0.371715000	-1.969187000	-0.234387000
N	-1.318746000	1.013572000	0.042854000
C	-0.589859000	1.542664000	1.078468000
C	0.480631000	2.310542000	0.634171000
C	0.385686000	2.296969000	-0.804239000
C	-0.722778000	1.515292000	-1.090925000
H	1.180847000	2.865646000	1.253514000
H	1.010544000	2.824789000	-1.520212000
C	-3.472242000	-0.898727000	-1.504221000
H	-4.240515000	-0.105341000	-1.539466000
H	-4.010411000	-1.862686000	-1.496313000
H	-2.901072000	-0.845282000	-2.444030000
C	-2.996015000	-1.065759000	1.916609000
H	-3.740851000	-0.311618000	2.228111000

H	-2.195315000	-1.068851000	2.672806000
H	-3.498526000	-2.047849000	1.963670000
C	2.383483000	-0.510959000	1.420153000
C	3.766517000	-0.521075000	0.755652000
H	2.322297000	0.148497000	2.303585000
H	4.154679000	0.512967000	0.680925000
H	2.080004000	-1.527980000	1.730771000
H	4.511357000	-1.078757000	1.355243000
C	3.636389000	-1.104394000	-0.659758000
C	2.551588000	-0.327299000	-1.414016000
H	4.606449000	-1.090275000	-1.193007000
H	2.909818000	0.682706000	-1.695900000
H	3.347222000	-2.168967000	-0.585030000
H	2.188132000	-0.831946000	-2.325678000
F	-0.940577000	1.291612000	2.327220000
F	-1.220506000	1.220062000	-2.279902000

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F-4-q SCF Done: -1512.731827 A.U.

Cr	-1.255184000	0.214709000	-0.013631000
Al	2.801350000	-0.011611000	0.584715000
Cl	0.821049000	0.682669000	1.599842000
N	1.709039000	-0.625543000	-0.986572000
C	0.775003000	-1.595592000	-0.837262000
C	-0.402000000	-1.339691000	-1.540530000
C	-0.130469000	-0.107105000	-2.263204000
C	1.141938000	0.253173000	-1.877806000
H	-1.206156000	-2.050718000	-1.713224000
H	-0.748138000	0.375227000	-3.016505000
C	3.884402000	1.556142000	0.115992000
H	4.663421000	1.292840000	-0.622087000
H	4.410717000	1.935646000	1.009719000
H	3.305438000	2.392127000	-0.307089000
C	3.553008000	-1.536041000	1.560972000
H	4.282218000	-2.085285000	0.938222000
H	2.794672000	-2.261159000	1.895492000
H	4.098860000	-1.189551000	2.456242000
C	-2.132429000	-1.027259000	1.370330000
C	-3.429283000	-1.574501000	0.772747000
H	-1.408468000	-1.804102000	1.670144000
H	-3.199042000	-2.400030000	0.073654000
H	-2.324226000	-0.387963000	2.252055000
H	-4.095591000	-2.010791000	1.542088000
C	-4.120581000	-0.445269000	-0.000875000

C	-3.104818000	0.168096000	-0.976940000
H	-5.034627000	-0.802502000	-0.512957000
H	-3.005912000	-0.474155000	-1.870707000
H	-4.465642000	0.318544000	0.721342000
H	-3.413845000	1.165982000	-1.340496000
C	-1.437330000	2.784496000	0.202358000
C	-2.123040000	2.360647000	1.280348000
H	-0.362708000	2.981129000	0.259427000
H	-1.622441000	2.191041000	2.237590000
H	-1.939852000	3.004807000	-0.743753000
H	-3.205271000	2.213458000	1.247851000
F	1.815904000	1.329919000	-2.243833000
F	1.008090000	-2.620559000	-0.042749000

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F-5-q SCF Done: -1512.767084 A.U.

Cr	-0.726890000	-0.030118000	0.082895000
Al	2.754437000	-0.276770000	-0.766054000
Cl	0.674594000	-0.991971000	-1.660815000
N	1.830685000	0.458221000	0.870254000
C	1.132202000	1.637498000	0.912530000
C	0.084741000	1.605983000	1.823496000
C	0.150404000	0.297927000	2.426887000
C	1.226911000	-0.329490000	1.817777000
H	-0.577515000	2.429636000	2.079209000
H	-0.456539000	-0.096652000	3.237832000
C	3.804701000	-1.865424000	-0.314715000
H	4.640735000	-1.606502000	0.359834000
H	4.253553000	-2.300323000	-1.224890000
H	3.218555000	-2.656796000	0.177600000
C	3.424381000	1.185540000	-1.881250000
H	4.227805000	1.741644000	-1.365475000
H	2.651465000	1.916401000	-2.166007000
H	3.861561000	0.784557000	-2.812503000
C	-1.830441000	1.256798000	-1.009466000
C	-3.217568000	1.539388000	-0.421660000
H	-1.222606000	2.179926000	-1.065881000
H	-3.169932000	1.637484000	0.683386000
H	-1.899362000	0.851282000	-2.034310000
H	-3.554281000	2.534643000	-0.769856000
C	-4.314944000	0.528581000	-0.793654000
C	-4.340267000	-0.830570000	-0.076031000
H	-5.291461000	1.008414000	-0.605391000
H	-4.460798000	-0.664767000	1.011852000

H	-4.275657000	0.358288000	-1.885941000
H	-5.266252000	-1.338403000	-0.396970000
C	-3.167862000	-1.804377000	-0.299247000
C	-1.937157000	-1.572970000	0.581731000
H	-3.546265000	-2.824921000	-0.097570000
H	-2.240285000	-1.436281000	1.638216000
H	-2.887197000	-1.813842000	-1.369294000
H	-1.258176000	-2.446616000	0.549332000
F	1.484125000	2.641467000	0.126907000
F	1.684412000	-1.549652000	2.047510000

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F-6-q SCF Done: -1512.767132 A.U.

Cr	-0.448663000	-0.563376000	-0.286167000
Al	2.717585000	0.599148000	-0.460857000
Cl	0.885423000	0.684610000	-1.932470000
N	1.524653000	-0.118711000	1.028553000
C	0.534540000	0.615964000	1.660561000
C	-0.434127000	-0.189870000	2.229267000
C	-0.020440000	-1.543934000	1.943347000
C	1.191681000	-1.429865000	1.271030000
H	-1.303180000	0.136298000	2.794427000
H	-0.491099000	-2.467030000	2.272446000
C	3.932760000	-0.816558000	-1.053727000
H	4.646623000	-1.094781000	-0.257953000
H	4.532837000	-0.461275000	-1.909980000
H	3.420103000	-1.738026000	-1.372321000
C	3.288000000	2.422611000	-0.038738000
H	3.942748000	2.436519000	0.851331000
H	2.451241000	3.111082000	0.156564000
H	3.876878000	2.843065000	-0.872719000
C	-2.722719000	2.294503000	-0.196008000
C	-3.777085000	1.446231000	0.517999000
H	-2.362765000	3.114917000	0.445351000
H	-3.363173000	1.050657000	1.464555000
H	-3.132427000	2.744199000	-1.115545000
H	-4.606049000	2.110607000	0.818861000
C	-4.364107000	0.281469000	-0.298568000
C	-3.537512000	-1.013062000	-0.388078000
H	-5.339482000	0.013466000	0.143064000
H	-3.324148000	-1.379911000	0.635709000
H	-4.591255000	0.635587000	-1.321651000
H	-4.195429000	-1.787837000	-0.830443000
C	-2.251102000	-0.970004000	-1.202290000

C	-1.367906000	-2.115597000	-1.236686000
H	-2.331824000	-0.387842000	-2.133521000
H	-1.603528000	-2.982488000	-0.603219000
H	-0.853620000	-2.378312000	-2.170216000
H	-1.844996000	1.701404000	-0.499728000
F	0.611921000	1.936621000	1.675192000
F	1.983100000	-2.401834000	0.854540000

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F-7-q SCF Done: -1591.294100 A.U.

Al	-3.109720000	0.612584000	0.331820000
Cl	-2.259351000	-0.455541000	2.087100000
N	-1.528973000	0.249923000	-0.956000000
C	-0.530144000	1.085205000	-1.348231000
C	0.443156000	0.441159000	-2.117271000
C	-0.036095000	-0.915305000	-2.259363000
C	-1.221352000	-0.949714000	-1.540538000
H	1.281213000	0.913146000	-2.623495000
H	0.396382000	-1.721098000	-2.847056000
C	-4.651300000	-0.319095000	-0.463528000
H	-4.874119000	0.054653000	-1.479831000
H	-5.557371000	-0.137482000	0.141975000
H	-4.523996000	-1.411694000	-0.534183000
C	-3.175046000	2.557979000	0.618510000
H	-3.347946000	3.118491000	-0.317571000
H	-2.266303000	2.970272000	1.087180000
H	-4.019591000	2.797418000	1.289836000
C	0.990681000	-2.012545000	1.995402000
C	0.281351000	-2.646156000	1.038234000
H	2.065490000	-2.170978000	2.121250000
H	0.748429000	-3.359586000	0.351960000
H	0.482936000	-1.361817000	2.712487000
H	-0.805247000	-2.520877000	0.989597000
Cr	0.993095000	-0.548245000	-0.077094000
C	1.519537000	0.967332000	1.172679000
C	2.463969000	2.040817000	0.622116000
H	0.529646000	1.397281000	1.421092000
H	2.219661000	2.283514000	-0.429555000
H	1.923758000	0.549363000	2.111557000
H	2.283792000	2.983762000	1.172708000
C	3.961738000	1.726518000	0.733826000
C	4.547666000	0.647641000	-0.188635000
H	4.518109000	2.660366000	0.539661000
H	4.366279000	0.928222000	-1.243846000

H	4.189691000	1.460861000	1.783636000
H	5.643648000	0.680565000	-0.063017000
C	4.091681000	-0.807949000	0.026510000
C	2.814424000	-1.224315000	-0.708508000
H	4.910406000	-1.467340000	-0.320604000
H	2.906241000	-0.964477000	-1.779012000
H	4.008207000	-1.007286000	1.111284000
H	2.692056000	-2.325314000	-0.665872000
F	-0.548231000	2.354690000	-1.004121000
F	-2.015004000	-1.989174000	-1.359158000

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F-8-q SCF Done: -1591.328443 A.U.

C	-4.614612000	0.505576000	-1.027666000
C	-4.919075000	-0.758261000	-0.203064000
H	-5.554858000	0.804099000	-1.523007000
H	-5.651908000	-0.500828000	0.583567000
H	-3.931478000	0.254686000	-1.857379000
H	-5.436670000	-1.474831000	-0.866866000
Cr	-0.319785000	-0.083550000	0.051098000
Al	3.205969000	-0.165817000	-0.779528000
Cl	1.129772000	-0.353028000	-1.901892000
N	2.256595000	0.286706000	0.941652000
C	1.572525000	1.458704000	1.141198000
C	0.496611000	1.312808000	2.003433000
C	0.510460000	-0.075132000	2.391446000
C	1.600486000	-0.625660000	1.725668000
H	-0.166463000	2.099479000	2.354006000
H	-0.119770000	-0.573699000	3.123870000
C	4.013071000	-1.946456000	-0.670214000
H	4.838884000	-1.962244000	0.063744000
H	4.449714000	-2.225104000	-1.645431000
H	3.306344000	-2.741280000	-0.384711000
C	4.146892000	1.399699000	-1.483871000
H	4.978348000	1.692492000	-0.817456000
H	3.501778000	2.282760000	-1.611560000
H	4.594179000	1.168692000	-2.466558000
C	-1.537550000	1.352060000	-0.701484000
C	-2.653061000	1.700529000	0.293272000
H	-0.919564000	2.223904000	-0.976434000
H	-2.650266000	1.001109000	1.153186000
H	-1.910744000	0.909956000	-1.640641000
H	-2.442296000	2.684745000	0.746905000
C	-4.087053000	1.745881000	-0.283905000

C	-3.728801000	-1.476067000	0.455756000
H	-4.784086000	1.993886000	0.537930000
H	-3.279766000	-0.813117000	1.211858000
H	-4.134618000	2.597452000	-0.985823000
H	-4.116242000	-2.333845000	1.032702000
C	-2.629960000	-1.977308000	-0.505641000
C	-1.219991000	-1.925185000	0.094362000
H	-2.869878000	-3.014048000	-0.809754000
H	-1.220867000	-2.307311000	1.132703000
H	-2.651597000	-1.403235000	-1.447647000
H	-0.515237000	-2.551492000	-0.482938000
F	1.960514000	2.560005000	0.520637000
F	2.037529000	-1.871561000	1.795816000

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F-9-q SCF Done: -1434.201344 A.U.

Cr	0.788028000	0.459952000	-0.519854000
Al	-2.285650000	-0.826373000	-0.136279000
Cl	-0.786889000	-0.754394000	-1.946901000
N	-1.072648000	0.410175000	0.939801000
C	-0.025268000	0.054834000	1.764408000
C	0.884012000	1.088305000	1.918723000
C	0.322289000	2.215705000	1.206362000
C	-0.865873000	1.752462000	0.668903000
H	1.789461000	1.068542000	2.520342000
H	0.712990000	3.228250000	1.148876000
C	-3.934046000	0.111717000	-0.616071000
H	-4.531056000	0.344181000	0.284348000
H	-4.565653000	-0.525448000	-1.259625000
H	-3.763600000	1.058390000	-1.151904000
C	-2.235265000	-2.619557000	0.646674000
H	-2.678110000	-2.629126000	1.658595000
H	-1.220948000	-3.041249000	0.728548000
H	-2.831832000	-3.315683000	0.031092000
C	3.458966000	-1.905397000	0.565134000
C	3.696474000	-0.558487000	-0.123477000
H	4.274826000	-2.153879000	1.263087000
H	3.776215000	0.242871000	0.634781000
H	3.395242000	-2.721101000	-0.174217000
H	4.687401000	-0.582592000	-0.620139000
C	2.641219000	-0.185045000	-1.149645000
C	2.406780000	1.184450000	-1.544403000
H	2.485555000	-0.953274000	-1.923052000
H	2.964901000	1.982355000	-1.034540000

H	2.158875000	1.418084000	-2.588291000
H	2.514876000	-1.908870000	1.135193000
F	0.029634000	-1.163908000	2.274176000
F	-1.760573000	2.420807000	-0.041499000

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F-2-3-q SCF Done: -1434.164628 A.U.

Cr	-1.441374000	0.140922000	0.108349000
Al	2.315773000	-0.590678000	-0.400414000
Cl	0.353601000	-1.406569000	-1.265227000
N	1.277527000	0.818273000	0.631565000
C	0.606750000	1.838710000	0.022912000
C	-0.530018000	2.238935000	0.719667000
C	-0.568347000	1.387599000	1.883690000
C	0.543603000	0.557574000	1.754704000
H	-1.170768000	3.083802000	0.481279000
H	-1.236060000	1.446464000	2.739656000
C	3.105935000	-1.869856000	0.861455000
H	3.854392000	-1.382392000	1.512101000
H	3.637206000	-2.666308000	0.310599000
H	2.370237000	-2.360104000	1.518608000
C	3.390555000	0.280316000	-1.792065000
H	4.137861000	0.964243000	-1.350248000
H	2.794021000	0.865101000	-2.510169000
H	3.954779000	-0.474023000	-2.368648000
C	-2.430097000	0.891587000	-1.509518000
C	-2.967230000	-0.459005000	-1.561879000
H	-1.668852000	1.165231000	-2.251564000
H	-2.452025000	-1.138004000	-2.248536000
H	-3.131628000	1.705743000	-1.282014000
H	-4.052764000	-0.547645000	-1.645527000
C	-3.043119000	-1.594783000	0.079345000
C	-2.174498000	-1.394694000	1.226503000
H	-2.898615000	-2.517591000	-0.490871000
H	-1.361390000	-2.113496000	1.386881000
H	-4.100119000	-1.393399000	0.272653000
H	-2.641685000	-1.043619000	2.155719000
F	0.937771000	-0.375637000	2.599537000
F	1.050921000	2.334320000	-1.115747000

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F-3-9-q SCF Done: -1434.158795 A.U.

Cr	1.455447000	0.162404000	-0.105224000
Al	-2.455500000	-0.755969000	-0.200300000
Cl	-0.309579000	-1.442092000	-0.911714000

N	-1.608241000	0.879997000	0.569460000
C	-0.703286000	0.774056000	1.579768000
C	0.396469000	1.610686000	1.418839000
C	0.112132000	2.357106000	0.203390000
C	-1.097946000	1.868167000	-0.236437000
H	1.154840000	1.827966000	2.167775000
H	0.672999000	3.189625000	-0.213645000
C	-3.535845000	-0.339345000	-1.782106000
H	-4.421856000	0.260717000	-1.506495000
H	-3.912734000	-1.268216000	-2.245265000
H	-2.990043000	0.221493000	-2.556725000
C	-3.077442000	-1.977266000	1.200584000
H	-3.927437000	-1.540728000	1.755816000
H	-2.301653000	-2.234078000	1.938596000
H	-3.440464000	-2.920628000	0.755979000
H	2.698187000	1.218925000	0.061453000
C	2.619769000	-1.079517000	1.047812000
C	3.975505000	-0.772204000	0.380784000
H	2.588890000	-0.804895000	2.113153000
H	4.625612000	-0.176136000	1.038006000
H	2.286420000	-2.122239000	0.929657000
H	4.538850000	-1.680751000	0.099787000
C	3.656387000	0.024205000	-0.879814000
C	2.760636000	-0.503999000	-1.797245000
H	4.272132000	0.889828000	-1.143013000
H	2.564724000	0.000075000	-2.748057000
H	2.455305000	-1.551633000	-1.726932000
F	-0.909012000	-0.084815000	2.562215000
F	-1.756626000	2.218685000	-1.327920000

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F-4-5-q SCF Done: -1512.706141 A.U.

Cr	1.164036000	0.220460000	-0.058198000
Al	-2.751297000	-0.302356000	-0.333942000
Cl	-1.664597000	-1.863878000	-1.440181000
N	-1.121880000	0.489310000	0.723076000
C	-0.425030000	-0.155727000	1.715100000
C	0.542910000	0.661513000	2.298912000
C	0.406432000	1.935111000	1.648543000
C	-0.614059000	1.765461000	0.720948000
H	1.200398000	0.393720000	3.122650000
H	0.959951000	2.850730000	1.843476000
C	-3.384946000	1.145960000	-1.509760000
H	-3.726882000	2.036700000	-0.954105000

H	-4.253387000	0.780053000	-2.087408000
H	-2.635772000	1.481459000	-2.246651000
C	-3.919002000	-0.995246000	1.093191000
H	-4.271551000	-0.191333000	1.765254000
H	-3.434315000	-1.763290000	1.718518000
H	-4.822455000	-1.458900000	0.658065000
C	1.789542000	-1.729710000	-0.103064000
C	3.199929000	-1.782217000	0.480646000
H	1.071765000	-2.379331000	0.422538000
H	3.165784000	-1.620217000	1.575013000
H	1.782425000	-2.025321000	-1.167420000
H	3.676587000	-2.771253000	0.343485000
C	4.059369000	-0.685983000	-0.157854000
C	3.334152000	0.656096000	-0.144620000
H	5.034823000	-0.588237000	0.354711000
H	3.027854000	0.936942000	0.887189000
H	4.299313000	-0.961840000	-1.201118000
H	3.969179000	1.483020000	-0.480687000
C	2.293817000	1.018365000	-1.972482000
C	0.913048000	0.723145000	-2.060184000
H	2.591388000	2.069964000	-1.979232000
H	0.200878000	1.554376000	-2.109807000
H	3.018821000	0.348242000	-2.441066000
H	0.573843000	-0.213183000	-2.513976000
F	-0.739949000	-1.389028000	2.052499000
F	-1.107199000	2.677632000	-0.097626000

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F-5-6-q SCF Done: -1512.733208 A.U.

Cr	-0.931594000	-0.265940000	0.274392000
Al	2.733224000	0.337974000	-0.829107000
Cl	0.711920000	0.236683000	-1.893334000
N	1.826198000	-0.064573000	0.945647000
C	1.051336000	0.830902000	1.628970000
C	0.047357000	0.224466000	2.377183000
C	0.203044000	-1.188571000	2.127385000
C	1.291657000	-1.278700000	1.263339000
H	-0.624842000	0.712798000	3.078969000
H	-0.318893000	-2.017470000	2.598537000
C	3.877547000	-1.177215000	-1.328708000
H	4.681972000	-1.334919000	-0.587472000
H	4.373544000	-0.978431000	-2.295371000
H	3.332055000	-2.129050000	-1.428653000
C	3.423589000	2.175903000	-0.796503000

H	4.186685000	2.305325000	-0.007735000
H	2.645354000	2.937343000	-0.628611000
H	3.916560000	2.414580000	-1.755660000
C	-2.118843000	1.603240000	-0.024907000
C	-3.634476000	1.575384000	0.236007000
H	-1.583297000	2.118500000	0.788813000
H	-3.827200000	1.215261000	1.263814000
H	-1.882056000	2.148688000	-0.953509000
H	-4.042717000	2.601136000	0.196008000
C	-4.406412000	0.679308000	-0.749872000
C	-3.972176000	-0.795605000	-0.689959000
H	-5.486662000	0.748573000	-0.540876000
H	-4.141603000	-1.177263000	0.333439000
H	-4.268034000	1.061386000	-1.778608000
H	-4.614678000	-1.402515000	-1.351795000
C	-2.507705000	-1.037913000	-1.073665000
C	-1.736758000	-2.053555000	-0.398332000
H	-2.299016000	-0.902928000	-2.144807000
H	-2.222545000	-2.637878000	0.393721000
H	-0.979070000	-2.606681000	-0.965180000
H	-2.116230000	0.312559000	-0.690841000
F	1.306207000	2.124036000	1.547101000
F	1.816242000	-2.381545000	0.765157000

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F-7-8-q SCF Done: -1591.26505450 A.U.

C	4.591836000	0.740091000	-0.244297000
C	4.268872000	-0.715677000	0.123625000
H	4.470848000	0.868420000	-1.336743000
H	4.986442000	-1.357329000	-0.418522000
H	5.669657000	0.880433000	-0.053130000
H	4.494535000	-0.883636000	1.192125000
Cr	0.812794000	-0.487217000	-0.002893000
Al	-3.082726000	0.655190000	0.245754000
Cl	-2.360270000	0.419343000	2.309734000
N	-1.480989000	-0.216175000	-0.801334000
C	-0.675255000	0.346985000	-1.762372000
C	0.112754000	-0.596627000	-2.413288000
C	-0.247311000	-1.860850000	-1.830485000
C	-1.225738000	-1.563078000	-0.888056000
H	0.809764000	-0.405392000	-3.225811000
H	0.117415000	-2.850389000	-2.095537000
C	-4.586748000	-0.536052000	-0.207379000
H	-4.437797000	-1.575883000	0.127433000

H	-4.783842000	-0.560542000	-1.295024000
H	-5.514727000	-0.174508000	0.271005000
C	-3.122185000	2.542888000	-0.313521000
H	-3.314095000	2.673257000	-1.393128000
H	-2.198102000	3.094269000	-0.071923000
H	-3.945237000	3.053312000	0.219198000
C	1.258820000	1.403842000	0.624673000
C	2.407031000	2.208821000	0.005302000
H	0.301512000	1.929575000	0.452993000
H	2.369060000	2.166918000	-1.100855000
H	1.381163000	1.353677000	1.722151000
H	2.234394000	3.275125000	0.244432000
C	3.838520000	1.874639000	0.472099000
C	2.860810000	-1.201669000	-0.222489000
H	4.446372000	2.784440000	0.332104000
H	2.544266000	-0.646118000	-1.135812000
H	3.837116000	1.692963000	1.563456000
H	2.843212000	-2.266599000	-0.493815000
C	2.049077000	-1.499253000	1.698992000
C	0.638489000	-1.509306000	1.798994000
H	2.595872000	-2.444769000	1.671795000
H	0.101556000	-2.455741000	1.670445000
H	2.596026000	-0.690305000	2.187778000
H	0.121181000	-0.761369000	2.409402000
F	-1.894864000	-2.412623000	-0.132809000
F	-0.736305000	1.640601000	-2.009003000

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G-0-s SCF Done: -1752.337195 A.U.

Cr	0.001101000	-0.977287000	1.879580000
Al	-0.000341000	1.865019000	-0.254291000
Cl	0.000660000	1.440790000	2.094683000
N	-0.000272000	-0.146959000	-0.708395000
C	1.097789000	-0.963768000	-0.516640000
C	0.710554000	-2.263091000	-0.165264000
C	-0.710673000	-2.263208000	-0.165231000
C	-1.098155000	-0.963961000	-0.516508000
C	2.533947000	-0.559117000	-0.722324000
H	1.374724000	-3.114524000	-0.035472000
H	-1.374691000	-3.114737000	-0.035290000
C	-2.534409000	-0.559485000	-0.721780000
C	-1.664961000	2.796188000	-0.698970000
H	-1.871807000	2.764592000	-1.782533000
H	-1.510802000	3.858034000	-0.434650000

H	-2.569058000	2.454894000	-0.177248000
C	1.663612000	2.796296000	-0.701305000
H	1.870290000	2.762543000	-1.784831000
H	2.567985000	2.456466000	-0.179084000
H	1.509012000	3.858605000	-0.439147000
F	3.035818000	0.140612000	0.316072000
F	2.699673000	0.172783000	-1.828196000
F	3.293559000	-1.662761000	-0.841030000
F	-2.700335000	0.173461000	-1.826927000
F	-3.036425000	0.139095000	0.317332000
F	-3.293755000	-1.663198000	-0.841538000

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G-1-q SCF Done: -1830.884762 A.U.

Cr	0.033263000	1.364849000	0.730662000
Al	-0.000966000	-1.989820000	0.729276000
Cl	0.103180000	-0.370509000	2.428893000
N	-0.012038000	-0.456483000	-0.699343000
C	-1.118248000	0.264705000	-1.140710000
C	-0.723288000	1.457037000	-1.747094000
C	0.696083000	1.467728000	-1.736201000
C	1.096591000	0.280696000	-1.117468000
C	-2.554242000	-0.170899000	-1.003056000
H	-1.387948000	2.204094000	-2.173096000
H	1.356736000	2.219247000	-2.159793000
C	2.535717000	-0.153550000	-0.997587000
C	1.636517000	-3.061173000	0.691955000
H	1.795419000	-3.537148000	-0.290926000
H	1.491290000	-3.879974000	1.419759000
H	2.564055000	-2.539857000	0.964007000
C	-1.688584000	-2.966943000	0.886338000
H	-1.928561000	-3.529830000	-0.031787000
H	-2.574170000	-2.378937000	1.161600000
H	-1.529956000	-3.716356000	1.683459000
C	-0.772541000	3.012489000	1.649160000
C	0.645515000	3.182230000	1.459378000
H	-1.472394000	3.582199000	1.023412000
H	1.007317000	3.881472000	0.694042000
H	-1.166012000	2.769052000	2.643793000
H	1.327659000	3.070662000	2.312120000
F	-2.753209000	-1.398393000	-1.496749000
F	-3.339467000	0.678191000	-1.683294000
F	-2.976814000	-0.163874000	0.274597000
F	2.749710000	-1.336604000	-1.585000000

F	2.949654000	-0.244286000	0.279251000
F	3.319005000	0.752386000	-1.602931000

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G-2-q SCF Done: -1909.422641 A.U.

Cr	-0.002205000	1.745187000	0.042373000
Al	0.002229000	-1.908139000	1.287870000
Cl	0.000549000	0.163842000	2.272474000
N	0.001179000	-0.980529000	-0.569580000
C	-1.093146000	-0.362269000	-1.134075000
C	-0.705578000	0.608997000	-2.070960000
C	0.704477000	0.610499000	-2.070985000
C	1.094131000	-0.359977000	-1.134159000
C	-2.527133000	-0.798287000	-0.951607000
H	-1.372217000	1.186599000	-2.705658000
H	1.369869000	1.189561000	-2.705659000
C	2.529107000	-0.792732000	-0.951531000
C	1.652030000	-2.917772000	1.642184000
H	1.953963000	-3.547148000	0.787434000
H	1.427744000	-3.606545000	2.476463000
H	2.527009000	-2.320384000	1.934558000
C	-1.645678000	-2.920690000	1.642898000
H	-1.948216000	-3.549163000	0.787707000
H	-2.520932000	-2.324772000	1.937507000
H	-1.419268000	-3.610393000	2.475837000
C	-2.032130000	2.462391000	0.346377000
C	-1.309671000	3.434960000	1.017370000
H	-2.493513000	1.638503000	0.897265000
H	-1.184912000	3.383250000	2.100966000
H	-2.445032000	2.668368000	-0.647239000
H	-1.142955000	4.415356000	0.566979000
C	1.300885000	3.437788000	1.017982000
C	2.025776000	2.467869000	0.345799000
H	1.176505000	3.384523000	2.101559000
H	2.489731000	1.644822000	0.895773000
H	1.131411000	4.418217000	0.568751000
H	2.437756000	2.675957000	-0.647759000
F	-2.997448000	-0.616349000	0.291893000
F	-2.689455000	-2.089092000	-1.265734000
F	-3.312641000	-0.075168000	-1.772214000
F	2.694249000	-2.083309000	-1.265073000
F	2.999030000	-0.609194000	0.291891000
F	3.313040000	-0.068188000	-1.772374000

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G-3-q SCF Done: -1909.451191 A.U.

Cr	1.328799000	-0.191796000	0.203621000
Al	-1.951292000	0.278672000	1.270568000
Cl	0.161789000	-0.009092000	2.302709000
N	-1.037094000	0.140253000	-0.588807000
C	-0.304351000	1.142959000	-1.204082000
C	0.552459000	0.613251000	-2.175275000
C	0.331975000	-0.781896000	-2.182349000
C	-0.646766000	-1.032392000	-1.215259000
C	-0.448895000	2.619721000	-0.936975000
H	1.221387000	1.184606000	-2.813330000
H	0.794281000	-1.524735000	-2.827060000
C	-1.237656000	-2.396780000	-0.964172000
C	-3.086843000	-1.243089000	1.741763000
H	-3.962059000	-1.323846000	1.074300000
H	-3.479803000	-1.029123000	2.752507000
H	-2.602398000	-2.227494000	1.779311000
C	-2.662259000	2.055745000	1.681255000
H	-3.411658000	2.378342000	0.938082000
H	-1.927826000	2.865567000	1.785605000
H	-3.193210000	1.963295000	2.645944000
C	2.965289000	1.018752000	0.407978000
C	4.203653000	0.121439000	0.299063000
H	2.959928000	1.857439000	-0.310318000
H	4.428940000	-0.080451000	-0.765720000
H	2.857325000	1.439398000	1.424685000
H	5.108021000	0.608913000	0.710501000
C	3.906176000	-1.208846000	1.003882000
C	2.598060000	-1.770430000	0.438536000
H	4.746860000	-1.921676000	0.902072000
H	2.743920000	-2.153903000	-0.592207000
H	3.791979000	-1.026206000	2.088221000
H	2.150744000	-2.575398000	1.045613000
F	-0.031231000	2.969890000	0.293084000
F	0.301056000	3.302330000	-1.816137000
F	-1.715512000	3.029528000	-1.073216000
F	-2.573907000	-2.381674000	-1.030857000
F	-0.788698000	-3.250201000	-1.897656000
F	-0.888000000	-2.904559000	0.232215000

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G-4-q SCF Done: -1987.972764 A.U.

Cr	-1.481742000	0.422368000	0.092693000
Al	2.518596000	-0.604804000	0.814636000

Cl	1.175896000	-0.525663000	2.573536000
N	0.975574000	-0.185695000	-0.610414000
C	0.073959000	-1.092986000	-1.121301000
C	-0.787543000	-0.484696000	-2.052044000
C	-0.400273000	0.872294000	-2.119857000
C	0.660558000	1.014565000	-1.216820000
C	0.079417000	-2.586946000	-0.883443000
H	-1.561355000	-0.987018000	-2.625592000
H	-0.832581000	1.657135000	-2.734747000
C	1.377896000	2.320638000	-0.988005000
C	3.874804000	0.822095000	0.859136000
H	4.391634000	0.965601000	-0.104931000
H	4.640505000	0.458168000	1.570029000
H	3.550026000	1.808775000	1.218776000
C	3.279501000	-2.369731000	0.385824000
H	3.494406000	-2.494124000	-0.689924000
H	2.693752000	-3.241798000	0.710342000
H	4.254183000	-2.420924000	0.904869000
C	-2.467937000	-1.006305000	1.200506000
C	-3.927308000	-1.079758000	0.742794000
H	-1.942295000	-1.972453000	1.166319000
H	-4.011202000	-1.752071000	-0.130505000
H	-2.385823000	-0.631281000	2.236342000
H	-4.585854000	-1.508897000	1.521037000
C	-4.380567000	0.324971000	0.327699000
C	-3.354064000	0.859709000	-0.671542000
H	-5.404989000	0.321635000	-0.091579000
H	-3.421654000	0.294909000	-1.618258000
H	-4.426271000	0.975084000	1.222652000
H	-3.469198000	1.930493000	-0.916463000
C	-1.736600000	2.714375000	1.184792000
C	-1.204348000	1.936516000	2.148437000
H	-1.107934000	3.243113000	0.461507000
H	-0.128330000	1.763753000	2.243597000
H	-2.808011000	2.922381000	1.145454000
H	-1.833257000	1.478094000	2.915887000
F	2.613030000	2.324685000	-1.487415000
F	1.446403000	2.648320000	0.315727000
F	0.690372000	3.309401000	-1.598784000
F	0.237586000	-2.928287000	0.395326000
F	-1.098546000	-3.094844000	-1.299006000
F	1.041164000	-3.183414000	-1.600735000

G-5-q SCF Done: -1988.019346 A.U.

Cr	-1.110806000	0.031608000	0.252391000
Al	2.323737000	0.128502000	1.266227000
Cl	0.168840000	0.229904000	2.277785000
N	1.436505000	-0.008647000	-0.582721000
C	0.909705000	-1.158352000	-1.139424000
C	-0.051994000	-0.856504000	-2.107505000
C	-0.119578000	0.552846000	-2.171960000
C	0.803333000	1.034312000	-1.236535000
C	1.367802000	-2.561193000	-0.833373000
H	-0.593659000	-1.576899000	-2.715040000
H	-0.719980000	1.160147000	-2.844218000
C	1.131351000	2.496213000	-1.070802000
C	3.298211000	1.802671000	1.555961000
H	4.061700000	1.964516000	0.775396000
H	3.840027000	1.696869000	2.512811000
H	2.691218000	2.715931000	1.617793000
C	3.187881000	-1.501554000	1.920482000
H	4.062851000	-1.776773000	1.307076000
H	2.551254000	-2.391217000	2.013161000
H	3.570828000	-1.261708000	2.929230000
C	-2.256976000	-1.568022000	0.666362000
C	-3.482834000	-1.676350000	-0.247377000
H	-1.576175000	-2.429217000	0.540160000
H	-3.239391000	-1.349981000	-1.281507000
H	-2.537270000	-1.526476000	1.732874000
H	-3.748041000	-2.744985000	-0.358159000
C	-4.738996000	-0.932786000	0.231582000
C	-4.777203000	0.596894000	0.094150000
H	-5.601873000	-1.330964000	-0.330534000
H	-4.673440000	0.869589000	-0.973910000
H	-4.922674000	-1.204210000	1.287937000
H	-5.795211000	0.915250000	0.377512000
C	-3.775042000	1.426685000	0.917612000
C	-2.386232000	1.601539000	0.299777000
H	-4.213428000	2.433995000	1.052766000
H	-2.474097000	1.947537000	-0.749923000
H	-3.696391000	1.011790000	1.939305000
H	-1.806608000	2.369127000	0.844498000
F	0.800494000	2.977601000	0.142616000
F	2.432783000	2.742705000	-1.264674000
F	0.438999000	3.209376000	-1.974219000
F	0.937359000	-3.009821000	0.362398000

F	2.701863000	-2.665029000	-0.852230000
F	0.876137000	-3.400130000	-1.759730000

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G-6-q SCF Done: -1988.021843 A.U.

Cr	0.467819000	-0.920806000	0.379120000
Al	-1.890124000	1.405926000	1.083010000
Cl	-0.246746000	0.307648000	2.357971000
N	-1.146465000	0.471477000	-0.631884000
C	0.017686000	0.830706000	-1.311354000
C	0.447750000	-0.206479000	-2.140002000
C	-0.491603000	-1.256957000	-1.990110000
C	-1.463863000	-0.798026000	-1.096275000
C	0.670905000	2.188481000	-1.266753000
H	1.320278000	-0.185343000	-2.787334000
H	-0.501572000	-2.215707000	-2.501750000
C	-2.705296000	-1.575400000	-0.737283000
C	-3.654624000	0.772539000	1.644761000
H	-4.433317000	0.993979000	0.895154000
H	-3.912841000	1.353671000	2.548962000
H	-3.733012000	-0.291207000	1.905325000
C	-1.618957000	3.344905000	1.088695000
H	-2.066891000	3.822411000	0.200129000
H	-0.580456000	3.693800000	1.165230000
H	-2.165592000	3.734951000	1.966188000
C	3.869414000	0.969070000	1.149695000
C	4.284256000	0.179611000	-0.095734000
H	3.775890000	2.043455000	0.926655000
H	3.548833000	0.344808000	-0.904954000
H	4.619457000	0.858254000	1.950607000
H	5.229131000	0.607683000	-0.473133000
C	4.486294000	-1.333038000	0.116348000
C	3.255251000	-2.241516000	-0.033415000
H	5.238981000	-1.691434000	-0.606872000
H	2.874475000	-2.164059000	-1.071382000
H	4.935246000	-1.499165000	1.113262000
H	3.609241000	-3.287982000	0.055317000
C	2.113527000	-2.040828000	0.956618000
C	0.920382000	-2.848383000	0.864855000
H	2.435879000	-1.758232000	1.969433000
H	0.825525000	-3.562098000	0.033697000
H	0.401632000	-3.164028000	1.778854000
H	2.903429000	0.634428000	1.556830000
F	-3.816746000	-0.861149000	-0.952366000

F	-2.716508000	-1.982000000	0.544830000
F	-2.770485000	-2.677191000	-1.500575000
F	1.148998000	2.506730000	-0.051668000
F	-0.173504000	3.157389000	-1.641536000
F	1.711893000	2.202404000	-2.116555000

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G-7-q SCF Done: -2066.545083 A.U.

Al	2.714922000	-0.473015000	1.088308000
Cl	0.630941000	-0.057847000	2.073703000
N	1.784863000	-0.308352000	-0.715499000
C	0.796607000	-1.183016000	-1.074487000
C	-0.230377000	-0.533982000	-1.774185000
C	0.193804000	0.817798000	-1.910620000
C	1.415205000	0.905435000	-1.256607000
C	0.830357000	-2.673729000	-0.846081000
H	-1.064269000	-1.019998000	-2.274351000
H	-0.289929000	1.608274000	-2.477223000
C	2.213445000	2.175189000	-1.172743000
C	3.919123000	0.988666000	1.601235000
H	4.838236000	0.994239000	0.990100000
H	4.233363000	0.778513000	2.640304000
H	3.501150000	2.004113000	1.584151000
C	3.390207000	-2.277002000	1.465855000
H	4.044892000	-2.635384000	0.652050000
H	2.632034000	-3.052271000	1.641915000
H	4.017876000	-2.212539000	2.372592000
C	-1.511520000	2.553111000	1.802450000
C	-2.162447000	1.644604000	2.552257000
H	-0.422778000	2.656566000	1.856782000
H	-1.623350000	0.978020000	3.229960000
H	-2.052939000	3.260972000	1.169530000
H	-3.253217000	1.573977000	2.542342000
Cr	-1.310327000	0.438274000	0.292588000
C	-2.393435000	-1.189021000	0.874665000
C	-3.553732000	-1.709993000	0.031165000
H	-1.584711000	-1.936971000	0.944045000
H	-3.260720000	-1.796609000	-1.032230000
H	-2.722870000	-0.976837000	1.907905000
H	-3.750484000	-2.751976000	0.350425000
C	-4.879447000	-0.937162000	0.137988000
C	-5.059518000	0.302210000	-0.749476000
H	-5.698104000	-1.632872000	-0.114796000
H	-4.945466000	0.003115000	-1.808804000

H	-5.048501000	-0.660132000	1.196138000
H	-6.109218000	0.629667000	-0.648151000
C	-4.160847000	1.518966000	-0.486289000
C	-2.695060000	1.362876000	-0.908627000
H	-4.598624000	2.370088000	-1.042326000
H	-2.657374000	0.869146000	-1.896758000
H	-4.247090000	1.807458000	0.578212000
H	-2.233423000	2.361810000	-1.050587000
F	0.556302000	-3.035014000	0.422201000
F	2.018526000	-3.196056000	-1.169216000
F	-0.102681000	-3.261318000	-1.618327000
F	3.530652000	1.961718000	-1.227377000
F	1.953684000	2.873544000	-0.040652000
F	1.882980000	2.986285000	-2.193832000

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G-8-q SCF Done: -2066.580540 A.U.

C	5.150491000	0.664344000	0.696619000
C	5.392549000	-0.711360000	0.048745000
H	6.138153000	1.069217000	0.977593000
H	5.985580000	-0.570687000	-0.873413000
H	4.619959000	0.536862000	1.655587000
H	6.039857000	-1.292252000	0.730904000
Cr	0.744637000	-0.196374000	0.302581000
Al	-2.733782000	0.093233000	1.223852000
Cl	-0.626874000	-0.162929000	2.291710000
N	-1.783678000	0.111490000	-0.599082000
C	-1.098385000	1.188249000	-1.128972000
C	-0.141733000	0.770627000	-2.058760000
C	-0.232144000	-0.637130000	-2.114819000
C	-1.244780000	-1.000969000	-1.217994000
C	-1.399537000	2.637572000	-0.845022000
H	0.504234000	1.419274000	-2.643831000
H	0.320233000	-1.315170000	-2.760276000
C	-1.746651000	-2.414476000	-1.064132000
C	-3.838691000	-1.491413000	1.548348000
H	-4.616146000	-1.609377000	0.773859000
H	-4.366999000	-1.317311000	2.503002000
H	-3.308211000	-2.449105000	1.633709000
C	-3.511474000	1.801496000	1.782648000
H	-4.304664000	2.133416000	1.090677000
H	-2.815008000	2.639411000	1.917299000
H	-3.999665000	1.615343000	2.756486000
C	2.008269000	1.331446000	0.711738000

C	2.949410000	1.547843000	-0.480399000
H	1.410981000	2.224233000	0.956697000
H	2.871809000	0.711494000	-1.204224000
H	2.526613000	1.016119000	1.631564000
H	2.611899000	2.430440000	-1.050721000
C	4.445509000	1.744778000	-0.142199000
C	4.156991000	-1.562311000	-0.292474000
H	4.998482000	1.880480000	-1.089980000
H	3.575754000	-1.058738000	-1.080702000
H	4.539010000	2.701801000	0.401124000
H	4.501752000	-2.501265000	-0.759459000
C	3.228374000	-1.903788000	0.892867000
C	1.744213000	-1.972930000	0.520258000
H	3.545469000	-2.872070000	1.324602000
H	1.597676000	-2.554769000	-0.410314000
H	3.365635000	-1.178372000	1.711658000
H	1.155392000	-2.471796000	1.310472000
F	-1.030753000	3.025067000	0.390691000
F	-2.701630000	2.913507000	-0.986561000
F	-0.718942000	3.407856000	-1.710559000
F	-1.134616000	-3.201205000	-1.965277000
F	-3.065766000	-2.500509000	-1.273981000
F	-1.488491000	-2.939019000	0.148070000

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G-9-q SCF Done: -1909.457217 A.U.

Cr	0.669299000	-0.938477000	0.541009000
Al	-1.678617000	1.450762000	0.926397000
Cl	-0.363583000	0.208149000	2.423490000
N	-0.738837000	0.472232000	-0.670587000
C	0.509622000	0.779312000	-1.207202000
C	1.009269000	-0.292916000	-1.946494000
C	0.017295000	-1.307597000	-1.907932000
C	-1.041835000	-0.798300000	-1.152175000
C	1.223010000	2.098005000	-1.054348000
H	1.960938000	-0.315681000	-2.470593000
H	0.038369000	-2.274931000	-2.402676000
C	-2.343866000	-1.527202000	-0.936680000
C	-3.566863000	0.981197000	1.141514000
H	-4.162871000	1.248875000	0.252287000
H	-3.944481000	1.602988000	1.973639000
H	-3.786565000	-0.066015000	1.388827000
C	-1.233076000	3.351932000	1.066339000
H	-1.546420000	3.916647000	0.171570000

H	-0.180971000	3.596271000	1.264796000
H	-1.828027000	3.743975000	1.911349000
C	4.428557000	-0.502086000	0.257981000
C	3.656619000	-1.820034000	0.360333000
H	5.345648000	-0.617520000	-0.341916000
H	3.373493000	-2.170854000	-0.650298000
H	4.728620000	-0.142269000	1.256109000
H	4.339938000	-2.600605000	0.750641000
C	2.424069000	-1.767180000	1.248550000
C	1.378864000	-2.757534000	1.148033000
H	2.618735000	-1.354190000	2.250515000
H	1.448910000	-3.518763000	0.357940000
H	0.861178000	-3.104858000	2.051279000
H	3.823668000	0.294206000	-0.205118000
F	-2.334214000	-2.665976000	-1.646379000
F	-2.543460000	-1.864868000	0.350595000
F	-3.393589000	-0.801834000	-1.339691000
F	1.604509000	2.339641000	0.213010000
F	0.468257000	3.124691000	-1.461389000
F	2.337551000	2.085737000	-1.804865000

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G-2-3-q SCF Done: -1909.413060 A.U.

Cr	-0.928325000	-1.419926000	-0.032076000
Al	1.017440000	1.602525000	1.314984000
Cl	-0.148278000	-0.177923000	2.203461000
N	0.580015000	0.884403000	-0.577565000
C	1.186107000	-0.212584000	-1.145764000
C	0.342954000	-0.842226000	-2.073529000
C	-0.859031000	-0.099715000	-2.074402000
C	-0.676233000	0.934312000	-1.141274000
C	2.622545000	-0.624427000	-0.930639000
H	0.606565000	-1.686808000	-2.704174000
H	-1.727384000	-0.236371000	-2.713095000
C	-1.677402000	2.045324000	-0.936610000
C	0.172480000	3.329867000	1.711611000
H	0.419698000	4.092124000	0.952339000
H	0.610315000	3.681074000	2.663566000
H	-0.919408000	3.326678000	1.833555000
C	2.918780000	1.503027000	1.792623000
H	3.552413000	2.079697000	1.096937000
H	3.352130000	0.497730000	1.882627000
H	3.012857000	1.990524000	2.780350000
C	0.043212000	-3.202884000	0.220066000

C	-1.022859000	-3.421186000	1.175430000
H	1.036236000	-2.948260000	0.608302000
H	-0.790541000	-3.160138000	2.212955000
H	0.064337000	-3.842213000	-0.672658000
H	-1.568098000	-4.364058000	1.102469000
C	-2.808837000	-2.481201000	0.942617000
C	-2.949203000	-1.237315000	0.220190000
H	-2.979868000	-2.454588000	2.023085000
H	-3.121703000	-0.320137000	0.794931000
H	-3.276049000	-3.347225000	0.467448000
H	-3.482527000	-1.267156000	-0.738664000
F	2.969127000	-1.519367000	-1.873421000
F	3.455046000	0.416603000	-1.029581000
F	2.837452000	-1.215811000	0.257822000
F	-1.122493000	3.247606000	-1.126515000
F	-2.245733000	2.040631000	0.280031000
F	-2.674551000	1.907274000	-1.829750000

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G-3-9-q SCF Done: -1909.411404 A.U.

Cr	1.615270000	-0.926265000	-0.351599000
Al	-1.562752000	0.828322000	1.498697000
Cl	0.544444000	-0.187009000	1.871229000
N	-1.245241000	0.538508000	-0.486315000
C	-0.162861000	1.100874000	-1.111767000
C	0.378113000	0.232356000	-2.071570000
C	-0.461199000	-0.917272000	-2.069202000
C	-1.427850000	-0.683943000	-1.101540000
C	0.326764000	2.513032000	-0.902198000
H	1.161172000	0.472894000	-2.786598000
H	-0.399481000	-1.777863000	-2.729745000
C	-2.541932000	-1.647732000	-0.798941000
C	-2.860940000	-0.337544000	2.392628000
H	-3.897526000	-0.098757000	2.099727000
H	-2.778810000	-0.116490000	3.473055000
H	-2.718455000	-1.419595000	2.267716000
C	-1.627740000	2.707270000	2.057849000
H	-1.195219000	3.469469000	1.398185000
H	-1.131460000	2.804335000	3.040580000
H	-2.689234000	2.969690000	2.219681000
H	2.122114000	-1.800397000	-1.603583000
C	3.303552000	0.221919000	-0.250854000
C	4.144239000	-0.623522000	0.724165000
H	3.743451000	0.280659000	-1.258157000

H	5.228912000	-0.539399000	0.537830000
H	3.072988000	1.228671000	0.127428000
H	3.954556000	-0.312236000	1.763305000
C	3.676811000	-2.045089000	0.516635000
C	2.699447000	-2.648680000	1.232899000
H	4.092854000	-2.574712000	-0.347631000
H	2.350461000	-3.652149000	0.971355000
H	2.295675000	-2.202256000	2.145364000
F	-3.665733000	-1.026669000	-0.426847000
F	-2.817696000	-2.376165000	-1.895108000
F	-2.211997000	-2.529480000	0.169211000
F	-0.672353000	3.398023000	-1.020512000
F	0.911136000	2.717290000	0.291274000
F	1.247758000	2.806989000	-1.837857000

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G-4-5-q SCF Done: -1987.980116 A.U.

Cr	-1.420180000	0.483460000	0.623711000
Al	1.640477000	-1.073789000	1.350055000
Cl	-0.528722000	-1.102715000	2.243869000
N	1.074328000	-0.429962000	-0.505564000
C	0.417821000	-1.217138000	-1.451666000
C	0.705569000	-0.807726000	-2.744384000
C	1.594232000	0.280719000	-2.627604000
C	1.788987000	0.482053000	-1.270733000
C	-0.652711000	-2.199583000	-1.134779000
H	0.298637000	-1.239039000	-3.655738000
H	2.039320000	0.864088000	-3.429513000
C	2.670690000	1.552945000	-0.710657000
C	2.551415000	0.215145000	2.520933000
H	3.636091000	0.245270000	2.329118000
H	2.415787000	-0.160605000	3.551924000
H	2.190923000	1.254317000	2.507730000
C	2.431061000	-2.864183000	1.212221000
H	1.890508000	-3.581070000	0.577904000
H	2.524325000	-3.314234000	2.216628000
H	3.458406000	-2.775063000	0.813417000
C	-3.419454000	0.387977000	1.059350000
C	-4.170464000	0.532676000	-0.263101000
H	-3.605758000	-0.571941000	1.569003000
H	-4.062575000	-0.391294000	-0.857813000
H	-3.657203000	1.207762000	1.759529000
H	-5.258161000	0.661963000	-0.107438000
C	-3.601273000	1.714308000	-1.059982000

C	-2.076425000	1.669724000	-1.104351000
H	-4.012381000	1.732131000	-2.086869000
H	-1.704106000	0.739390000	-1.587497000
H	-3.924705000	2.664612000	-0.596123000
H	-1.643988000	2.483959000	-1.695896000
C	-1.232111000	2.852223000	0.569928000
C	-0.876281000	2.178040000	1.748143000
H	-0.433455000	3.225671000	-0.073940000
H	0.182668000	2.041112000	1.982495000
H	-2.169507000	3.409397000	0.514176000
H	-1.561945000	2.159164000	2.600499000
F	-0.355577000	-3.142022000	-0.244593000
F	-1.763744000	-1.522124000	-0.587101000
F	-1.114691000	-2.792977000	-2.232520000
F	2.020913000	2.332767000	0.188977000
F	3.763708000	1.071103000	-0.091863000
F	3.097934000	2.363635000	-1.690466000

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G-5-6-q SCF Done: -1987.982279 A.U.

Cr	1.221126000	-0.337001000	-0.117065000
Al	-2.238358000	0.372753000	1.359225000
Cl	-0.167943000	-0.065035000	2.228870000
N	-1.427280000	0.212572000	-0.546344000
C	-0.640071000	1.170504000	-1.149509000
C	0.178760000	0.609588000	-2.141958000
C	-0.093953000	-0.775653000	-2.136160000
C	-1.066668000	-0.975109000	-1.143121000
C	-0.722228000	2.655281000	-0.893240000
H	0.843632000	1.154793000	-2.806809000
H	0.307832000	-1.538720000	-2.797028000
C	-1.723879000	-2.312577000	-0.895939000
C	-3.547184000	-1.034458000	1.766029000
H	-4.386815000	-1.030502000	1.049027000
H	-3.977670000	-0.780737000	2.752094000
H	-3.168953000	-2.063638000	1.829898000
C	-2.868898000	2.185301000	1.782031000
H	-3.597872000	2.553191000	1.039221000
H	-2.098776000	2.959539000	1.902903000
H	-3.411571000	2.109047000	2.741958000
C	2.690455000	1.298955000	0.281486000
C	4.175260000	1.137846000	-0.085289000
H	2.187067000	1.973058000	-0.427752000
H	4.266566000	0.916832000	-1.164928000

H	2.565948000	1.739619000	1.284403000
H	4.701919000	2.096129000	0.070639000
C	4.888445000	0.025213000	0.702599000
C	4.275038000	-1.362455000	0.452724000
H	5.955910000	0.006209000	0.428554000
H	4.338494000	-1.593191000	-0.626068000
H	4.852275000	0.256329000	1.783601000
H	4.871116000	-2.136505000	0.966730000
C	2.817053000	-1.497971000	0.905409000
C	1.883990000	-2.287749000	0.140533000
H	2.690961000	-1.525979000	1.997254000
H	2.236434000	-2.755094000	-0.788153000
H	1.115955000	-2.859905000	0.670847000
H	2.579063000	-0.078204000	0.755564000
F	0.050119000	3.297353000	-1.792565000
F	-1.969281000	3.116742000	-1.024626000
F	-0.270931000	3.009035000	0.321021000
F	-1.263543000	-3.200000000	-1.796901000
F	-3.052050000	-2.241412000	-1.036531000
F	-1.462156000	-2.822023000	0.318241000

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G-7-8-q SCF Done: -2066.515065 A.U.

C	-4.923940000	-0.129902000	-0.167695000
C	-4.389070000	1.301157000	-0.327380000
H	-4.720888000	-0.693625000	-1.098031000
H	-4.949043000	1.769923000	-1.156112000
H	-6.023145000	-0.050893000	-0.109473000
H	-4.657808000	1.896317000	0.563752000
Cr	-1.022479000	0.645882000	0.110479000
Al	2.692536000	-0.885586000	0.911363000
Cl	1.564888000	-0.162256000	2.666061000
N	1.264062000	-0.249163000	-0.568809000
C	0.352315000	-1.013022000	-1.275047000
C	-0.283111000	-0.253991000	-2.268491000
C	0.236767000	1.050968000	-2.162899000
C	1.169682000	1.017071000	-1.115983000
C	0.162706000	-2.504595000	-1.144267000
H	-1.023798000	-0.622402000	-2.973791000
H	-0.013685000	1.919989000	-2.766406000
C	2.036036000	2.203572000	-0.769926000
C	4.381576000	0.051153000	0.512829000
H	4.645636000	0.027095000	-0.559134000
H	5.174643000	-0.511527000	1.038855000

H	4.451494000	1.096150000	0.848303000
C	2.897553000	-2.843458000	0.936831000
H	3.206302000	-3.274469000	-0.030295000
H	2.036120000	-3.418952000	1.304378000
H	3.731688000	-3.027644000	1.640133000
C	-1.872372000	-0.688238000	1.394467000
C	-3.043125000	-1.586497000	0.983286000
H	-0.984739000	-1.292842000	1.647691000
H	-2.877266000	-2.032023000	-0.015696000
H	-2.128252000	-0.126973000	2.310931000
H	-3.048799000	-2.453907000	1.670170000
C	-4.453789000	-0.968765000	1.032764000
C	-2.899059000	1.428161000	-0.651224000
H	-5.171075000	-1.801513000	1.128492000
H	-2.612707000	0.504261000	-1.205335000
H	-4.565012000	-0.381196000	1.963727000
H	-2.688479000	2.265509000	-1.331213000
C	-2.189536000	2.435696000	1.081936000
C	-0.817570000	2.293607000	1.379601000
H	-2.539945000	3.339450000	0.578137000
H	-0.113534000	3.027401000	0.978230000
H	-2.922734000	1.990945000	1.756961000
H	-0.500133000	1.790145000	2.298876000
F	-0.015705000	-2.916632000	0.114597000
F	1.195207000	-3.180645000	-1.662848000
F	-0.937771000	-2.863411000	-1.840767000
F	3.205109000	2.171172000	-1.420518000
F	2.285532000	2.325550000	0.534967000
F	1.399825000	3.332548000	-1.165047000

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H-0-s SCF Done : -1577.608197 A.U.

Cr	-1.612641000	-0.125023000	1.291041000
Al	1.451382000	0.419986000	-0.185434000
Cl	0.660424000	0.483636000	2.019422000
N	-0.274366000	-0.045777000	-0.990036000
C	-0.894270000	-1.289346000	-0.851207000
C	-2.282361000	-1.105382000	-0.819604000
C	-2.524566000	0.301657000	-0.977159000
C	-1.278879000	0.919025000	-1.095634000
C	-0.170989000	-2.603144000	-0.843344000
H	0.421223000	-2.730229000	-1.763365000
H	-0.906254000	-3.418784000	-0.789852000
H	0.531114000	-2.710126000	-0.004805000

H	-3.024783000	-1.902453000	-0.806931000
H	-3.489633000	0.794576000	-1.085768000
C	-1.018229000	2.373850000	-1.349808000
H	-0.371798000	2.516329000	-2.229809000
H	-0.531670000	2.882021000	-0.503588000
H	-1.971997000	2.885657000	-1.541605000
C	2.233207000	2.150486000	-0.646172000
H	2.265111000	2.301692000	-1.739348000
H	3.278639000	2.160081000	-0.293235000
H	1.729459000	3.022350000	-0.200863000
Cl	2.836228000	-1.214390000	-0.324560000

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H-1-q SCF Done : -1656.159948 A.U.

Cr	-1.413896000	-0.111958000	0.430841000
Al	1.836995000	0.327052000	0.227804000
Cl	0.446615000	0.169346000	2.058428000
N	0.311634000	0.220762000	-1.040928000
C	-0.323463000	-0.929089000	-1.536873000
C	-1.603330000	-0.569943000	-1.966731000
C	-1.737014000	0.847560000	-1.806382000
C	-0.542847000	1.318579000	-1.263996000
C	0.303615000	-2.287301000	-1.618466000
H	1.189643000	-2.271468000	-2.272357000
H	-0.427165000	-2.991040000	-2.040724000
H	0.637863000	-2.672192000	-0.645597000
H	-2.335329000	-1.250246000	-2.397869000
H	-2.591802000	1.460517000	-2.084758000
C	-0.169874000	2.743218000	-0.984881000
H	0.703028000	3.051918000	-1.581200000
H	0.071622000	2.927475000	0.072321000
H	-1.013989000	3.393686000	-1.252670000
C	2.858628000	1.990480000	0.213294000
H	3.161117000	2.266804000	-0.812148000
H	3.788756000	1.832613000	0.785542000
H	2.342860000	2.855980000	0.656659000
C	-2.873080000	-1.230751000	1.331778000
C	-3.202003000	0.177046000	1.387925000
H	-3.441459000	-1.888047000	0.660560000
H	-4.013416000	0.564206000	0.757660000
H	-2.514294000	-1.736796000	2.237910000
H	-3.090994000	0.718991000	2.336820000
Cl	3.032261000	-1.447652000	0.119849000

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H-2-q SCF Done : -1734.701588 A.U.

Cr	1.652152000	-0.039588000	0.064590000
Al	-1.996592000	0.324531000	-0.518156000
Cl	-0.560191000	-0.519087000	-1.998768000
N	-0.740291000	0.225653000	1.015118000
C	-0.195516000	-0.956468000	1.492061000
C	0.942040000	-0.663189000	2.266209000
C	1.096615000	0.747636000	2.261942000
C	0.056294000	1.270313000	1.475753000
C	-0.808289000	-2.306412000	1.287861000
H	-1.792643000	-2.360190000	1.776516000
H	-0.156019000	-3.077335000	1.720884000
H	-0.972841000	-2.535825000	0.225246000
H	1.539853000	-1.392984000	2.808161000
H	1.842184000	1.334852000	2.795324000
C	-0.304272000	2.715455000	1.329842000
H	-1.228113000	2.933642000	1.890247000
H	-0.478325000	3.017073000	0.290119000
H	0.497684000	3.342329000	1.743596000
C	-2.613332000	2.113311000	-1.024502000
H	-3.088924000	2.658431000	-0.191452000
H	-3.388344000	1.986622000	-1.800889000
H	-1.833893000	2.762238000	-1.457123000
C	2.337539000	-2.097976000	-0.182167000
C	2.943278000	-1.475910000	-1.262387000
H	1.409930000	-2.658946000	-0.323215000
H	2.477755000	-1.513042000	-2.249420000
H	2.922678000	-2.354560000	0.707656000
H	4.010789000	-1.249285000	-1.249460000
C	2.907331000	1.090620000	-1.524752000
C	2.063776000	1.907480000	-0.780816000
H	2.634508000	0.791169000	-2.538094000
H	1.115689000	2.243049000	-1.211647000
H	3.974046000	1.042596000	-1.291656000
H	2.463897000	2.519742000	0.034322000
Cl	-3.617256000	-1.034272000	-0.097311000

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H-3-q SCF Done : -1734.726548 A.U.

Cr	1.168847000	0.085232000	-0.035527000
Al	-2.155436000	-0.067446000	-0.523661000
Cl	-0.359222000	-0.421742000	-1.932237000
N	-0.987480000	0.655517000	0.908791000
C	-0.304386000	-0.041894000	1.904821000

C	0.811263000	0.714980000	2.294402000
C	0.778006000	1.935306000	1.557528000
C	-0.336014000	1.884658000	0.719628000
C	-0.741874000	-1.350457000	2.486582000
H	-1.742978000	-1.261696000	2.936642000
H	-0.033535000	-1.648650000	3.271607000
H	-0.799684000	-2.155146000	1.741431000
H	1.525038000	0.431117000	3.065281000
H	1.476550000	2.766288000	1.631142000
C	-0.823669000	2.958870000	-0.204826000
H	-1.824567000	3.313885000	0.086692000
H	-0.881422000	2.627964000	-1.252275000
H	-0.132598000	3.811971000	-0.162020000
C	-3.459644000	1.174267000	-1.276679000
H	-3.999788000	1.716566000	-0.480570000
H	-4.215117000	0.596499000	-1.835769000
H	-3.040309000	1.922443000	-1.966787000
C	2.218420000	-1.671754000	0.155100000
C	3.684614000	-1.373261000	-0.184354000
H	2.089720000	-2.157312000	1.138484000
H	4.194109000	-0.947828000	0.701389000
H	1.761450000	-2.331969000	-0.606930000
H	4.250846000	-2.287414000	-0.448060000
C	3.723003000	-0.339736000	-1.317718000
C	2.856190000	0.855074000	-0.904729000
H	4.761061000	-0.043820000	-1.565229000
H	3.360656000	1.451617000	-0.119345000
H	3.311493000	-0.798013000	-2.236480000
H	2.610308000	1.534255000	-1.741292000
Cl	-2.948189000	-1.976757000	0.035901000

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H-4-q SCF Done : -1813.256484 A.U.

Cr	-1.496724000	0.195958000	-0.084467000
Al	2.504977000	0.136815000	0.404256000
Cl	1.790213000	-0.916806000	2.180356000
N	0.870132000	0.128057000	-0.774486000
C	0.236220000	-1.026454000	-1.216496000
C	-0.782994000	-0.666022000	-2.116664000
C	-0.718414000	0.751012000	-2.281899000
C	0.300012000	1.214392000	-1.447780000
C	0.660363000	-2.410333000	-0.844976000
H	1.614425000	-2.647183000	-1.342359000
H	-0.100462000	-3.133342000	-1.168702000

H	0.825151000	-2.514839000	0.235813000
H	-1.438338000	-1.362016000	-2.636304000
H	-1.343322000	1.367496000	-2.924809000
C	0.794772000	2.623900000	-1.340215000
H	1.808117000	2.714668000	-1.761465000
H	0.849273000	2.989262000	-0.305513000
H	0.130677000	3.288716000	-1.910372000
C	-2.212908000	-1.410380000	0.997006000
C	-3.624660000	-1.731005000	0.494369000
H	-1.532662000	-2.277471000	0.974422000
H	-3.568149000	-2.283843000	-0.462546000
H	-2.254870000	-1.062059000	2.046780000
H	-4.182537000	-2.387553000	1.189512000
C	-4.358406000	-0.406485000	0.258537000
C	-3.479460000	0.468268000	-0.641248000
H	-5.368113000	-0.563933000	-0.167081000
H	-3.521169000	0.098094000	-1.682169000
H	-4.520890000	0.089473000	1.234949000
H	-3.787088000	1.529715000	-0.664277000
C	-1.998982000	2.085300000	1.502234000
C	-0.887583000	1.503860000	1.997056000
H	-1.945227000	2.935253000	0.814908000
H	0.113046000	1.853815000	1.730542000
H	-2.996475000	1.784930000	1.830675000
H	-0.926211000	0.699370000	2.735057000
C	3.151980000	1.933470000	0.857581000
H	4.023802000	1.787620000	1.520598000
H	3.510641000	2.516140000	-0.006747000
H	2.441810000	2.563141000	1.420932000
Cl	3.913004000	-1.020875000	-0.757626000

41

H-5-q SCF Done : -1813.293655 A.U.

Cr	0.839627000	-0.046435000	0.054644000
Al	-2.508320000	0.474053000	-0.492857000
Cl	-0.659069000	0.344116000	-1.882609000
N	-1.466970000	-0.104185000	1.077965000
C	-0.932881000	-1.384356000	1.243542000
C	0.172238000	-1.302158000	2.097774000
C	0.313683000	0.062088000	2.481154000
C	-0.714457000	0.776393000	1.853496000
C	-1.496852000	-2.630403000	0.632082000
H	-2.540642000	-2.788662000	0.941275000
H	-0.898795000	-3.492023000	0.960045000

H	-1.493100000	-2.608700000	-0.467772000
H	0.779887000	-2.143746000	2.424928000
H	1.043966000	0.480994000	3.170842000
C	-1.029728000	2.231555000	2.022663000
H	-2.054269000	2.374410000	2.399718000
H	-0.941100000	2.804301000	1.088456000
H	-0.333819000	2.670764000	2.750497000
C	-3.228687000	2.288106000	-0.483076000
H	-3.836801000	2.484248000	0.416857000
H	-3.903460000	2.392228000	-1.350069000
H	-2.471780000	3.084171000	-0.560647000
C	2.024099000	-1.503460000	-0.706869000
C	3.425371000	-1.608229000	-0.094689000
H	1.456687000	-2.441880000	-0.560467000
H	3.393213000	-1.424615000	0.999297000
H	2.076153000	-1.329870000	-1.797321000
H	3.782851000	-2.651645000	-0.189815000
C	4.494473000	-0.702760000	-0.724656000
C	4.452968000	0.801715000	-0.416604000
H	5.483746000	-1.072885000	-0.401785000
H	4.550035000	0.952483000	0.675838000
H	4.469459000	-0.844396000	-1.821541000
H	5.368046000	1.238718000	-0.853051000
C	3.249272000	1.617487000	-0.925076000
C	2.016122000	1.615995000	-0.015486000
H	3.588925000	2.664395000	-1.044729000
H	2.316944000	1.858497000	1.022315000
H	2.981669000	1.287389000	-1.946250000
H	1.308706000	2.407353000	-0.333714000
Cl	-3.921774000	-1.037782000	-1.044362000

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H-6-q SCF Done : -1813.296951 A.U.

Cr	0.636678000	0.533443000	-0.232435000
Al	-2.558778000	-0.091130000	-0.456479000
Cl	-0.837668000	-0.566145000	-1.924712000
N	-1.296716000	0.266490000	1.026137000
C	-0.414481000	-0.704649000	1.546594000
C	0.637745000	-0.049249000	2.185330000
C	0.406744000	1.354131000	2.058370000
C	-0.813653000	1.524294000	1.389534000
C	-0.658503000	-2.181864000	1.486274000
H	-1.552853000	-2.457664000	2.065984000
H	0.209797000	-2.705684000	1.909553000

H	-0.817129000	-2.550878000	0.462946000
H	1.471185000	-0.533434000	2.689808000
H	1.017808000	2.158194000	2.464427000
C	-1.540463000	2.810673000	1.140891000
H	-2.519040000	2.810515000	1.647706000
H	-1.718989000	3.007751000	0.075620000
H	-0.948929000	3.644124000	1.543792000
C	-3.609176000	1.411136000	-1.124013000
H	-4.242986000	1.860670000	-0.340806000
H	-4.291478000	1.026712000	-1.901940000
H	-3.012519000	2.214480000	-1.584657000
C	2.955487000	-2.380871000	-0.315623000
C	4.020598000	-1.560468000	0.415328000
H	2.640880000	-3.252908000	0.280760000
H	3.624994000	-1.214534000	1.388691000
H	3.337519000	-2.758523000	-1.278545000
H	4.860385000	-2.233120000	0.663678000
C	4.583495000	-0.354146000	-0.356447000
C	3.747497000	0.937227000	-0.375881000
H	5.564382000	-0.099302000	0.081034000
H	3.558235000	1.262193000	0.666180000
H	4.796558000	-0.660721000	-1.397920000
H	4.392377000	1.730502000	-0.804583000
C	2.441190000	0.912586000	-1.160818000
C	1.576425000	2.075832000	-1.181424000
H	2.504077000	0.343739000	-2.102306000
H	1.837126000	2.933762000	-0.545317000
H	1.072478000	2.359380000	-2.115099000
H	2.054965000	-1.786961000	-0.539227000
Cl	-3.678534000	-1.866176000	-0.031097000

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H-7-q SCF Done : -1891.821143 A.U.

Al	2.895828000	-0.104281000	0.380223000
Cl	2.064038000	-1.316149000	1.999338000
N	1.276745000	0.264282000	-0.754717000
C	0.508251000	-0.718187000	-1.361518000
C	-0.461898000	-0.101411000	-2.172585000
C	-0.224139000	1.306808000	-2.110863000
C	0.841231000	1.503746000	-1.233467000
C	0.763463000	-2.184361000	-1.224323000
H	-1.186347000	-0.621881000	-2.795598000
H	-0.765828000	2.089133000	-2.638450000
C	1.495674000	2.810182000	-0.905316000

C	3.767531000	1.505949000	1.087741000
H	4.205953000	2.158024000	0.314561000
H	4.607571000	1.152125000	1.712309000
H	3.139793000	2.132366000	1.744814000
C	-1.411001000	2.154606000	1.905939000
C	-0.346543000	1.405193000	2.250847000
H	-1.293563000	3.114101000	1.393195000
H	0.675299000	1.723958000	2.028537000
H	-2.427899000	1.871242000	2.188140000
H	-0.441249000	0.475867000	2.817357000
Cr	-1.152836000	0.501866000	-0.035220000
C	-1.787149000	-1.173589000	0.929738000
C	-2.735378000	-2.150356000	0.224104000
H	-0.834989000	-1.667531000	1.198639000
H	-2.499515000	-2.226020000	-0.855321000
H	-2.239914000	-0.835738000	1.881492000
H	-2.563382000	-3.168764000	0.621226000
C	-4.231117000	-1.848494000	0.387787000
C	-4.804733000	-0.628968000	-0.346285000
H	-4.798032000	-2.733282000	0.047787000
H	-4.655651000	-0.753356000	-1.435783000
H	-4.453367000	-1.752911000	1.467770000
H	-5.898354000	-0.648951000	-0.196607000
C	-4.295204000	0.764938000	0.064972000
C	-2.994864000	1.220026000	-0.606538000
H	-5.087460000	1.493474000	-0.193971000
H	-3.069347000	1.027502000	-1.692776000
H	-4.218410000	0.811326000	1.168161000
H	-2.876110000	2.318036000	-0.504396000
H	1.602298000	2.983528000	0.174170000
H	2.508663000	2.859676000	-1.334581000
H	0.906803000	3.632853000	-1.335100000
H	0.930655000	-2.480184000	-0.179849000
H	-0.084277000	-2.751903000	-1.631124000
H	1.674019000	-2.452106000	-1.783631000
Cl	4.154959000	-1.241862000	-0.960336000

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H-8-q SCF Done : -1891.855008 A.U.

C	4.740437000	-0.786472000	-1.020123000
C	5.074771000	0.578756000	-0.391083000
H	5.671575000	-1.175421000	-1.467915000
H	5.792244000	0.422486000	0.435414000
H	4.058370000	-0.645789000	-1.876114000

H	5.620871000	1.170899000	-1.148382000
Cr	0.443415000	0.123837000	0.058945000
Al	-2.958350000	0.274655000	-0.581176000
Cl	-1.078473000	0.063699000	-1.914782000
N	-1.910938000	0.038829000	1.070217000
C	-1.276580000	-1.150239000	1.431318000
C	-0.185149000	-0.848252000	2.254218000
C	-0.147555000	0.566287000	2.407299000
C	-1.225089000	1.088185000	1.677085000
C	-1.743764000	-2.517817000	1.038535000
H	0.480770000	-1.577544000	2.710696000
H	0.541915000	1.147065000	3.017201000
C	-1.649073000	2.524378000	1.608301000
C	-3.815901000	2.002707000	-0.877337000
H	-4.488751000	2.274969000	-0.045805000
H	-4.447491000	1.916376000	-1.778380000
H	-3.124222000	2.843022000	-1.043159000
C	1.643186000	-1.430064000	-0.484469000
C	2.782751000	-1.702828000	0.509244000
H	1.007129000	-2.318023000	-0.645125000
H	2.842213000	-0.901420000	1.269110000
H	2.005190000	-1.117266000	-1.478912000
H	2.546100000	-2.610252000	1.092515000
C	4.190038000	-1.892418000	-0.101159000
C	3.901303000	1.424215000	0.133892000
H	4.906074000	-2.058010000	0.725261000
H	3.422705000	0.898659000	0.974524000
H	4.181394000	-2.831170000	-0.683802000
H	4.311918000	2.347734000	0.578790000
C	2.828285000	1.805607000	-0.907292000
C	1.413807000	1.903364000	-0.323431000
H	3.113150000	2.769180000	-1.372349000
H	1.419355000	2.512951000	0.600178000
H	2.831499000	1.085106000	-1.742053000
H	0.731436000	2.404957000	-1.035864000
H	-1.543531000	2.958313000	0.603259000
H	-2.701058000	2.642362000	1.909455000
H	-1.028584000	3.118635000	2.293029000
H	-1.760816000	-2.667390000	-0.050754000
H	-1.071587000	-3.267110000	1.479261000
H	-2.765810000	-2.707069000	1.399580000
Cl	-4.247861000	-1.407412000	-0.897015000

H-9-q SCF Done : -1734.731819 A.U.

Cr	1.003354000	0.270265000	-0.311487000
Al	-2.254687000	0.121245000	-0.380598000
Cl	-0.699832000	-0.413372000	-2.000995000
N	-0.865995000	0.198595000	1.030484000
C	-0.100609000	-0.911154000	1.446886000
C	1.063536000	-0.441112000	2.053748000
C	1.011673000	0.988566000	2.029121000
C	-0.204900000	1.358769000	1.445265000
C	-0.538407000	-2.337182000	1.305918000
H	-1.442067000	-2.532979000	1.903267000
H	0.266844000	-2.995479000	1.660920000
H	-0.778054000	-2.613414000	0.269041000
H	1.848882000	-1.060419000	2.481871000
H	1.744038000	1.677339000	2.446200000
C	-0.765664000	2.741870000	1.309759000
H	-1.718446000	2.833574000	1.855674000
H	-0.954113000	3.033208000	0.267659000
H	-0.056499000	3.463031000	1.738790000
C	-3.156110000	1.787433000	-0.847021000
H	-3.662459000	2.249530000	0.017365000
H	-3.942432000	1.548784000	-1.584137000
H	-2.502229000	2.545784000	-1.306143000
C	4.272715000	-1.685278000	-0.075731000
C	4.092308000	-0.193296000	-0.366310000
H	5.199119000	-1.881146000	0.488361000
H	4.068438000	0.373424000	0.583516000
H	4.326013000	-2.265998000	-1.011834000
H	4.994791000	0.172838000	-0.896266000
C	2.860846000	0.141784000	-1.191624000
C	2.339401000	1.492106000	-1.260281000
H	2.775562000	-0.459391000	-2.111686000
H	2.806257000	2.265142000	-0.633508000
H	1.950178000	1.876028000	-2.212563000
H	3.429289000	-2.089253000	0.508939000
Cl	-3.553665000	-1.542411000	-0.019815000

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H-2-3-q SCF Done: -1734.691451 A.U.

Cr	1.598919000	-0.038571000	0.167489000
Al	-2.025217000	0.278931000	-0.573832000
Cl	-0.469665000	-0.620429000	-1.905216000
N	-0.826948000	0.355178000	1.002773000
C	-0.292315000	-0.763098000	1.625159000

C	0.840071000	-0.382027000	2.367724000
C	1.007868000	1.017301000	2.183652000
C	-0.019672000	1.441292000	1.323477000
C	-0.886582000	-2.134892000	1.559027000
H	-1.904006000	-2.140492000	1.976593000
H	-0.260512000	-2.832386000	2.132395000
H	-0.968557000	-2.504325000	0.526466000
H	1.433654000	-1.044560000	2.994119000
H	1.755747000	1.662553000	2.640931000
C	-0.325921000	2.854115000	0.934620000
H	-1.289162000	3.172973000	1.363721000
H	-0.389971000	2.996173000	-0.151824000
H	0.458032000	3.519772000	1.321179000
C	-2.693541000	1.991190000	-1.247129000
H	-3.185478000	2.594635000	-0.464959000
H	-3.464596000	1.772830000	-2.006672000
H	-1.932210000	2.621233000	-1.735050000
C	2.426081000	-1.904090000	0.034096000
C	2.896629000	-1.389348000	-1.241776000
H	1.610091000	-2.636178000	0.010651000
H	2.278958000	-1.658488000	-2.104146000
H	3.182422000	-2.118607000	0.801374000
H	3.961388000	-1.513111000	-1.454434000
C	3.110644000	0.558371000	-1.545157000
C	2.315070000	1.568823000	-0.868835000
H	2.939383000	0.440718000	-2.619670000
H	1.503404000	2.035004000	-1.440424000
H	4.177637000	0.588696000	-1.304797000
H	2.845636000	2.267447000	-0.208898000
Cl	-3.605597000	-1.118181000	-0.130374000

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H-3-9-q SCF Done: -1734.681834 A.U.

Cr	1.619708000	0.237847000	0.145420000
Al	-2.152045000	-0.242330000	-0.281364000
Cl	-1.287763000	-1.196320000	-2.051175000
N	-0.600114000	0.895491000	0.374110000
C	-0.000672000	0.964845000	1.640507000
C	0.976419000	1.972371000	1.620064000
C	0.957186000	2.562208000	0.323332000
C	-0.028989000	1.899893000	-0.417478000
C	-0.419816000	0.169400000	2.837255000
H	-1.422537000	0.478927000	3.173325000
H	0.289728000	0.353496000	3.656245000

H	-0.472503000	-0.906693000	2.636396000
H	1.606996000	2.253560000	2.461399000
H	1.573741000	3.384039000	-0.035923000
C	-0.489343000	2.239785000	-1.801795000
H	-1.446582000	2.784322000	-1.760377000
H	-0.642486000	1.346345000	-2.422360000
H	0.248848000	2.892837000	-2.288026000
C	-3.664365000	0.959612000	-0.612884000
H	-3.872258000	1.604178000	0.259697000
H	-4.575138000	0.362272000	-0.791584000
H	-3.534728000	1.615565000	-1.489708000
H	3.234808000	0.385251000	0.347941000
C	1.881995000	-1.672912000	0.844534000
C	3.192706000	-1.951419000	0.075710000
H	2.007068000	-1.737409000	1.936366000
H	4.058020000	-2.014071000	0.752292000
H	1.039511000	-2.314099000	0.539474000
H	3.162285000	-2.887501000	-0.510114000
C	3.377655000	-0.780094000	-0.885718000
C	2.339497000	-0.486751000	-1.775067000
H	4.379574000	-0.368420000	-1.048526000
H	2.476521000	0.267684000	-2.555588000
H	1.521911000	-1.200574000	-1.925251000
Cl	-2.539416000	-1.767670000	1.199555000

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H-4-5-q SCF Done: -1392.980028 A.U.

Cr	1.153728000	0.191020000	-0.027907000
Al	-2.703116000	-0.144190000	-0.331733000
Cl	-1.831585000	-1.720876000	-1.614227000
N	-1.061041000	0.349799000	0.805417000
C	-0.384797000	-0.553629000	1.623452000
C	0.607326000	0.136505000	2.342787000
C	0.497561000	1.510082000	1.992769000
C	-0.532689000	1.618053000	1.050745000
C	-0.778626000	-1.988254000	1.783987000
H	-1.648650000	-2.064033000	2.456218000
H	0.048221000	-2.555707000	2.233274000
H	-1.052829000	-2.449386000	0.825807000
H	1.287021000	-0.311244000	3.065801000
H	1.095362000	2.337558000	2.371992000
C	-1.079885000	2.886968000	0.473217000
H	-2.081271000	3.100906000	0.879633000
H	-1.182622000	2.853821000	-0.618635000

H	-0.421479000	3.726063000	0.740409000
C	-3.281337000	1.373285000	-1.462450000
H	-3.698241000	2.231077000	-0.906816000
H	-4.103185000	0.986558000	-2.093587000
H	-2.520052000	1.760306000	-2.161330000
C	-4.045560000	-0.823857000	0.951753000
H	-4.219464000	-0.120593000	1.787385000
H	-3.809081000	-1.806378000	1.392866000
H	-5.015672000	-0.938465000	0.434780000
C	1.949610000	-1.678888000	-0.385775000
C	3.369503000	-1.695078000	0.180896000
H	1.317964000	-2.481170000	0.025678000
H	3.336483000	-1.686642000	1.287485000
H	1.963467000	-1.809816000	-1.482827000
H	3.925985000	-2.612160000	-0.091914000
C	4.126753000	-0.453710000	-0.301341000
C	3.293015000	0.806467000	-0.095884000
H	5.099606000	-0.349390000	0.215405000
H	3.007933000	0.923917000	0.970919000
H	4.371362000	-0.562432000	-1.374137000
H	3.841263000	1.722637000	-0.343110000
C	2.172756000	1.284500000	-1.858062000
C	0.838383000	0.839177000	-1.992448000
H	2.344049000	2.357031000	-1.734107000
H	0.034212000	1.580583000	-1.971014000
H	2.970526000	0.768035000	-2.396956000
H	0.612273000	-0.074512000	-2.548867000

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H-5-6-q SCF Done: -1813.260821 A.U.

Cr	1.112571000	0.309193000	0.371159000
Al	-2.425099000	-0.025049000	-0.757559000
Cl	-0.751167000	-0.973452000	-1.865596000
N	-1.367274000	0.390393000	0.876452000
C	-0.767880000	-0.567233000	1.685507000
C	0.169518000	0.061932000	2.524336000
C	0.152285000	1.447028000	2.207318000
C	-0.793344000	1.619375000	1.181847000
C	-1.137352000	-2.017707000	1.688294000
H	-2.185913000	-2.151956000	1.991868000
H	-0.491110000	-2.561466000	2.391417000
H	-1.034576000	-2.470776000	0.691496000
H	0.762275000	-0.432702000	3.291727000
H	0.724130000	2.243898000	2.679101000

C	-1.254332000	2.922189000	0.606306000
H	-2.292715000	3.131156000	0.909871000
H	-1.226715000	2.939090000	-0.490267000
H	-0.617822000	3.735967000	0.980162000
C	-3.177243000	1.509023000	-1.714872000
H	-3.807486000	2.153734000	-1.078918000
H	-3.836228000	1.107780000	-2.505119000
H	-2.431315000	2.146801000	-2.217041000
C	2.295516000	-1.600303000	0.360669000
C	3.832751000	-1.527592000	0.391292000
H	1.902063000	-1.917237000	1.337888000
H	4.156754000	-0.949539000	1.276869000
H	1.944238000	-2.338608000	-0.379659000
H	4.253333000	-2.540465000	0.524990000
C	4.447266000	-0.882681000	-0.864061000
C	3.987808000	0.569229000	-1.079187000
H	5.546929000	-0.909033000	-0.789232000
H	4.276684000	1.172134000	-0.198980000
H	4.186037000	-1.486475000	-1.753278000
H	4.521598000	1.009547000	-1.939540000
C	2.480532000	0.718377000	-1.312372000
C	1.772472000	1.875593000	-0.819115000
H	2.140511000	0.324771000	-2.280991000
H	2.335191000	2.634231000	-0.259455000
H	0.955690000	2.283067000	-1.425001000
H	2.176783000	-0.486327000	-0.576103000
Cl	-3.931823000	-1.451767000	-0.164539000

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H-7-8-q SCF Done: -1891.798629 A.U.

C	-4.846968000	-0.450976000	-0.370242000
C	-4.387417000	0.919494000	0.149058000
H	-4.690241000	-0.489554000	-1.465155000
H	-5.042893000	1.679646000	-0.312495000
H	-5.941447000	-0.489862000	-0.232433000
H	-4.596533000	0.990578000	1.232001000
Cr	-0.967285000	0.363723000	0.008064000
Al	2.865628000	-0.057933000	0.519394000
Cl	2.000174000	-1.540063000	1.871615000
N	1.321382000	0.360352000	-0.704937000
C	0.666443000	-0.579844000	-1.501917000
C	-0.251016000	0.089498000	-2.327157000
C	-0.110945000	1.482594000	-2.069453000
C	0.862075000	1.627495000	-1.077509000

C	1.020100000	-2.032270000	-1.540986000
H	-0.895288000	-0.385633000	-3.065071000
H	-0.651057000	2.298510000	-2.547118000
C	1.433351000	2.914290000	-0.568278000
C	3.563179000	1.487796000	1.504296000
H	4.012514000	2.267385000	0.867734000
H	4.372202000	1.105971000	2.152682000
H	2.829210000	1.968517000	2.173383000
C	-1.667972000	-1.473554000	0.604241000
C	-2.831272000	-2.152078000	-0.132510000
H	-0.765715000	-2.105390000	0.547049000
H	-2.719697000	-2.057446000	-1.230918000
H	-1.905639000	-1.404608000	1.681474000
H	-2.766874000	-3.240140000	0.058117000
C	-4.258161000	-1.722973000	0.262304000
C	-2.940837000	1.306926000	-0.164565000
H	-4.935653000	-2.548440000	-0.015942000
H	-2.673692000	0.803655000	-1.120729000
H	-4.324135000	-1.652244000	1.364586000
H	-2.835243000	2.383917000	-0.354360000
C	-2.095337000	1.413394000	1.775821000
C	-0.703553000	1.200714000	1.906859000
H	-2.485414000	2.433745000	1.790723000
H	-0.036979000	2.068425000	1.877625000
H	-2.773921000	0.676340000	2.208079000
H	-0.333399000	0.342854000	2.477713000
H	2.458999000	3.058750000	-0.943806000
H	1.485708000	2.960612000	0.526728000
H	0.821859000	3.754751000	-0.926687000
H	1.174308000	-2.450889000	-0.537609000
H	1.965033000	-2.164819000	-2.091463000
H	0.227652000	-2.596669000	-2.051763000
Cl	4.295609000	-0.924037000	-0.858275000

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I-0-s SCF Done : -1997.857943 A.U.

Cr	1.824208000	-0.000349000	1.249788000
Al	-1.333756000	0.000039000	-0.056133000
Cl	-0.511726000	-0.001706000	2.089391000
N	0.375897000	0.000333000	-0.969714000
C	1.200978000	1.130840000	-0.990638000
C	2.535687000	0.718592000	-0.977563000
C	2.535736000	-0.717828000	-0.977812000
C	1.201035000	-1.130125000	-0.991066000

C	0.706894000	2.542335000	-1.105402000
H	0.057438000	2.662034000	-1.986437000
H	1.568942000	3.215311000	-1.216975000
H	0.120693000	2.875567000	-0.236856000
H	3.399808000	1.375140000	-1.069446000
H	3.399893000	-1.374297000	-1.069949000
C	0.707048000	-2.541595000	-1.106481000
H	0.059154000	-2.661365000	-1.988680000
H	0.119257000	-2.874636000	-0.238954000
H	1.569223000	-3.214669000	-1.216444000
Cl	-2.469952000	1.770853000	-0.353920000
Cl	-2.470800000	-1.769786000	-0.356627000

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I-1-q SCF Done : -2076.409235 A.U.

Cr	-1.566537000	-0.001361000	-0.446521000
Al	1.663803000	-0.103120000	-0.195294000
Cl	3.087397000	1.467351000	-0.139290000
N	0.165631000	0.204159000	1.031418000
C	-0.512504000	1.443699000	1.105312000
C	-1.768223000	1.222346000	1.666331000
C	-1.858630000	-0.171934000	1.981327000
C	-0.645062000	-0.770705000	1.636580000
C	0.077802000	2.759135000	0.695776000
H	0.952992000	3.010501000	1.314379000
H	-0.680385000	3.543787000	0.826278000
H	0.412083000	2.778780000	-0.351858000
H	-2.520622000	1.985488000	1.853424000
H	-2.692789000	-0.679252000	2.462520000
C	-0.233240000	-2.187472000	1.894626000
H	0.644043000	-2.224618000	2.559833000
H	0.036453000	-2.736037000	0.982366000
H	-1.062402000	-2.714494000	2.386569000
C	-3.358890000	0.276509000	-1.400790000
C	-3.043630000	-1.130761000	-1.302833000
H	-4.159093000	0.693718000	-0.775790000
H	-3.608786000	-1.760467000	-0.603187000
H	-3.248796000	0.787562000	-2.366952000
H	-2.694923000	-1.669192000	-2.193999000
Cl	2.515042000	-2.038984000	-0.028862000
Cl	0.367240000	0.000070000	-2.050447000

32

I-2-q SCF Done : -2154.954036 A.U.

Cr	1.794797000	0.085120000	0.056584000
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Al	-1.869983000	0.011760000	-0.377782000
Cl	-0.592384000	-0.446697000	-2.094964000
N	-0.535761000	-0.195566000	1.052107000
C	0.157706000	-1.385634000	1.224436000
C	1.281892000	-1.152760000	2.035626000
C	1.265967000	0.222926000	2.385528000
C	0.144995000	0.796466000	1.765643000
C	-0.305295000	-2.709085000	0.700287000
H	-1.279719000	-2.973553000	1.137847000
H	0.423451000	-3.487256000	0.965034000
H	-0.435660000	-2.703473000	-0.391964000
H	1.980536000	-1.914730000	2.374264000
H	1.954283000	0.746338000	3.046956000
C	-0.389309000	2.169030000	2.027359000
H	-1.294047000	2.104098000	2.654196000
H	-0.674861000	2.708917000	1.117553000
H	0.361273000	2.754772000	2.576236000
C	2.824176000	-1.709010000	-0.621968000
C	3.153508000	-0.799869000	-1.616683000
H	2.021541000	-2.433254000	-0.785147000
H	2.582304000	-0.773725000	-2.547409000
H	3.557069000	-1.974480000	0.148202000
H	4.150866000	-0.359413000	-1.661727000
C	2.635629000	1.715613000	-1.368406000
C	1.745226000	2.200555000	-0.420229000
H	2.312037000	1.551055000	-2.397713000
H	0.709309000	2.413620000	-0.703013000
H	3.712787000	1.833799000	-1.225937000
H	2.114815000	2.719339000	0.470810000
Cl	-3.429130000	-1.406850000	-0.043860000
Cl	-2.584249000	2.022474000	-0.523489000

32

I-3-q SCF Done : -2154.97572 A.U.

Cr	1.328661000	0.143258000	-0.045351000
Al	-1.959430000	-0.242505000	-0.373596000
Cl	-0.316014000	-0.117412000	-1.933807000
N	-0.802122000	0.363723000	1.084929000
C	-0.016260000	-0.439516000	1.914316000
C	1.066824000	0.322848000	2.373639000
C	0.907694000	1.644678000	1.861612000
C	-0.247569000	1.657300000	1.081027000
C	-0.335696000	-1.854982000	2.283846000
H	-1.335723000	-1.922340000	2.739156000

H	0.403915000	-2.209579000	3.014590000
H	-0.329876000	-2.538430000	1.423757000
H	1.840896000	-0.031010000	3.051795000
H	1.551423000	2.501921000	2.047701000
C	-0.858106000	2.841163000	0.394653000
H	-1.851363000	3.070932000	0.809273000
H	-0.988943000	2.692884000	-0.687154000
H	-0.206416000	3.713410000	0.542121000
C	2.461394000	-1.559124000	-0.229396000
C	3.898245000	-1.122447000	-0.541789000
H	2.389041000	-2.232847000	0.642337000
H	4.413353000	-0.836814000	0.395200000
H	2.008801000	-2.079828000	-1.095414000
H	4.501183000	-1.940645000	-0.980584000
C	3.845966000	0.098985000	-1.468790000
C	2.930416000	1.148799000	-0.828400000
H	4.858167000	0.495048000	-1.679481000
H	3.433019000	1.638098000	0.028804000
H	3.432742000	-0.209216000	-2.447405000
H	2.606537000	1.941253000	-1.527519000
Cl	-2.590447000	-2.257373000	-0.172449000
Cl	-3.531458000	1.121212000	-0.774380000

38

I-4-q SCF Done : -2233.511166 A.U.

Cr	1.596872000	0.194437000	0.121387000
Al	-2.326722000	-0.096488000	-0.330479000
Cl	-1.655594000	-0.799092000	-2.257526000
N	-0.726903000	-0.189375000	0.841640000
C	-0.005331000	-1.367460000	1.023120000
C	1.017361000	-1.130609000	1.954952000
C	0.866412000	0.211681000	2.416055000
C	-0.207929000	0.771205000	1.725466000
C	-0.362418000	-2.679224000	0.400883000
H	-1.296393000	-3.057308000	0.847880000
H	0.437288000	-3.407706000	0.590361000
H	-0.527704000	-2.598944000	-0.681521000
H	1.731388000	-1.873103000	2.305200000
H	1.469362000	0.720155000	3.165489000
C	-0.782241000	2.135722000	1.952910000
H	-1.812830000	2.070166000	2.334619000
H	-0.832901000	2.747299000	1.042662000
H	-0.170440000	2.658323000	2.701778000
C	2.366606000	-1.104426000	-1.285785000

C	3.813773000	-1.420801000	-0.893052000
H	1.744334000	-2.004154000	-1.421979000
H	3.827897000	-2.158473000	-0.068370000
H	2.342793000	-0.548891000	-2.242868000
H	4.384914000	-1.883206000	-1.720929000
C	4.472435000	-0.124844000	-0.408253000
C	3.575583000	0.486612000	0.672860000
H	5.504738000	-0.296935000	-0.047745000
H	3.682519000	-0.080385000	1.615903000
H	4.568755000	0.568733000	-1.265512000
H	3.811699000	1.541711000	0.901778000
C	1.907196000	2.391334000	-1.060161000
C	0.800413000	1.867892000	-1.625821000
H	1.844081000	3.087531000	-0.218102000
H	-0.204379000	2.117587000	-1.270059000
H	2.902590000	2.210509000	-1.472222000
H	0.849298000	1.227022000	-2.509694000
Cl	-3.758573000	-1.352518000	0.636994000
Cl	-2.939797000	1.954613000	-0.516778000

38

I-5-q SCF Done : -2233.542942 A.U.

Cr	-0.990033000	0.081672000	0.029691000
Al	2.373945000	-0.191234000	-0.426505000
Cl	0.613486000	-0.266057000	-1.865875000
N	1.288029000	0.357964000	1.095872000
C	0.676693000	1.616961000	1.149745000
C	-0.443689000	1.534896000	1.979710000
C	-0.521529000	0.196272000	2.460266000
C	0.562673000	-0.506261000	1.919021000
C	1.187093000	2.843242000	0.456813000
H	2.210240000	3.087766000	0.778657000
H	0.531047000	3.690069000	0.701186000
H	1.213374000	2.738087000	-0.638246000
H	-1.107450000	2.361549000	2.225371000
H	-1.243932000	-0.209524000	3.165850000
C	0.943008000	-1.923712000	2.219848000
H	1.961735000	-1.979681000	2.632538000
H	0.922530000	-2.574873000	1.334610000
H	0.243918000	-2.330973000	2.963069000
C	-2.269326000	1.397076000	-0.823736000
C	-3.665694000	1.443457000	-0.193407000
H	-1.768654000	2.381038000	-0.755283000
H	-3.603249000	1.333112000	0.909357000

H	-2.319963000	1.137257000	-1.897054000
H	-4.097538000	2.451184000	-0.346112000
C	-4.677027000	0.425752000	-0.742083000
C	-4.510106000	-1.051817000	-0.355210000
H	-5.683093000	0.738142000	-0.410460000
H	-4.560797000	-1.148417000	0.746410000
H	-4.690560000	0.507555000	-1.845250000
H	-5.401640000	-1.580125000	-0.735162000
C	-3.262445000	-1.799171000	-0.864078000
C	-2.011452000	-1.678759000	0.012444000
H	-3.527103000	-2.871454000	-0.938166000
H	-2.261945000	-1.932272000	1.060651000
H	-3.042498000	-1.489405000	-1.902680000
H	-1.245004000	-2.408147000	-0.316281000
Cl	3.214746000	-2.129316000	-0.229438000
Cl	3.777926000	1.285471000	-1.015753000

38

I-6-q SCF Done : -2233.546042 A.U.

Cr	-0.767592000	-0.539405000	-0.177041000
Al	2.363376000	0.320517000	-0.341833000
Cl	0.730488000	0.550939000	-1.897161000
N	1.119234000	-0.097196000	1.110636000
C	0.168598000	0.849797000	1.559616000
C	-0.862048000	0.168903000	2.202884000
C	-0.551682000	-1.224139000	2.151683000
C	0.694696000	-1.364004000	1.525769000
C	0.335961000	2.334186000	1.439708000
H	1.203359000	2.681946000	2.021668000
H	-0.565793000	2.827029000	1.828377000
H	0.489202000	2.671358000	0.404519000
H	-1.733849000	0.630424000	2.661740000
H	-1.129166000	-2.039677000	2.582893000
C	1.482910000	-2.627402000	1.366124000
H	2.448081000	-2.554336000	1.892018000
H	1.704963000	-2.867436000	0.318235000
H	0.913960000	-3.459984000	1.802044000
C	-3.188134000	2.260745000	-0.531088000
C	-4.241940000	1.450467000	0.227155000
H	-2.919654000	3.180682000	0.013509000
H	-3.862874000	1.188362000	1.232842000
H	-3.558321000	2.560445000	-1.525459000
H	-5.113402000	2.104606000	0.405342000
C	-4.736046000	0.173083000	-0.474266000

C	-3.850643000	-1.081853000	-0.385942000
H	-5.717555000	-0.091881000	-0.044468000
H	-3.681878000	-1.332696000	0.679725000
H	-4.933061000	0.400569000	-1.538838000
H	-4.450620000	-1.926067000	-0.780737000
C	-2.522694000	-1.056194000	-1.133285000
C	-1.611331000	-2.178480000	-1.050852000
H	-2.576148000	-0.550440000	-2.110883000
H	-1.854286000	-3.004214000	-0.367400000
H	-1.061341000	-2.497263000	-1.946306000
H	-2.261662000	1.687233000	-0.695013000
Cl	3.622921000	-1.302353000	-0.873925000
Cl	3.400582000	2.140829000	-0.011295000

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I-7-q SCF Done : -2312.07609 A.U.

Al	2.690011000	-0.316039000	0.282300000
Cl	1.957765000	-1.475212000	1.949512000
N	1.111587000	0.063957000	-0.857002000
C	0.286179000	-0.943251000	-1.348387000
C	-0.678353000	-0.368720000	-2.190645000
C	-0.380486000	1.025650000	-2.278638000
C	0.718024000	1.269760000	-1.457770000
C	0.501719000	-2.401521000	-1.098774000
H	-1.440767000	-0.916875000	-2.739879000
H	-0.902784000	1.772322000	-2.872977000
C	1.426019000	2.581303000	-1.309620000
C	-1.320198000	2.298881000	1.693397000
C	-0.291772000	1.518257000	2.078922000
H	-1.158655000	3.198799000	1.091757000
H	0.742873000	1.748455000	1.804922000
H	-2.342942000	2.111735000	2.030263000
H	-0.432547000	0.654300000	2.733334000
Cr	-1.260695000	0.481149000	-0.087854000
C	-1.946110000	-1.065131000	1.045765000
C	-2.969427000	-2.040901000	0.451489000
H	-1.015770000	-1.591186000	1.330456000
H	-2.775180000	-2.215977000	-0.624816000
H	-2.347790000	-0.622496000	1.977264000
H	-2.837615000	-3.032110000	0.925370000
C	-4.440434000	-1.643833000	0.636580000
C	-4.976552000	-0.460370000	-0.180213000
H	-5.065119000	-2.521273000	0.392357000
H	-4.878989000	-0.686373000	-1.259271000

H	-4.616969000	-1.446120000	1.711002000
H	-6.062620000	-0.404578000	0.009600000
C	-4.375944000	0.932058000	0.088409000
C	-3.078806000	1.249299000	-0.662127000
H	-5.135313000	1.680033000	-0.210437000
H	-3.204363000	0.968767000	-1.724132000
H	-4.255820000	1.072264000	1.179620000
H	-2.892491000	2.342578000	-0.659202000
H	1.494834000	2.927672000	-0.270176000
H	2.461394000	2.513784000	-1.677759000
H	0.897799000	3.339425000	-1.904999000
H	0.628206000	-2.633973000	-0.033226000
H	-0.345894000	-2.975920000	-1.495392000
H	1.419708000	-2.729054000	-1.613593000
Cl	4.025919000	-1.367361000	-1.013441000
Cl	3.470969000	1.539641000	1.036118000

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I-8-q SCF Done : -2312.104461 A.U.

C	-4.901374000	0.546053000	-1.128762000
C	-5.179105000	-0.783163000	-0.402786000
H	-5.840678000	0.850138000	-1.622647000
H	-5.915873000	-0.602121000	0.401350000
H	-4.193970000	0.376864000	-1.958747000
H	-5.683597000	-1.456806000	-1.119541000
Cr	-0.600956000	-0.076166000	0.096994000
Al	2.789088000	-0.029796000	-0.503305000
Cl	0.973794000	-0.047201000	-1.868558000
N	1.740714000	0.193520000	1.123009000
C	1.047101000	1.376081000	1.398402000
C	-0.040372000	1.078495000	2.225107000
C	-0.018060000	-0.323664000	2.468847000
C	1.091757000	-0.847052000	1.790337000
C	1.460830000	2.737089000	0.928553000
H	-0.743795000	1.805604000	2.625337000
H	-0.688206000	-0.893293000	3.109891000
C	1.573585000	-2.264698000	1.839890000
C	-1.855562000	1.382042000	-0.570047000
C	-3.033850000	1.673909000	0.371452000
H	-1.256208000	2.284462000	-0.782939000
H	-3.079899000	0.930474000	1.188957000
H	-2.176664000	0.979513000	-1.546575000
H	-2.856750000	2.633716000	0.887861000
C	-4.429929000	1.746747000	-0.288387000

C	-3.973721000	-1.528354000	0.196971000
H	-5.176230000	1.942137000	0.503863000
H	-3.533834000	-0.920739000	1.002725000
H	-4.447503000	2.635775000	-0.944124000
H	-4.344422000	-2.437232000	0.702661000
C	-2.867058000	-1.928134000	-0.800492000
C	-1.461994000	-1.925419000	-0.188055000
H	-3.099693000	-2.931242000	-1.206993000
H	-1.456247000	-2.476340000	0.771178000
H	-2.884164000	-1.262840000	-1.679964000
H	-0.741790000	-2.434607000	-0.856388000
H	1.586078000	-2.753179000	0.855591000
H	2.600102000	-2.317041000	2.233485000
H	0.916252000	-2.842916000	2.503536000
H	1.463157000	2.833981000	-0.167321000
H	0.763074000	3.482429000	1.334595000
H	2.476552000	2.984163000	1.271872000
Cl	4.037280000	1.633039000	-0.926631000
Cl	3.801902000	-1.891120000	-0.628329000

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I-9-q SCF Done : -2154.98083 A.U.

Cr	-1.130450000	-0.337865000	-0.287547000
Al	2.079865000	0.174499000	-0.291498000
Cl	0.598206000	0.305148000	-2.000537000
N	0.691477000	0.008082000	1.081298000
C	-0.184711000	1.070129000	1.403192000
C	-1.316541000	0.535555000	2.013429000
C	-1.132550000	-0.881905000	2.093398000
C	0.127548000	-1.181299000	1.566819000
C	0.120827000	2.519194000	1.173402000
H	0.990785000	2.839722000	1.767137000
H	-0.749294000	3.118242000	1.476198000
H	0.348147000	2.753674000	0.123296000
H	-2.166579000	1.106747000	2.380127000
H	-1.809535000	-1.604297000	2.545458000
C	0.801949000	-2.518985000	1.553404000
H	1.744319000	-2.488004000	2.122569000
H	1.051604000	-2.870755000	0.543423000
H	0.137142000	-3.256282000	2.024099000
C	-4.473819000	1.499959000	-0.284982000
C	-4.233091000	-0.002788000	-0.446883000
H	-5.420796000	1.706383000	0.239583000
H	-4.214027000	-0.490272000	0.545993000

H	-4.523552000	1.999696000	-1.266905000
H	-5.106983000	-0.444897000	-0.966332000
C	-2.970402000	-0.357908000	-1.214112000
C	-2.396561000	-1.686098000	-1.157907000
H	-2.883106000	0.168258000	-2.179031000
H	-2.844806000	-2.422994000	-0.476800000
H	-1.966664000	-2.131583000	-2.064803000
H	-3.660571000	1.981914000	0.283238000
Cl	3.206387000	1.960000000	-0.0914445000
Cl	3.270127000	-1.568498000	-0.506506000

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I-2-3-q SCF Done: -2154.943078 A.U.

Cr	1.776728000	0.011772000	0.155000000
Al	-1.911761000	0.051653000	-0.398677000
Cl	-0.499300000	-0.253591000	-2.050000000
N	-0.623910000	-0.165136000	1.069803000
C	0.047708000	-1.363018000	1.281413000
C	1.161915000	-1.127594000	2.105477000
C	1.173166000	0.261783000	2.405748000
C	0.075158000	0.836529000	1.744427000
C	-0.404966000	-2.691934000	0.762466000
H	-1.379587000	-2.966181000	1.192749000
H	0.331926000	-3.460018000	1.034201000
H	-0.526120000	-2.694614000	-0.330733000
H	1.846435000	-1.890840000	2.469206000
H	1.866778000	0.795878000	3.052532000
C	-0.387946000	2.252210000	1.884036000
H	-1.329114000	2.291188000	2.455779000
H	-0.585763000	2.739411000	0.921818000
H	0.370882000	2.830251000	2.429312000
C	2.849416000	-1.565143000	-0.573734000
C	3.061762000	-0.638271000	-1.677132000
H	2.169715000	-2.407377000	-0.750308000
H	2.370467000	-0.759534000	-2.517233000
H	3.726037000	-1.835669000	0.031027000
H	4.091873000	-0.520312000	-2.022538000
C	2.986886000	1.308834000	-1.393420000
C	2.141487000	1.940616000	-0.393626000
H	2.717459000	1.484226000	-2.439743000
H	1.211750000	2.406599000	-0.741738000
H	4.059470000	1.441817000	-1.222515000
H	2.641259000	2.501510000	0.406650000
Cl	-3.404395000	-1.465283000	-0.244093000

Cl	-2.757022000	2.010728000	-0.462860000
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I-3-9-q SCF Done: -2154.935583 A.U.

Cr	1.789492000	0.289837000	0.175223000
Al	-1.908196000	-0.422599000	-0.249485000
Cl	-1.114146000	-0.999193000	-2.176560000
N	-0.464689000	0.701456000	0.542707000
C	0.159292000	0.599127000	1.797434000
C	1.044117000	1.676888000	1.942222000
C	0.940639000	2.480818000	0.769552000
C	-0.004229000	1.877786000	-0.067575000
C	-0.162921000	-0.427403000	2.837740000
H	-1.182210000	-0.274553000	3.226661000
H	0.544405000	-0.323957000	3.672542000
H	-0.119456000	-1.453595000	2.454392000
H	1.669542000	1.862549000	2.813290000
H	1.474502000	3.404908000	0.556275000
C	-0.529592000	2.408650000	-1.364827000
H	-1.563533000	2.764722000	-1.231784000
H	-0.553089000	1.640880000	-2.150480000
H	0.092934000	3.250025000	-1.699142000
H	3.396148000	0.513216000	0.374832000
C	2.201819000	-1.694910000	0.494289000
C	3.502672000	-1.727485000	-0.338375000
H	2.367354000	-1.953064000	1.551649000
H	4.391589000	-1.853446000	0.297392000
H	1.398589000	-2.331588000	0.089744000
H	3.516532000	-2.536550000	-1.090358000
C	3.576532000	-0.386219000	-1.063550000
C	2.491438000	-0.005129000	-1.859062000
H	4.542260000	0.120549000	-1.164531000
H	2.551933000	0.891115000	-2.483557000
H	1.721419000	-0.736906000	-2.128024000
Cl	-2.268114000	-2.149274000	0.956019000
Cl	-3.585737000	0.903201000	-0.352223000

38

I-4-5-q SCF Done: -2233.493685 A.U.

Cr	1.463934000	0.143893000	0.074549000
Al	-2.304460000	-0.037376000	-0.394116000
Cl	-1.613582000	-0.917809000	-2.237529000
N	-0.752423000	-0.131773000	0.848362000
C	-0.086489000	-1.330077000	1.132385000
C	0.886329000	-1.080762000	2.111844000

C	0.772506000	0.287314000	2.481564000
C	-0.241116000	0.854026000	1.704135000
C	-0.487711000	-2.663359000	0.584797000
H	-1.453739000	-2.964620000	1.021730000
H	0.267856000	-3.414421000	0.852473000
H	-0.613411000	-2.651464000	-0.505749000
H	1.554360000	-1.828362000	2.535589000
H	1.355027000	0.816487000	3.234054000
C	-0.776902000	2.246443000	1.836716000
H	-1.819432000	2.233800000	2.190960000
H	-0.780945000	2.803206000	0.891184000
H	-0.170766000	2.792907000	2.573350000
C	2.328469000	-1.318910000	-1.091605000
C	3.762836000	-1.512149000	-0.597072000
H	1.746238000	-2.253810000	-1.075966000
H	3.761434000	-2.015910000	0.388438000
H	2.320172000	-0.947731000	-2.132014000
H	4.355217000	-2.167738000	-1.263253000
C	4.445787000	-0.147663000	-0.454478000
C	3.558961000	0.829216000	0.310735000
H	5.425428000	-0.239367000	0.051343000
H	3.289240000	0.421805000	1.309290000
H	4.666898000	0.263469000	-1.456625000
H	4.058342000	1.781718000	0.521415000
C	2.378782000	2.016195000	-1.021414000
C	1.086422000	1.581708000	-1.397342000
H	2.456452000	2.907706000	-0.392961000
H	0.214786000	2.160989000	-1.076395000
H	3.212486000	1.890563000	-1.716264000
H	0.951115000	1.027022000	-2.330087000
Cl	-3.814061000	-1.168915000	0.617565000
Cl	-2.835502000	2.014180000	-0.722759000

38

I-5-6-q SCF Done: -2233.512999 A.U.

Cr	1.282513000	0.129714000	0.519156000
Al	-2.280696000	-0.027848000	-0.625000000
Cl	-0.749912000	-0.466512000	-2.117698000
N	-1.170374000	-0.128052000	1.000928000
C	-0.507792000	-1.297245000	1.367748000
C	0.408649000	-1.002008000	2.390890000
C	0.312051000	0.391489000	2.651882000
C	-0.659590000	0.910592000	1.779708000
C	-0.806563000	-2.649665000	0.799264000

H	-1.835348000	-2.954073000	1.042943000
H	-0.109688000	-3.387641000	1.219915000
H	-0.716274000	-2.665964000	-0.296651000
H	1.039843000	-1.728222000	2.899887000
H	0.849128000	0.964477000	3.405370000
C	-1.195384000	2.307661000	1.796804000
H	-2.233835000	2.313716000	2.164656000
H	-1.211474000	2.776318000	0.805513000
H	-0.584838000	2.921029000	2.473880000
C	2.572399000	-1.540082000	-0.237141000
C	4.099142000	-1.346105000	-0.283415000
H	2.292240000	-2.208644000	0.590671000
H	4.467102000	-1.084123000	0.726108000
H	2.201384000	-2.006456000	-1.165386000
H	4.589057000	-2.301682000	-0.542455000
C	4.555992000	-0.255146000	-1.268002000
C	3.998361000	1.135614000	-0.921879000
H	5.657451000	-0.211804000	-1.281989000
H	4.337265000	1.417106000	0.091689000
H	4.247280000	-0.531400000	-2.293618000
H	4.420379000	1.891864000	-1.606412000
C	2.469563000	1.229996000	-0.978282000
C	1.750521000	2.069186000	-0.050930000
H	2.057860000	1.179885000	-1.996756000
H	2.321106000	2.615884000	0.711253000
H	0.861674000	2.599791000	-0.409197000
H	2.308337000	-0.182691000	-0.706284000
Cl	-3.800718000	-1.520609000	-0.462674000
Cl	-3.089451000	1.928424000	-0.916936000

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I-7-8-q SCF Done: -2312.052239 A.U.

C	5.039214000	-0.182021000	0.162199000
C	4.414451000	1.198159000	-0.091454000
H	4.957626000	-0.418714000	1.240276000
H	5.011945000	1.934999000	0.474642000
H	6.120865000	-0.078598000	-0.031355000
H	4.557359000	1.477679000	-1.150940000
Cr	1.085942000	0.251562000	0.088463000
Al	-2.704103000	-0.155656000	-0.397320000
Cl	-1.961412000	-1.364247000	-2.025167000
N	-1.177107000	0.048653000	0.858778000
C	-0.491160000	-1.046151000	1.395851000
C	0.445194000	-0.577402000	2.327957000

C	0.285447000	0.833328000	2.411348000
C	-0.716562000	1.201473000	1.511288000
C	-0.844238000	-2.473267000	1.118480000
H	1.113266000	-1.204897000	2.915163000
H	0.832639000	1.520253000	3.054898000
C	-1.293302000	2.574510000	1.352367000
C	1.918159000	-1.393892000	-0.818637000
C	3.194915000	-2.034587000	-0.256252000
H	1.094710000	-2.128451000	-0.799062000
H	3.147348000	-2.118910000	0.847532000
H	2.067966000	-1.148524000	-1.885742000
H	3.234266000	-3.082065000	-0.610803000
C	4.538380000	-1.388801000	-0.649267000
C	2.954210000	1.365182000	0.332639000
H	5.314009000	-2.167781000	-0.553596000
H	2.790753000	0.683670000	1.199018000
H	4.518280000	-1.130794000	-1.725019000
H	2.746129000	2.377412000	0.705696000
C	2.001646000	1.681906000	-1.526355000
C	0.637657000	1.326812000	-1.645209000
H	2.272688000	2.731412000	-1.389082000
H	-0.131925000	2.082566000	-1.458488000
H	2.734418000	1.109649000	-2.097746000
H	0.343014000	0.531459000	-2.337209000
H	-2.342603000	2.600319000	1.685655000
H	-1.292639000	2.930877000	0.314568000
H	-0.719056000	3.276503000	1.973953000
H	-0.955749000	-2.680873000	0.045981000
H	-1.808185000	-2.712821000	1.596247000
H	-0.071691000	-3.134238000	1.534596000
Cl	-4.200720000	-1.117139000	0.795015000
Cl	-3.291339000	1.768672000	-1.138572000

26

J-0-s SCF Done : -939.788795 A.U.

Cr	-1.735136000	0.109785000	0.158880000
Cl	-3.460821000	-0.334098000	-1.224730000
N	1.332484000	0.058812000	0.231945000
C	1.310502000	1.449240000	-0.018554000
C	0.392317000	2.037870000	0.816139000
C	-0.177877000	1.014322000	1.644548000
C	0.388069000	-0.205553000	1.260115000
C	2.064746000	2.135581000	-1.114404000
H	3.148434000	2.175130000	-0.928228000

H	1.703673000	3.170138000	-1.196442000
H	1.915703000	1.652250000	-2.092577000
H	0.137808000	3.096008000	0.822735000
H	-0.787166000	1.164166000	2.536900000
C	0.366969000	-1.470147000	2.077703000
H	1.365555000	-1.688167000	2.494991000
H	0.038266000	-2.358908000	1.524073000
H	-0.321150000	-1.332542000	2.923950000
C	1.643349000	-2.446182000	-0.588707000
H	2.098745000	-3.064038000	0.207664000
H	2.007193000	-2.875949000	-1.537096000
H	0.554603000	-2.589791000	-0.541358000
C	3.515041000	-0.583284000	-1.146510000
H	4.054543000	0.261533000	-0.697514000
H	3.363505000	-0.346962000	-2.216311000
H	4.176161000	-1.465768000	-1.132323000
B	2.135055000	-0.951006000	-0.473353000

32

J-1-q SCF Done : -1018.325056 A.U.

Cr	-1.202490000	-0.194488000	-0.011200000
Cl	-1.160107000	-2.225856000	-1.047388000
N	1.257166000	0.400133000	0.396961000
C	0.394787000	1.488513000	0.693181000
C	-0.369153000	1.141728000	1.804681000
C	-0.000434000	-0.181962000	2.198264000
C	0.988435000	-0.625679000	1.338446000
C	0.506055000	2.856782000	0.092093000
H	1.529432000	3.253712000	0.194708000
H	-0.168974000	3.532816000	0.634681000
H	0.232374000	2.894614000	-0.969190000
H	-1.074549000	1.800808000	2.305349000
H	-0.427687000	-0.765316000	3.011226000
C	1.625558000	-1.978132000	1.347489000
H	2.684646000	-1.938523000	1.641767000
H	1.546410000	-2.475581000	0.370370000
H	1.094592000	-2.605339000	2.076243000
C	3.486279000	-0.577252000	-0.679909000
H	3.900576000	-0.739417000	0.324409000
H	4.272744000	-0.145258000	-1.320254000
H	3.265515000	-1.571914000	-1.110528000
C	1.921767000	1.131260000	-2.072493000
H	2.456153000	2.099366000	-2.043771000
H	0.863412000	1.335692000	-2.285742000

H	2.348751000	0.582857000	-2.928274000
C	-2.399084000	1.039645000	-1.134856000
C	-3.114914000	0.559904000	0.030897000
H	-2.114315000	2.099786000	-1.183591000
H	-3.354515000	1.260580000	0.841850000
H	-2.623127000	0.603460000	-2.116262000
H	-3.859652000	-0.237313000	-0.088895000
B	2.194771000	0.318494000	-0.753033000

38

J-2-q SCF Done : -1096.85542 A.U.

Cr	1.267862000	0.092666000	0.132924000
Cl	-0.498924000	-0.589792000	-1.881388000
N	-1.318431000	0.011667000	0.722874000
C	-0.684599000	-1.092955000	1.281810000
C	0.276500000	-0.658098000	2.203865000
C	0.230263000	0.759228000	2.218745000
C	-0.750570000	1.151825000	1.297721000
C	-1.009332000	-2.525421000	0.999586000
H	-2.033016000	-2.769990000	1.319794000
H	-0.315718000	-3.166005000	1.562115000
H	-0.924958000	-2.764935000	-0.068946000
H	0.880632000	-1.308054000	2.832913000
H	0.784448000	1.433369000	2.869313000
C	-1.255925000	2.555981000	1.157384000
H	-2.345848000	2.594421000	1.293950000
H	-1.032687000	3.013862000	0.186316000
H	-0.792905000	3.176144000	1.938161000
C	-2.618583000	1.347215000	-1.271765000
H	-3.428374000	1.788393000	-0.662674000
H	-3.055476000	1.137356000	-2.261505000
H	-1.853621000	2.119435000	-1.429667000
C	-3.239819000	-1.186339000	-0.754776000
H	-3.994697000	-1.019243000	0.037459000
H	-2.915231000	-2.231101000	-0.679447000
H	-3.771307000	-1.092401000	-1.715643000
C	2.334861000	-1.814839000	0.106482000
C	3.012068000	-1.110514000	-0.876932000
H	1.549694000	-2.524526000	-0.167389000
H	2.736935000	-1.228804000	-1.927280000
H	2.788916000	-1.957873000	1.093186000
H	4.009450000	-0.709770000	-0.689703000
C	2.634347000	1.438185000	-1.182931000
C	1.557500000	2.100248000	-0.605758000

H	2.595247000	1.123145000	-2.227299000
H	0.657690000	2.293056000	-1.196445000
H	3.636461000	1.539397000	-0.759069000
H	1.705614000	2.736291000	0.273534000
B	-2.103894000	-0.049692000	-0.665791000

38

J-3-q SCF Done : -1096.893932 A.U.

Cr	0.936385000	-0.277146000	-0.026821000
Cl	0.409620000	-1.931641000	-1.490733000
N	-1.699603000	0.408058000	0.476777000
C	-1.447691000	-0.695893000	1.323626000
C	-0.437217000	-0.347861000	2.198199000
C	-0.058425000	1.004688000	1.920709000
C	-0.836813000	1.455357000	0.866380000
C	-2.106762000	-2.033982000	1.218959000
H	-3.169173000	-2.002441000	1.501580000
H	-1.597081000	-2.725840000	1.903470000
H	-2.023117000	-2.452262000	0.205145000
H	-0.011499000	-1.003228000	2.955005000
H	0.661757000	1.609498000	2.468195000
C	-0.905947000	2.858998000	0.349415000
H	-1.929641000	3.260561000	0.416548000
H	-0.575457000	2.956387000	-0.692900000
H	-0.254652000	3.493809000	0.965518000
C	-2.345315000	1.329126000	-1.937089000
H	-2.879006000	2.293961000	-1.846990000
H	-2.767553000	0.840045000	-2.830373000
H	-1.286442000	1.544896000	-2.132416000
C	-3.948855000	-0.435325000	-0.670252000
H	-4.368110000	-0.658748000	0.320257000
H	-3.748913000	-1.401288000	-1.170388000
H	-4.723824000	0.058890000	-1.278802000
C	2.694905000	-0.795418000	0.882794000
C	3.806388000	-0.255850000	-0.023265000
H	2.755895000	-1.882710000	1.061564000
H	3.915574000	-0.916367000	-0.902385000
H	2.700118000	-0.279350000	1.863908000
H	4.793664000	-0.246532000	0.479515000
C	3.408161000	1.148098000	-0.501343000
C	2.010808000	1.080935000	-1.136652000
H	4.163841000	1.567571000	-1.193958000
H	2.056764000	0.644059000	-2.149762000
H	3.392821000	1.828378000	0.372621000

H	1.532585000	2.074598000	-1.219517000
B	-2.635504000	0.430375000	-0.679202000

44

J-4-q SCF Done : -1175.418205 A.U.

Cr	1.238653000	0.206712000	-0.087194000
Cl	-0.340806000	0.828465000	-1.772120000
N	-2.205287000	-0.405415000	0.563948000
C	-1.280970000	-1.422880000	0.343218000
C	-0.204630000	-1.241386000	1.206780000
C	-0.509456000	-0.099277000	2.030190000
C	-1.713821000	0.406547000	1.608553000
C	-1.389926000	-2.492542000	-0.692745000
H	-2.230819000	-3.175426000	-0.503323000
H	-0.465456000	-3.085349000	-0.686049000
H	-1.508176000	-2.065552000	-1.699427000
H	0.589164000	-1.969445000	1.359983000
H	0.074630000	0.276150000	2.867509000
C	-2.446796000	1.564493000	2.209921000
H	-3.503041000	1.329065000	2.412450000
H	-2.426412000	2.462171000	1.573979000
H	-1.972629000	1.824064000	3.167174000
C	-3.875100000	1.381814000	-0.501638000
H	-4.659074000	1.619284000	0.241388000
H	-4.359886000	1.470194000	-1.487659000
H	-3.093782000	2.149286000	-0.433509000
C	-4.149524000	-1.238103000	-1.059913000
H	-4.121035000	-2.231126000	-0.591702000
H	-3.751670000	-1.343909000	-2.086287000
H	-5.203654000	-0.937992000	-1.180571000
C	2.337734000	-1.247982000	-1.045501000
C	3.356942000	-1.858400000	-0.082616000
H	1.643970000	-1.977230000	-1.498282000
H	2.864269000	-2.617219000	0.555519000
H	2.829499000	-0.702326000	-1.871926000
H	4.168264000	-2.396433000	-0.611753000
C	3.900696000	-0.739355000	0.813428000
C	2.701284000	0.006174000	1.421084000
H	4.598278000	-1.135240000	1.577578000
H	2.279141000	-0.601053000	2.243838000
H	4.505324000	-0.051566000	0.191282000
H	2.999152000	0.969972000	1.876899000
C	2.065496000	2.709855000	-0.338853000
C	2.769038000	2.075214000	-1.293011000

H	1.044639000	3.051621000	-0.533545000
H	2.332445000	1.880444000	-2.275974000
H	2.504188000	2.941270000	0.635334000
H	3.801922000	1.760272000	-1.124254000
B	-3.360402000	-0.095205000	-0.312197000

44

J-5-q SCF Done : -1175.461839 A.U.

Cr	-0.599404000	-0.276938000	0.254938000
Cl	0.225793000	-0.736711000	2.322024000
N	2.139950000	0.131647000	-0.688489000
C	1.898809000	-1.248180000	-0.867273000
C	0.843891000	-1.392833000	-1.744875000
C	0.417985000	-0.085512000	-2.143606000
C	1.220244000	0.836134000	-1.490114000
C	2.596564000	-2.351832000	-0.137824000
H	3.650329000	-2.459327000	-0.433543000
H	2.085648000	-3.296948000	-0.368374000
H	2.551206000	-2.208603000	0.952016000
H	0.422813000	-2.343369000	-2.064602000
H	-0.338901000	0.161017000	-2.886087000
C	1.231954000	2.316421000	-1.716511000
H	2.244346000	2.686270000	-1.939767000
H	0.848366000	2.888842000	-0.860135000
H	0.592680000	2.546274000	-2.580008000
C	2.861619000	2.147183000	0.899405000
H	3.381782000	2.925762000	0.310191000
H	3.324700000	2.173724000	1.899438000
H	1.810776000	2.447287000	1.000665000
C	4.440116000	-0.022355000	0.644508000
H	4.838313000	-0.707786000	-0.116064000
H	4.268957000	-0.612501000	1.564060000
H	5.221923000	0.710665000	0.902419000
C	-2.095616000	-1.614844000	-0.008061000
C	-3.246786000	-1.189337000	-0.927011000
H	-1.581533000	-2.510947000	-0.406472000
H	-2.870113000	-0.653612000	-1.822960000
H	-2.467164000	-1.880587000	0.996483000
H	-3.730765000	-2.098854000	-1.333304000
C	-4.349520000	-0.349249000	-0.260917000
C	-4.084492000	1.141940000	-0.002133000
H	-5.250420000	-0.408793000	-0.897501000
H	-3.882852000	1.646204000	-0.967362000
H	-4.628688000	-0.835359000	0.692663000

H	-5.034792000	1.573819000	0.358503000
C	-2.980497000	1.530822000	0.996947000
C	-1.552397000	1.503210000	0.443902000
H	-3.204617000	2.558346000	1.343886000
H	-1.524687000	1.994769000	-0.550232000
H	-3.056019000	0.899451000	1.901303000
H	-0.873585000	2.072120000	1.108765000
B	3.111724000	0.730360000	0.260777000

44

J-6-q SCF Done : -1175.462132 A.U.

Cr	-0.288935000	0.024729000	0.556323000
Cl	0.199404000	-1.564132000	2.131345000
N	1.952119000	0.146939000	-0.781675000
C	1.365841000	-1.074510000	-1.195099000
C	0.158110000	-0.793568000	-1.807230000
C	-0.028487000	0.624520000	-1.786802000
C	1.068029000	1.191739000	-1.145822000
C	1.934894000	-2.434042000	-0.945261000
H	2.841848000	-2.623105000	-1.537849000
H	1.182017000	-3.181422000	-1.229995000
H	2.163749000	-2.590057000	0.118693000
H	-0.524320000	-1.537926000	-2.211445000
H	-0.840690000	1.184887000	-2.243761000
C	1.397553000	2.651784000	-1.082615000
H	2.337904000	2.869990000	-1.614756000
H	1.490042000	3.034873000	-0.059144000
H	0.594989000	3.214452000	-1.578689000
C	3.419512000	1.496340000	0.982439000
H	3.932721000	2.335707000	0.476740000
H	4.098451000	1.178715000	1.790880000
H	2.498642000	1.886592000	1.437229000
C	4.395603000	-0.729835000	-0.197421000
H	4.444079000	-1.237595000	-1.170228000
H	4.317220000	-1.511920000	0.580697000
H	5.358623000	-0.225501000	-0.014150000
C	-3.338565000	-1.885046000	-0.477921000
C	-3.855392000	-0.633514000	-1.192644000
H	-3.109246000	-2.690817000	-1.195437000
H	-3.112755000	-0.290803000	-1.937824000
H	-4.093477000	-2.276446000	0.224138000
H	-4.746142000	-0.916889000	-1.780970000
C	-4.233627000	0.547075000	-0.279103000
C	-3.101833000	1.482048000	0.181933000

H	-4.972825000	1.169908000	-0.812819000
H	-2.604218000	1.912403000	-0.709196000
H	-4.763817000	0.157465000	0.610007000
H	-3.585705000	2.351019000	0.673931000
C	-2.069494000	0.911274000	1.143390000
C	-0.915708000	1.697764000	1.547996000
H	-2.511440000	0.277079000	1.926416000
H	-0.754273000	2.664935000	1.048462000
H	-0.605749000	1.694308000	2.600932000
H	-2.428786000	-1.688041000	0.110680000
B	3.218854000	0.298839000	-0.018095000

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J-7-q SCF Done : -1253.973201 A.U.

Cl	-1.941773000	0.934127000	1.831067000
N	-1.821689000	0.082783000	-0.847353000
C	-0.924419000	1.036606000	-1.296328000
C	0.069135000	0.405119000	-2.067737000
C	-0.282324000	-0.972553000	-2.144676000
C	-1.435826000	-1.150719000	-1.384232000
C	-1.013521000	2.509914000	-1.054851000
H	-1.792654000	2.955182000	-1.693020000
H	-0.054508000	2.976536000	-1.318804000
H	-1.253671000	2.744243000	-0.010429000
H	0.870404000	0.914816000	-2.598159000
H	0.229416000	-1.754572000	-2.700485000
C	-2.189060000	-2.443180000	-1.291587000
H	-3.217976000	-2.332402000	-1.662658000
H	-2.257978000	-2.845335000	-0.273306000
H	-1.679179000	-3.187525000	-1.919705000
C	-3.863881000	-0.897773000	0.700872000
H	-4.511855000	-1.299185000	-0.097773000
H	-4.538610000	-0.545903000	1.498174000
H	-3.298977000	-1.738886000	1.130893000
C	-3.970251000	1.579777000	-0.248072000
H	-4.455650000	1.317485000	-1.207411000
H	-3.509297000	2.567912000	-0.375149000
H	-4.781017000	1.705305000	0.488610000
C	-0.055879000	-2.087328000	1.724597000
C	0.778481000	-1.321878000	2.454281000
H	-1.122455000	-1.848312000	1.688242000
H	0.396164000	-0.452273000	2.994809000
H	0.286064000	-2.998910000	1.225510000
H	1.837521000	-1.567385000	2.566922000

Cr	0.687918000	-0.365846000	0.046023000
C	1.645654000	1.257251000	0.845058000
C	2.757796000	1.951007000	0.049198000
H	0.798787000	1.943148000	1.022185000
H	2.522680000	1.979299000	-1.032637000
H	2.028647000	0.976000000	1.842818000
H	2.799231000	3.014630000	0.353785000
C	4.167682000	1.374945000	0.242342000
C	4.487734000	0.017385000	-0.397202000
H	4.893879000	2.104860000	-0.157594000
H	4.365106000	0.092310000	-1.494597000
H	4.375593000	1.316869000	1.327804000
H	5.563948000	-0.168752000	-0.235044000
C	3.712176000	-1.215559000	0.100957000
C	2.339355000	-1.438195000	-0.543905000
H	4.337778000	-2.103724000	-0.112518000
H	2.437087000	-1.311638000	-1.636916000
H	3.640909000	-1.179364000	1.204273000
H	2.012398000	-2.486170000	-0.387203000
B	-3.001393000	0.380698000	0.227175000

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J-8-q SCF Done : -1254.022431 A.U.

C	-4.689230000	-0.519671000	0.307748000
C	-4.738360000	0.928552000	-0.211812000
H	-5.730947000	-0.834477000	0.494613000
H	-5.272794000	0.940061000	-1.179880000
H	-4.207972000	-0.542147000	1.300132000
H	-5.370886000	1.512369000	0.482192000
Cr	-0.175839000	-0.115995000	0.414332000
Cl	0.850473000	-0.462267000	2.416036000
N	2.535647000	0.016078000	-0.765243000
C	2.148930000	-1.337588000	-0.840993000
C	1.004848000	-1.419404000	-1.610188000
C	0.670813000	-0.096757000	-2.044900000
C	1.614211000	0.770009000	-1.516159000
C	2.808221000	-2.467405000	-0.116294000
H	3.811486000	-2.695211000	-0.505177000
H	2.189396000	-3.367123000	-0.238373000
H	2.888344000	-2.264095000	0.961925000
H	0.469849000	-2.338100000	-1.839090000
H	-0.122161000	0.188338000	-2.733828000
C	1.745293000	2.230105000	-1.821297000
H	2.755164000	2.481323000	-2.181244000

H	1.530332000	2.874778000	-0.957409000
H	1.031689000	2.490905000	-2.614897000
C	3.572778000	2.014299000	0.661771000
H	4.096909000	2.726440000	-0.002982000
H	4.128901000	2.033222000	1.613545000
H	2.563507000	2.403735000	0.847633000
C	4.935015000	-0.292071000	0.343494000
H	5.184226000	-1.046327000	-0.415314000
H	4.820275000	-0.818728000	1.309114000
H	5.800790000	0.378263000	0.472074000
C	-1.652743000	-1.517776000	0.434466000
C	-2.523719000	-1.528226000	-0.830905000
H	-1.161815000	-2.490125000	0.615507000
H	-2.308332000	-0.650501000	-1.467889000
H	-2.222119000	-1.276859000	1.346498000
H	-2.248246000	-2.393287000	-1.460357000
C	-4.050789000	-1.589414000	-0.596820000
C	-3.398190000	1.663455000	-0.385722000
H	-4.556202000	-1.573291000	-1.580759000
H	-2.806699000	1.156732000	-1.163634000
H	-4.282706000	-2.575551000	-0.155607000
H	-3.605731000	2.665813000	-0.800520000
C	-2.538951000	1.817021000	0.888244000
C	-1.029905000	1.744503000	0.620461000
H	-2.794141000	2.779879000	1.371375000
H	-0.772630000	2.343511000	-0.276337000
H	-2.813324000	1.051711000	1.633062000
H	-0.460643000	2.166363000	1.468798000
B	3.641940000	0.560893000	0.062080000

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J-9-q SCF Done : -1096.841358 A.U.

Cr	-1.282245000	0.643809000	0.086572000
Cl	0.766748000	-2.227422000	0.163897000
N	1.177468000	0.577939000	0.102413000
C	0.719465000	1.641880000	-0.683489000
C	0.051063000	2.557921000	0.145602000
C	0.106513000	2.051595000	1.471567000
C	0.817583000	0.846295000	1.424240000
C	1.012754000	1.878036000	-2.133959000
H	2.095835000	1.969439000	-2.303146000
H	0.539298000	2.823698000	-2.433057000
H	0.640904000	1.084295000	-2.790569000
H	-0.395354000	3.492286000	-0.185698000

H	-0.298506000	2.511025000	2.370835000
C	1.180250000	0.015989000	2.616625000
H	2.215267000	0.227891000	2.927359000
H	1.103816000	-1.058309000	2.410658000
H	0.519989000	0.279110000	3.455718000
C	3.398831000	-0.879638000	0.401839000
H	4.043070000	-0.011828000	0.164388000
H	3.933995000	-1.774964000	0.044520000
H	3.350513000	-0.960009000	1.496852000
C	2.172867000	-0.923940000	-1.968134000
H	2.868614000	-0.189816000	-2.409424000
H	1.241539000	-0.914924000	-2.554364000
H	2.627565000	-1.915106000	-2.129457000
H	-2.486361000	1.691163000	0.121825000
C	-1.926739000	-0.207976000	-1.665676000
C	-2.752321000	-1.384278000	-1.093172000
H	-2.541620000	0.500673000	-2.242031000
H	-3.640018000	-1.633971000	-1.698532000
H	-1.086082000	-0.561425000	-2.282872000
H	-2.121269000	-2.282252000	-1.015063000
C	-3.161335000	-0.924001000	0.285928000
C	-2.408592000	-1.077048000	1.404685000
H	-4.076179000	-0.323346000	0.354097000
H	-2.735178000	-0.651680000	2.358387000
H	-1.522542000	-1.721580000	1.406927000
B	1.991514000	-0.756040000	-0.376913000

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J-2-3-q SCF Done: -1096.845892 A.U.

Cr	1.196834000	0.059675000	0.215361000
Cl	-0.434266000	-0.680084000	-1.818417000
N	-1.396857000	0.111365000	0.687261000
C	-0.824093000	-0.962601000	1.362952000
C	0.124951000	-0.482662000	2.274469000
C	0.137284000	0.932114000	2.160175000
C	-0.795062000	1.276072000	1.171217000
C	-1.173892000	-2.405686000	1.184410000
H	-2.225708000	-2.598103000	1.441579000
H	-0.542778000	-3.007165000	1.853498000
H	-1.010895000	-2.743412000	0.151898000
H	0.692851000	-1.097824000	2.968795000
H	0.702048000	1.641706000	2.761839000
C	-1.202400000	2.684010000	0.857505000
H	-2.293427000	2.802304000	0.911085000

H	-0.882963000	3.021060000	-0.136467000
H	-0.748428000	3.353558000	1.601914000
C	-2.578891000	1.305189000	-1.464069000
H	-3.404891000	1.803839000	-0.924588000
H	-2.979651000	1.024677000	-2.451474000
H	-1.793896000	2.049802000	-1.648207000
C	-3.245779000	-1.185492000	-0.800362000
H	-4.024435000	-0.986409000	-0.039151000
H	-2.919992000	-2.224073000	-0.669365000
H	-3.748087000	-1.135939000	-1.779820000
C	2.339662000	-1.643997000	0.270681000
C	2.948379000	-1.032861000	-0.895100000
H	1.666432000	-2.493208000	0.104800000
H	2.546937000	-1.361145000	-1.859246000
H	2.962152000	-1.745386000	1.170205000
H	4.039044000	-0.968498000	-0.909227000
C	2.907064000	0.964481000	-1.141856000
C	1.848943000	1.808061000	-0.624695000
H	2.964687000	0.851510000	-2.228882000
H	1.090519000	2.161830000	-1.332742000
H	3.890525000	1.135894000	-0.694485000
H	2.119227000	2.542832000	0.144783000
B	-2.115951000	-0.043588000	-0.727021000

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J-3-9-q SCF Done: -1096.848920 A.U.

Cr	1.477586000	-0.253870000	-0.000307000
B	-3.048150000	0.503559000	0.375904000
Cl	0.144346000	-0.304895000	1.906102000
N	-1.976366000	0.089994000	-0.552054000
C	-1.003637000	0.924460000	-1.110678000
C	-0.112446000	0.144765000	-1.833906000
C	-0.540244000	-1.222566000	-1.707913000
C	-1.670093000	-1.235806000	-0.926464000
C	-1.002368000	2.419573000	-1.049321000
H	-1.987228000	2.845167000	-1.294111000
H	-0.277663000	2.804410000	-1.780087000
H	-0.712007000	2.799566000	-0.059216000
H	0.641254000	0.533395000	-2.515460000
H	-0.068676000	-2.099014000	-2.148545000
C	-2.378731000	-2.458071000	-0.435519000
H	-3.402601000	-2.554034000	-0.825671000
H	-2.430875000	-2.484633000	0.663863000
H	-1.814060000	-3.342759000	-0.761767000

C	-4.374455000	-0.341526000	0.515947000
H	-5.209699000	0.328484000	0.779175000
H	-4.278557000	-1.043145000	1.365447000
H	-4.664611000	-0.929991000	-0.364912000
H	2.392468000	-0.707330000	-1.309737000
C	2.600961000	1.471954000	-0.033909000
C	3.967896000	0.819700000	-0.317457000
H	2.289267000	2.175459000	-0.821210000
H	4.299803000	1.008161000	-1.349295000
H	2.537524000	1.971049000	0.945888000
H	4.771012000	1.175727000	0.354678000
C	3.772884000	-0.678522000	-0.111652000
C	3.233206000	-1.123372000	1.084526000
H	4.238278000	-1.383725000	-0.806418000
H	3.140912000	-2.191277000	1.300998000
H	3.119173000	-0.444402000	1.933156000
C	-2.930629000	1.815236000	1.241386000
H	-1.905229000	2.059343000	1.547562000
H	-3.345003000	2.683221000	0.695520000
H	-3.548152000	1.709719000	2.148390000

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J-4-5-q SCF Done: -1175.388810 A.U.

Cr	1.241276000	0.177993000	-0.045680000
Cl	-2.708802000	-1.633444000	-1.238914000
N	-0.990985000	0.429049000	0.773666000
C	-0.306740000	-0.416073000	1.610138000
C	0.787355000	0.269612000	2.199880000
C	0.708203000	1.618458000	1.744648000
C	-0.388834000	1.673547000	0.866497000
C	-0.728405000	-1.827527000	1.879631000
H	-1.518910000	-1.844775000	2.648506000
H	0.117120000	-2.417897000	2.259702000
H	-1.126879000	-2.310875000	0.978345000
H	1.504688000	-0.148233000	2.904327000
H	1.375907000	2.439547000	2.000027000
C	-0.925347000	2.890454000	0.173287000
H	-1.850064000	3.240845000	0.661083000
H	-1.175754000	2.698902000	-0.879796000
H	-0.194331000	3.711252000	0.215820000
C	-3.631688000	1.088368000	-1.067011000
H	-3.739410000	1.973092000	-0.421656000
H	-4.612918000	0.930806000	-1.556050000
H	-2.918824000	1.308948000	-1.875014000

C	-3.990194000	-0.537233000	1.125872000
H	-5.067950000	-0.709342000	0.935790000
H	-3.926757000	0.320366000	1.814506000
H	-3.608365000	-1.435945000	1.628430000
C	1.996809000	-1.739235000	-0.326640000
C	3.488606000	-1.724086000	0.029406000
H	1.434050000	-2.510498000	0.225661000
H	3.612457000	-1.742995000	1.129015000
H	1.874999000	-1.969415000	-1.402662000
H	4.028232000	-2.613559000	-0.351034000
C	4.094765000	-0.424039000	-0.509397000
C	3.246893000	0.741349000	0.011472000
H	5.164323000	-0.325632000	-0.238110000
H	3.458159000	0.902402000	1.085018000
H	4.070412000	-0.452625000	-1.616633000
H	3.458109000	1.698876000	-0.499929000
C	1.320571000	1.168918000	-2.340050000
C	0.351692000	0.230937000	-2.393534000
H	1.106953000	2.204003000	-2.056785000
H	-0.688928000	0.446777000	-2.139379000
H	2.342257000	0.952536000	-2.659021000
H	0.557750000	-0.780452000	-2.750567000
B	-3.324508000	-0.230687000	-0.264521000

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J-5-6-q SCF Done: -1175.420236 A.U.

Cr	-1.157606000	0.064535000	0.430217000
Cl	0.396950000	-0.921766000	1.767188000
N	2.504127000	0.212767000	-0.553654000
C	1.524579000	-0.392534000	-1.353405000
C	0.594527000	0.567343000	-1.709706000
C	1.041174000	1.820745000	-1.168517000
C	2.187729000	1.582723000	-0.453399000
C	1.465218000	-1.844085000	-1.706508000
H	2.306220000	-2.162235000	-2.340018000
H	0.539235000	-2.032172000	-2.267055000
H	1.448135000	-2.483805000	-0.811132000
H	-0.229288000	0.401838000	-2.402267000
H	0.602048000	2.803732000	-1.329900000
C	3.025841000	2.613054000	0.238023000
H	4.093869000	2.524151000	-0.013958000
H	2.942982000	2.569991000	1.334510000
H	2.691160000	3.611270000	-0.079502000
C	4.108135000	0.080533000	1.568833000

H	4.981268000	0.733799000	1.385045000
H	4.480309000	-0.749796000	2.191038000
H	3.376554000	0.649301000	2.157314000
C	4.175563000	-1.850613000	-0.304732000
H	4.169272000	-2.001149000	-1.392442000
H	3.637066000	-2.702364000	0.150584000
H	5.215493000	-1.931747000	0.053078000
C	-2.154182000	-1.540944000	-0.340285000
C	-3.634329000	-1.418676000	-0.705908000
H	-1.556634000	-1.868331000	-1.212351000
H	-3.763359000	-0.880236000	-1.663730000
H	-2.015344000	-2.297895000	0.450552000
H	-4.040685000	-2.431010000	-0.895377000
C	-4.510007000	-0.755714000	0.369454000
C	-4.525645000	0.786726000	0.347861000
H	-5.557552000	-1.079283000	0.246099000
H	-5.064332000	1.106877000	-0.562293000
H	-4.189759000	-1.107005000	1.364086000
H	-5.124423000	1.139640000	1.202331000
C	-3.209021000	1.538223000	0.352299000
C	-2.379963000	1.676097000	-0.727722000
H	-3.038317000	2.199500000	1.206808000
H	-2.608774000	1.202841000	-1.686021000
H	-1.612027000	2.453289000	-0.731430000
H	-2.171646000	0.269969000	1.659201000
B	3.547267000	-0.496922000	0.211455000

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J-7-8-q SCF Done: -1253.947112 A.U.

C	4.520284000	-0.183381000	0.390337000
C	3.939877000	1.152510000	-0.096913000
H	4.374908000	-0.258030000	1.484966000
H	4.501910000	1.956329000	0.412053000
H	5.613075000	-0.125518000	0.245275000
H	4.173977000	1.284024000	-1.168988000
Cr	0.554160000	0.289630000	-0.068496000
Cl	-2.145488000	-1.509077000	-1.576834000
N	-1.789853000	0.191913000	0.676816000
C	-1.062318000	-0.698387000	1.469383000
C	-0.163395000	0.032304000	2.262689000
C	-0.383488000	1.406662000	1.989598000
C	-1.382713000	1.487469000	1.015104000
C	-1.291557000	-2.174336000	1.567474000
H	-2.126358000	-2.379170000	2.256434000

H	-0.392645000	-2.655759000	1.978424000
H	-1.535885000	-2.620192000	0.596480000
H	0.517822000	-0.401542000	2.992616000
H	0.121436000	2.259811000	2.439098000
C	-1.985956000	2.770421000	0.530204000
H	-3.043101000	2.846635000	0.823923000
H	-1.946554000	2.892625000	-0.558553000
H	-1.444385000	3.607501000	0.994139000
C	-3.594321000	0.932277000	-1.264728000
H	-4.190156000	1.677916000	-0.711313000
H	-4.286673000	0.452179000	-1.975619000
H	-2.851606000	1.467569000	-1.877102000
C	-4.174915000	-0.988016000	0.502385000
H	-4.601932000	-0.303431000	1.259819000
H	-3.883966000	-1.911906000	1.023404000
H	-4.998943000	-1.257664000	-0.179196000
C	1.422480000	-1.501229000	-0.579447000
C	2.655528000	-2.044570000	0.154447000
H	0.578247000	-2.201700000	-0.465740000
H	2.545382000	-1.938316000	1.251939000
H	1.624568000	-1.462856000	-1.665924000
H	2.694332000	-3.137783000	-0.013378000
C	4.031936000	-1.487918000	-0.262359000
C	2.452920000	1.381138000	0.179810000
H	4.783964000	-2.256792000	-0.015448000
H	2.210682000	0.828412000	1.113060000
H	4.068507000	-1.389991000	-1.363901000
H	2.230620000	2.437562000	0.384467000
C	1.690470000	1.415365000	-1.790523000
C	0.317229000	1.136679000	-1.966127000
H	2.035193000	2.452134000	-1.798838000
H	-0.396379000	1.966086000	-1.945921000
H	2.417444000	0.707655000	-2.192621000
H	-0.001959000	0.257313000	-2.533698000
B	-3.008295000	-0.251048000	-0.337101000

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K-0-s SCF Done : -2839.606386 A.U.

Cr	-1.619966000	-0.002464000	1.319572000
Cl	0.673304000	-0.007152000	2.098732000
N	-0.372107000	0.002256000	-1.027277000
C	-1.189644000	-1.121379000	-0.973966000
C	-2.522843000	-0.716018000	-0.843045000
C	-2.522846000	0.719966000	-0.841043000

C	-1.189678000	1.125695000	-0.970908000
C	-0.689242000	-2.528103000	-1.109479000
H	-0.086967000	-2.650576000	-2.023695000
H	-1.544700000	-3.215763000	-1.173023000
H	-0.064647000	-2.847683000	-0.262744000
H	-3.391196000	-1.373573000	-0.855251000
H	-3.391213000	1.377530000	-0.851343000
C	-0.689207000	2.532755000	-1.102750000
H	-0.082762000	2.656346000	-2.014031000
H	-0.068607000	2.851785000	-0.252869000
H	-1.544613000	3.220184000	-1.169497000
C	2.475419000	1.732537000	-0.450921000
H	2.419389000	2.111503000	-1.484052000
H	3.537873000	1.566671000	-0.209950000
H	2.093342000	2.509922000	0.225843000
C	2.476910000	-1.728150000	-0.466756000
H	2.407875000	-2.105443000	-1.499653000
H	2.104665000	-2.507282000	0.213558000
H	3.542125000	-1.561099000	-0.239258000
Ga	1.523033000	0.000922000	-0.258325000

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K-1-q SCF Done : -2918.158426 A.U.

Cr	1.453369000	-0.384809000	-0.251215000
Cl	-0.401685000	-1.717717000	-1.137001000
N	-0.222158000	1.059109000	0.367595000
C	0.647786000	1.091897000	1.455841000
C	1.858656000	1.659675000	1.037879000
C	1.698818000	2.064140000	-0.324465000
C	0.409614000	1.696031000	-0.714045000
C	0.286293000	0.633720000	2.835762000
H	-0.555103000	1.222743000	3.236676000
H	1.146722000	0.776341000	3.504109000
H	-0.002764000	-0.424481000	2.877479000
H	2.733327000	1.814206000	1.667274000
H	2.430855000	2.575296000	-0.946291000
C	-0.257677000	1.961192000	-2.029051000
H	-1.118077000	2.639061000	-1.911471000
H	-0.620475000	1.041832000	-2.511005000
H	0.460844000	2.438579000	-2.709957000
C	-3.195413000	0.582770000	-1.115451000
H	-4.159666000	0.072603000	-0.961260000
H	-2.916463000	0.471841000	-2.172791000
H	-3.344756000	1.654793000	-0.906999000

C	-2.338381000	-1.199440000	1.760480000
H	-2.637073000	-0.528740000	2.581949000
H	-1.526794000	-1.852241000	2.112399000
H	-3.203752000	-1.837909000	1.518920000
C	2.855382000	-1.725355000	0.408281000
C	3.238543000	-1.175264000	-0.876114000
H	3.411497000	-1.423292000	1.305911000
H	4.076645000	-0.467341000	-0.926628000
H	2.467132000	-2.751092000	0.459134000
H	3.138892000	-1.794894000	-1.777502000
Ga	-1.854833000	-0.198086000	0.119689000

38

K-2-q SCF Done : -2996.694731 A.U.

Cr	1.686859000	0.062363000	0.024932000
Cl	-0.366606000	-0.459703000	-1.908311000
N	-0.707920000	0.010242000	1.164774000
C	-0.001926000	-1.121030000	1.518955000
C	1.160060000	-0.749373000	2.221087000
C	1.163915000	0.669179000	2.285597000
C	0.009683000	1.108807000	1.611814000
C	-0.478357000	-2.513949000	1.249938000
H	-1.437594000	-2.705024000	1.755049000
H	0.256138000	-3.239453000	1.626115000
H	-0.629397000	-2.695644000	0.176019000
H	1.873321000	-1.435321000	2.673485000
H	1.881324000	1.307720000	2.798523000
C	-0.504249000	2.513561000	1.552998000
H	-1.444610000	2.601533000	2.121002000
H	-0.709234000	2.855961000	0.530848000
H	0.227651000	3.197728000	2.004496000
C	-2.817698000	1.814326000	-0.789533000
H	-3.302417000	2.278173000	0.084969000
H	-3.589460000	1.690980000	-1.567407000
H	-2.061215000	2.510200000	-1.181646000
C	-3.333945000	-1.539576000	-0.205515000
H	-3.665867000	-1.669841000	0.838134000
H	-2.896230000	-2.487936000	-0.549135000
H	-4.230570000	-1.341539000	-0.815276000
C	2.602891000	-1.887175000	-0.343085000
C	3.146883000	-1.134297000	-1.372549000
H	1.740637000	-2.532562000	-0.532411000
H	2.700173000	-1.157862000	-2.368369000
H	3.207320000	-2.137635000	0.535152000

H	4.182834000	-0.793677000	-1.325143000
C	2.794015000	1.425571000	-1.500957000
C	1.903472000	2.098217000	-0.672399000
H	2.507449000	1.163060000	-2.520667000
H	0.909587000	2.363601000	-1.044012000
H	3.868555000	1.471498000	-1.308836000
H	2.273566000	2.685881000	0.174358000
Ga	-2.091203000	0.006811000	-0.379157000

38

K-3-q SCF Done : -2996.725489 A.U.

Cr	-1.242463000	0.077336000	-0.112487000
Cl	0.255050000	-1.342705000	-1.422509000
N	0.894188000	0.980195000	0.619954000
C	0.352592000	1.952693000	-0.225067000
C	-0.804674000	2.466248000	0.365696000
C	-0.975325000	1.798306000	1.613622000
C	0.104261000	0.911610000	1.758570000
C	0.971216000	2.370754000	-1.523706000
H	1.977856000	2.790343000	-1.371553000
H	0.346795000	3.144793000	-1.991185000
H	1.060985000	1.535432000	-2.233351000
H	-1.442829000	3.239426000	-0.057509000
H	-1.753385000	1.974798000	2.354080000
C	0.419061000	0.057556000	2.948649000
H	1.441883000	0.247036000	3.309740000
H	0.335311000	-1.018075000	2.739041000
H	-0.279550000	0.294627000	3.762777000
C	2.515320000	-1.936155000	1.229712000
H	3.060609000	-1.547414000	2.104889000
H	3.159478000	-2.685039000	0.740865000
H	1.607902000	-2.448882000	1.578604000
C	3.520098000	0.209308000	-1.327091000
H	4.352574000	-0.509869000	-1.386202000
H	3.925427000	1.163267000	-0.952514000
H	3.137481000	0.372175000	-2.344638000
C	-2.864854000	0.381159000	-1.329597000
C	-3.806107000	-0.811687000	-1.125751000
H	-2.560547000	0.528868000	-2.381563000
H	-3.418512000	-1.688996000	-1.676426000
H	-3.341629000	1.318027000	-0.979535000
H	-4.821299000	-0.624675000	-1.527575000
C	-3.844053000	-1.140396000	0.372203000
C	-2.402727000	-1.310264000	0.871364000

H	-4.470958000	-2.030063000	0.577536000
H	-1.988658000	-2.285158000	0.551302000
H	-4.327913000	-0.300555000	0.907208000
H	-2.318795000	-1.254271000	1.971745000
Ga	2.142996000	-0.509743000	-0.094345000

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K-4-q SCF Done : -3075.249316 A.U.

Cr	1.482845000	0.176345000	-0.006634000
Cl	-0.605417000	0.286282000	-1.726513000
N	-1.279608000	-0.386587000	1.183653000
C	-0.396326000	-1.435960000	1.176783000
C	0.782754000	-1.062660000	1.847193000
C	0.570463000	0.275530000	2.323452000
C	-0.693062000	0.658391000	1.887142000
C	-0.676272000	-2.763340000	0.546928000
H	-1.629638000	-3.179393000	0.905744000
H	0.127189000	-3.470246000	0.795616000
H	-0.737957000	-2.691372000	-0.549208000
H	1.594204000	-1.736857000	2.114206000
H	1.234054000	0.860662000	2.957249000
C	-1.382298000	1.958900000	2.160431000
H	-2.396301000	1.795302000	2.556285000
H	-1.486978000	2.582586000	1.259866000
H	-0.811831000	2.532275000	2.904983000
C	-3.587748000	1.606335000	-0.303512000
H	-4.156530000	1.700704000	0.635927000
H	-4.315600000	1.598092000	-1.131368000
H	-2.959734000	2.501411000	-0.419533000
C	-3.468390000	-1.764252000	-0.974298000
H	-3.876377000	-2.322089000	-0.115093000
H	-2.809773000	-2.437877000	-1.540620000
H	-4.314726000	-1.490329000	-1.624737000
C	2.373614000	-1.235984000	-1.217653000
C	3.727656000	-1.620390000	-0.620123000
H	1.693631000	-2.091096000	-1.372784000
H	3.579731000	-2.322492000	0.222155000
H	2.493781000	-0.728343000	-2.193391000
H	4.377495000	-2.150915000	-1.343645000
C	4.392101000	-0.345197000	-0.090221000
C	3.390571000	0.368476000	0.828654000
H	5.351125000	-0.563995000	0.418368000
H	3.370056000	-0.127710000	1.814949000
H	4.653331000	0.300611000	-0.950104000

H	3.657583000	1.426099000	1.013321000
C	1.544633000	2.696498000	-0.666611000
C	2.236625000	2.144605000	-1.679622000
H	0.459015000	2.813051000	-0.728066000
H	1.729970000	1.788218000	-2.580276000
H	2.048059000	3.096403000	0.218248000
H	3.325765000	2.063415000	-1.650787000
Ga	-2.562077000	-0.097574000	-0.377555000

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K-5-q SCF Done : -3075.292099 A.U.

Cr	-0.894206000	0.176171000	-0.008185000
Cl	0.526869000	-0.640249000	-1.815557000
N	1.380956000	0.647513000	0.952360000
C	0.851286000	1.887376000	0.599612000
C	-0.264974000	2.146972000	1.400496000
C	-0.421787000	1.035734000	2.277698000
C	0.619620000	0.138074000	1.994214000
C	1.434073000	2.777726000	-0.454805000
H	2.475020000	3.050208000	-0.221591000
H	0.845827000	3.704021000	-0.515336000
H	1.426453000	2.308556000	-1.450040000
H	-0.879181000	3.044518000	1.360364000
H	-1.161720000	0.918114000	3.067350000
C	0.937332000	-1.129993000	2.725640000
H	1.975338000	-1.123903000	3.093032000
H	0.811222000	-2.028300000	2.105163000
H	0.270235000	-1.227799000	3.593143000
C	2.863908000	-2.317945000	0.247325000
H	3.423237000	-2.335920000	1.196430000
H	3.487632000	-2.809434000	-0.516955000
H	1.947293000	-2.912554000	0.366478000
C	3.868961000	0.628054000	-1.306884000
H	4.388736000	1.299528000	-0.603845000
H	3.444232000	1.238130000	-2.116397000
H	4.621943000	-0.045742000	-1.746043000
C	-2.295563000	1.187660000	-1.072863000
C	-3.689976000	1.297286000	-0.444509000
H	-1.857071000	2.191399000	-1.232168000
H	-3.620300000	1.449209000	0.652443000
H	-2.346056000	0.703496000	-2.065029000
H	-4.184728000	2.213572000	-0.821010000
C	-4.638615000	0.122676000	-0.730092000
C	-4.397345000	-1.208650000	-0.002623000

H	-5.664596000	0.447455000	-0.480455000
H	-4.467250000	-1.044684000	1.090060000
H	-4.644063000	-0.062413000	-1.821018000
H	-5.249456000	-1.864573000	-0.253787000
C	-3.099412000	-1.979994000	-0.305137000
C	-1.868637000	-1.543692000	0.495941000
H	-3.296194000	-3.048043000	-0.088555000
H	-2.125141000	-1.484051000	1.572002000
H	-2.890249000	-1.943473000	-1.390441000
H	-1.069844000	-2.305787000	0.401647000
Ga	2.509128000	-0.466312000	-0.365327000

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K-6-q SCF Done : -3075.295077 A.U.

Cr	0.668862000	0.519297000	-0.243336000
Cl	-0.676924000	-0.769555000	-1.841963000
N	-1.186305000	0.199342000	1.127784000
C	-0.229089000	-0.689392000	1.643425000
C	0.814407000	0.050814000	2.201898000
C	0.493897000	1.430550000	2.023691000
C	-0.764473000	1.494686000	1.404651000
C	-0.390900000	-2.178834000	1.640765000
H	-1.264439000	-2.486464000	2.237099000
H	0.502891000	-2.641678000	2.081614000
H	-0.517796000	-2.588402000	0.628212000
H	1.698564000	-0.360646000	2.684298000
H	1.073647000	2.287326000	2.362522000
C	-1.574124000	2.722769000	1.119604000
H	-2.541300000	2.687747000	1.647076000
H	-1.782912000	2.859474000	0.050495000
H	-1.028111000	3.608799000	1.471792000
C	-3.566233000	1.131913000	-1.106251000
H	-4.179250000	1.652669000	-0.353190000
H	-4.250111000	0.715636000	-1.863786000
H	-2.918259000	1.866623000	-1.604979000
C	-3.390445000	-2.124126000	0.127589000
H	-4.327250000	-2.225776000	-0.443256000
H	-3.641799000	-2.178929000	1.199418000
H	-2.745539000	-2.979171000	-0.119859000
C	3.211023000	-2.286054000	-0.245341000
C	4.228899000	-1.356976000	0.421588000
H	2.973813000	-3.147998000	0.400150000
H	3.831879000	-0.998842000	1.389878000
H	3.603333000	-2.684105000	-1.196074000

H	5.122250000	-1.954678000	0.675613000
C	4.682704000	-0.147169000	-0.413711000
C	3.760209000	1.083103000	-0.456491000
H	5.656655000	0.190525000	-0.018199000
H	3.570711000	1.429902000	0.578264000
H	4.885250000	-0.480376000	-1.449154000
H	4.342510000	1.902333000	-0.924993000
C	2.444988000	0.940390000	-1.213426000
C	1.515645000	2.052936000	-1.287750000
H	2.529739000	0.325584000	-2.123400000
H	1.738754000	2.960654000	-0.708496000
H	0.990584000	2.254528000	-2.230951000
H	2.265538000	-1.771476000	-0.478808000
Ga	-2.556427000	-0.379580000	-0.315929000

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K-7-q SCF Done : -3153.813417 A.U.

Cl	1.729320000	-1.040821000	1.962558000
N	1.207174000	0.169967000	-1.020302000
C	0.339396000	-0.780321000	-1.507158000
C	-0.724596000	-0.137478000	-2.177243000
C	-0.441691000	1.261377000	-2.141786000
C	0.742481000	1.419519000	-1.418260000
C	0.565030000	-2.252863000	-1.374399000
H	1.352747000	-2.581956000	-2.070788000
H	-0.355788000	-2.799114000	-1.619730000
H	0.881037000	-2.525501000	-0.357926000
H	-1.534867000	-0.633421000	-2.707413000
H	-1.024281000	2.062649000	-2.591167000
C	1.485434000	2.699893000	-1.191912000
H	2.439667000	2.699976000	-1.742621000
H	1.729596000	2.877097000	-0.136458000
H	0.885411000	3.545430000	-1.557454000
C	3.896247000	1.360084000	0.675051000
H	4.315244000	1.905618000	-0.185890000
H	4.744480000	1.029656000	1.297896000
H	3.305466000	2.063960000	1.280850000
C	3.880839000	-1.759763000	-0.786393000
H	3.895399000	-1.608688000	-1.879046000
H	3.450860000	-2.750573000	-0.578891000
H	4.927490000	-1.768699000	-0.440397000
C	-0.328959000	1.976222000	1.796708000
C	-1.115129000	1.144213000	2.507209000
H	0.737594000	1.758071000	1.694063000

H	-0.691050000	0.243151000	2.957656000
H	-0.702631000	2.921020000	1.390277000
H	-2.169648000	1.363799000	2.693689000
Cr	-1.200196000	0.433994000	0.021038000
C	-1.976554000	-1.300714000	0.781984000
C	-3.050447000	-2.045483000	-0.022302000
H	-1.074652000	-1.924307000	0.916874000
H	-2.860213000	-1.976319000	-1.110779000
H	-2.358033000	-1.096958000	1.798063000
H	-2.983210000	-3.126583000	0.206338000
C	-4.497002000	-1.615967000	0.257364000
C	-4.947896000	-0.235208000	-0.238832000
H	-5.170665000	-2.365087000	-0.195716000
H	-4.843086000	-0.188288000	-1.339664000
H	-4.676339000	-1.678758000	1.347609000
H	-6.032497000	-0.163588000	-0.045255000
C	-4.272048000	1.004948000	0.375442000
C	-2.962400000	1.443457000	-0.289754000
H	-4.990815000	1.843574000	0.297143000
H	-3.119938000	1.493928000	-1.381943000
H	-4.140103000	0.846711000	1.462286000
H	-2.704125000	2.474480000	0.028322000
Ga	2.908605000	-0.288530000	0.140951000

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K-8-q SCF Done : -3153.853132 A.U.

C	-4.882291000	0.479088000	-1.090126000
C	-5.144527000	-0.821216000	-0.308504000
H	-5.828737000	0.758588000	-1.585504000
H	-5.878448000	-0.613110000	0.492071000
H	-4.182296000	0.279020000	-1.919274000
H	-5.647470000	-1.527854000	-0.994259000
Cr	-0.517455000	-0.054738000	0.087944000
Cl	0.907046000	-0.138389000	-1.900499000
N	1.809954000	0.260004000	1.104313000
C	1.134469000	1.460087000	1.291596000
C	0.043456000	1.241357000	2.142239000
C	0.051179000	-0.139564000	2.486657000
C	1.156922000	-0.717048000	1.840746000
C	1.558443000	2.764971000	0.691230000
H	2.587279000	3.027135000	0.981875000
H	0.890556000	3.562896000	1.044391000
H	1.516439000	2.753915000	-0.407991000
H	-0.654165000	2.002025000	2.486544000

H	-0.625384000	-0.655364000	3.165517000
C	1.628719000	-2.133469000	1.963849000
H	2.676744000	-2.175175000	2.298027000
H	1.560725000	-2.689048000	1.017791000
H	1.013014000	-2.660508000	2.705593000
C	3.701613000	-1.947882000	-0.639264000
H	4.294295000	-2.187744000	0.258308000
H	4.375703000	-2.004369000	-1.509324000
H	2.926352000	-2.717140000	-0.762032000
C	4.027929000	1.470875000	-1.125234000
H	4.537693000	1.934796000	-0.265067000
H	3.421641000	2.239828000	-1.624163000
H	4.802947000	1.134786000	-1.832596000
C	-1.835481000	1.341327000	-0.607271000
C	-3.000685000	1.672562000	0.339061000
H	-1.252349000	2.240448000	-0.874847000
H	-3.034102000	0.967400000	1.189448000
H	-2.175217000	0.897204000	-1.558055000
H	-2.820181000	2.655558000	0.809450000
C	-4.405570000	1.714621000	-0.304657000
C	-3.929263000	-1.530276000	0.314773000
H	-5.144228000	1.940226000	0.487230000
H	-3.492673000	-0.886380000	1.093247000
H	-4.434769000	2.575447000	-0.997031000
H	-4.290148000	-2.421346000	0.858406000
C	-2.820631000	-1.960654000	-0.668460000
C	-1.414189000	-1.909575000	-0.059547000
H	-3.044515000	-2.984243000	-1.026790000
H	-1.414248000	-2.388885000	0.938291000
H	-2.849316000	-1.336299000	-1.577043000
H	-0.698108000	-2.474285000	-0.686404000
Ga	2.966835000	-0.106853000	-0.559377000

38

K-9-q SCF Done : -2996.682571 A.U.

Cr	1.886412000	0.416470000	0.034251000
Cl	-1.051197000	-2.206858000	-0.605267000
N	-0.437544000	1.027343000	-0.117256000
C	0.207024000	1.835421000	0.814300000
C	1.168192000	2.621078000	0.150847000
C	1.093411000	2.292445000	-1.233883000
C	0.086005000	1.323632000	-1.368181000
C	-0.175125000	1.921685000	2.259277000
H	-1.160183000	2.404014000	2.369614000

H	0.562293000	2.531841000	2.799368000
H	-0.232758000	0.938475000	2.741231000
H	1.823324000	3.352581000	0.618795000
H	1.684321000	2.716919000	-2.043274000
C	-0.427249000	0.725731000	-2.641493000
H	-1.381537000	1.198853000	-2.923280000
H	-0.612218000	-0.353196000	-2.544553000
H	0.289318000	0.900740000	-3.456579000
C	-3.491479000	0.325285000	-1.048919000
H	-3.518531000	1.426496000	-1.106920000
H	-4.472795000	-0.010647000	-0.675418000
H	-3.367845000	-0.074483000	-2.066401000
C	-2.421640000	-0.573391000	2.133982000
H	-2.783700000	0.338563000	2.634441000
H	-1.549860000	-0.959018000	2.683596000
H	-3.218977000	-1.331515000	2.211481000
H	3.362693000	1.010884000	0.203708000
C	2.047564000	-0.802143000	1.679701000
C	2.531608000	-2.106360000	1.000382000
H	2.784944000	-0.393365000	2.388117000
H	3.268944000	-2.665654000	1.599748000
H	1.084191000	-0.947353000	2.193797000
H	1.673223000	-2.765761000	0.800139000
C	3.138548000	-1.656225000	-0.307771000
C	2.419617000	-1.430583000	-1.437084000
H	4.202820000	-1.392928000	-0.302140000
H	2.901150000	-1.043032000	-2.339888000
H	1.373761000	-1.755250000	-1.508265000
Ga	-2.068134000	-0.311507000	0.193679000

38

K-2-3-q SCF Done: -2996.685344 A.U.

Cr	1.642185000	0.016999000	0.124458000
Cl	-0.266626000	-0.302067000	-1.868458000
N	-0.811717000	0.012807000	1.174492000
C	-0.126548000	-1.125011000	1.552582000
C	1.028099000	-0.761363000	2.269630000
C	1.054590000	0.660003000	2.310201000
C	-0.080527000	1.106005000	1.607640000
C	-0.599554000	-2.516832000	1.272482000
H	-1.589748000	-2.697241000	1.717922000
H	0.107017000	-3.241513000	1.700092000
H	-0.681788000	-2.712500000	0.193560000
H	1.726957000	-1.452100000	2.736831000

H	1.773858000	1.296278000	2.822709000
C	-0.535074000	2.524498000	1.459831000
H	-1.512174000	2.674823000	1.945815000
H	-0.641788000	2.826878000	0.409736000
H	0.190663000	3.197616000	1.936877000
C	-2.895402000	1.824281000	-0.796432000
H	-3.387452000	2.250841000	0.092925000
H	-3.667908000	1.700358000	-1.573256000
H	-2.159255000	2.550559000	-1.170373000
C	-3.300082000	-1.569626000	-0.432564000
H	-3.713124000	-1.763596000	0.571376000
H	-2.796728000	-2.482769000	-0.781039000
H	-4.149324000	-1.373132000	-1.107164000
C	2.639249000	-1.719172000	-0.321177000
C	3.096591000	-0.944847000	-1.459510000
H	1.883279000	-2.491678000	-0.506725000
H	2.537911000	-1.103137000	-2.386594000
H	3.389461000	-2.010241000	0.426462000
H	4.175136000	-0.916501000	-1.631820000
C	3.103230000	1.065665000	-1.418246000
C	2.241010000	1.852368000	-0.558127000
H	2.907760000	1.119793000	-2.493425000
H	1.381801000	2.351278000	-1.021614000
H	4.170002000	1.144189000	-1.190303000
H	2.721589000	2.441537000	0.233636000
Ga	-2.116691000	0.030708000	-0.428650000

38

K-3-9-q SCF Done: -2996.677476 A.U.

Cr	-1.684958000	0.168865000	0.038335000
Cl	0.121079000	-1.159041000	1.227744000
N	1.174210000	0.813917000	-0.868261000
C	0.285354000	0.321793000	-1.800810000
C	-0.817853000	1.183520000	-1.893300000
C	-0.568611000	2.264128000	-0.980757000
C	0.652144000	1.999648000	-0.370586000
C	0.517164000	-0.920306000	-2.605301000
H	1.504254000	-0.899426000	-3.091489000
H	-0.250472000	-1.003977000	-3.387372000
H	0.471914000	-1.831764000	-1.990648000
H	-1.609615000	1.123322000	-2.638061000
H	-1.175310000	3.156690000	-0.840327000
C	1.353760000	2.853549000	0.639678000
H	2.404449000	3.023904000	0.358618000

H	1.355040000	2.404097000	1.643941000
H	0.855276000	3.831002000	0.708745000
C	3.289687000	0.395009000	1.750775000
H	3.961850000	1.184403000	1.376675000
H	3.916531000	-0.381014000	2.219408000
H	2.648103000	0.827417000	2.531638000
C	3.045863000	-1.985726000	-0.719621000
H	3.539274000	-1.648872000	-1.646221000
H	2.305619000	-2.754033000	-0.984859000
H	3.813694000	-2.457655000	-0.085471000
H	-2.984885000	1.077351000	-0.363957000
C	-2.857066000	-1.397208000	-0.615277000
C	-4.187041000	-0.955324000	0.028888000
H	-2.911883000	-1.452317000	-1.713372000
H	-4.905115000	-0.602180000	-0.726103000
H	-2.467505000	-2.349384000	-0.222298000
H	-4.684099000	-1.760769000	0.600320000
C	-3.845156000	0.188186000	0.977209000
C	-2.884709000	-0.006700000	1.953027000
H	-4.481949000	1.077845000	1.000514000
H	-2.667391000	0.768000000	2.693984000
H	-2.512899000	-1.010847000	2.171313000
Ga	2.262422000	-0.451990000	0.273795000

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K-4-5-q SCF Done: -3075.229474 A.U.

Cr	1.472959000	-0.265422000	-0.199598000
Cl	-0.273497000	-1.865238000	-0.633694000
N	-1.426136000	0.912883000	0.515605000
C	-0.341578000	0.928835000	1.396925000
C	0.232894000	2.207246000	1.359032000
C	-0.506889000	2.977825000	0.435111000
C	-1.516079000	2.153621000	-0.064985000
C	-0.163362000	-0.090477000	2.496453000
H	-1.016525000	-0.070754000	3.196376000
H	0.737400000	0.146403000	3.082817000
H	-0.078575000	-1.130347000	2.141221000
H	1.052445000	2.546885000	1.992050000
H	-0.342317000	4.018703000	0.158632000
C	-2.551005000	2.520944000	-1.086257000
H	-3.568897000	2.260435000	-0.754658000
H	-2.391212000	2.019800000	-2.054834000
H	-2.525280000	3.605614000	-1.264926000
C	-3.372212000	-0.687444000	-1.721523000

H	-4.298353000	-0.094841000	-1.645665000
H	-3.656002000	-1.715892000	-1.998244000
H	-2.761214000	-0.274052000	-2.537189000
C	-3.079379000	-1.767172000	1.577952000
H	-3.805204000	-2.527017000	1.246865000
H	-3.595711000	-1.090022000	2.278940000
H	-2.278442000	-2.280977000	2.129374000
C	2.929155000	-1.611662000	-0.812045000
C	4.104008000	-1.557903000	0.165271000
H	2.487111000	-2.617131000	-0.893264000
H	3.822270000	-2.044794000	1.118550000
H	3.244225000	-1.303788000	-1.826612000
H	4.986412000	-2.115234000	-0.202508000
C	4.462539000	-0.095626000	0.445845000
C	3.190492000	0.693126000	0.717120000
H	5.166574000	-0.004791000	1.294787000
H	2.610848000	0.219230000	1.550694000
H	4.991775000	0.338620000	-0.422637000
H	3.362938000	1.728535000	1.033085000
C	2.483841000	1.608569000	-1.217118000
C	1.413139000	0.994912000	-1.881057000
H	2.300244000	2.546590000	-0.691496000
H	0.422040000	1.457630000	-1.821683000
H	3.508684000	1.448905000	-1.557519000
H	1.594884000	0.321176000	-2.723321000
Ga	-2.400068000	-0.753182000	0.008411000

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K-5-6-q SCF Done: -3075.253660 A.U.

Cr	1.158743000	0.248007000	0.328337000
Ga	-2.511920000	-0.192934000	-0.592536000
Cl	-0.550324000	-0.484567000	-1.852618000
N	-1.348403000	0.127096000	1.093332000
C	-0.620369000	-0.876597000	1.706436000
C	0.385720000	-0.303317000	2.504837000
C	0.282555000	1.105884000	2.346635000
C	-0.784152000	1.336621000	1.458042000
C	-0.927207000	-2.335124000	1.564297000
H	-1.947174000	-2.562583000	1.908899000
H	-0.223964000	-2.923857000	2.169993000
H	-0.848140000	-2.670630000	0.519918000
H	1.078056000	-0.849132000	3.143783000
H	0.871938000	1.875427000	2.841623000
C	-1.333865000	2.670120000	1.056801000

H	-2.357455000	2.803398000	1.441845000
H	-1.375354000	2.799118000	-0.032312000
H	-0.705467000	3.469476000	1.473297000
C	-3.456562000	1.447068000	-1.209277000
H	-4.024380000	1.929628000	-0.397033000
H	-4.181128000	1.144281000	-1.983202000
H	-2.784185000	2.193269000	-1.657004000
C	2.416102000	-1.595353000	0.001802000
C	3.945808000	-1.490035000	0.128846000
H	1.984998000	-2.104723000	0.876658000
H	4.206077000	-1.077473000	1.121625000
H	2.128372000	-2.185685000	-0.884201000
H	4.399264000	-2.497320000	0.094742000
C	4.591936000	-0.604310000	-0.951743000
C	4.090081000	0.849420000	-0.915577000
H	5.687800000	-0.614826000	-0.829356000
H	4.320186000	1.283260000	0.074755000
H	4.390500000	-1.037126000	-1.949703000
H	4.646555000	1.456875000	-1.651147000
C	2.589535000	1.000710000	-1.188541000
C	1.825756000	2.025614000	-0.516617000
H	2.305411000	0.793627000	-2.230187000
H	2.344510000	2.678461000	0.197516000
H	1.016374000	2.517381000	-1.067172000
H	2.292527000	-0.332050000	-0.705444000
C	-3.526844000	-1.901415000	-0.457076000
H	-2.905379000	-2.791461000	-0.630827000
H	-4.012767000	-2.003974000	0.527703000
H	-4.324114000	-1.892315000	-1.218241000

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K-7-8-q SCF Done: -3153.788529 A.U.

C	4.999077000	-0.275213000	0.170044000
C	4.433701000	1.001132000	-0.470272000
H	4.934760000	-0.181243000	1.270940000
H	5.074830000	1.840051000	-0.144568000
H	6.079162000	-0.291146000	-0.057536000
H	4.570499000	0.953872000	-1.566078000
Cr	1.050812000	0.324776000	0.000549000
Cl	-1.937419000	-1.816922000	-1.511037000
N	-1.187425000	0.428940000	0.851106000
C	-0.485428000	-0.415756000	1.700280000
C	0.487267000	0.332575000	2.389766000
C	0.330537000	1.687070000	1.985244000

C	-0.703720000	1.720731000	1.041309000
C	-0.834649000	-1.855424000	1.910472000
H	-1.684817000	-1.937377000	2.607290000
H	0.017556000	-2.390518000	2.352509000
H	-1.121831000	-2.347217000	0.971256000
H	1.179017000	-0.062220000	3.132234000
H	0.903362000	2.547596000	2.327961000
C	-1.301857000	2.941431000	0.412138000
H	-2.313566000	3.129679000	0.806402000
H	-1.394412000	2.861277000	-0.678599000
H	-0.682650000	3.819422000	0.646336000
C	-3.488946000	1.274648000	-1.505095000
H	-3.899717000	2.156738000	-0.988624000
H	-4.296683000	0.849983000	-2.124729000
H	-2.694078000	1.602783000	-2.192238000
C	-4.147391000	-0.909386000	1.112922000
H	-4.170041000	-0.275504000	2.015574000
H	-3.880502000	-1.933412000	1.413856000
H	-5.170173000	-0.938547000	0.702322000
C	1.794443000	-1.560781000	-0.360529000
C	3.059889000	-2.068947000	0.344608000
H	0.940504000	-2.211316000	-0.107864000
H	3.043602000	-1.819365000	1.424228000
H	1.918687000	-1.659117000	-1.454528000
H	3.043778000	-3.175240000	0.317157000
C	4.418183000	-1.637595000	-0.244596000
C	2.990300000	1.352850000	-0.105784000
H	5.160879000	-2.394829000	0.060260000
H	2.816061000	0.965249000	0.922727000
H	4.374298000	-1.703137000	-1.348324000
H	2.833099000	2.439000000	-0.049629000
C	2.027962000	1.133584000	-1.973102000
C	0.640098000	0.865187000	-1.975843000
H	2.378988000	2.149512000	-2.169701000
H	-0.057478000	1.707047000	-2.020213000
H	2.705065000	0.358400000	-2.335609000
H	0.258300000	-0.080905000	-2.373572000
Ga	-2.908215000	-0.174377000	-0.265545000

Table S2. Spin contamination (in e).

Model Catalyst	All	S²	A	B	C	D	E	F	G	H	I	J	K
Active Species	5	8.75	0.004	0.003	0.004	0.004	0.004	0.003	0.003	0.003	0.003	0.005	0.004
1	3	3.75	0.063	0.064	0.060	0.063	0.063	0.066	0.066	0.063	0.061	0.087	0.063
2	3	3.75	0.080	0.080	0.081	0.080	0.072	0.075	0.078	0.078	0.076	0.079	0.080
TS-2-3	3	3.75	0.087	0.090	0.090	0.091	0.079	0.090	0.097	0.087	0.087	0.087	0.087
3	3	3.75	0.051	0.054	0.050	0.053	0.054	0.061	0.063	0.053	0.054	0.058	0.051
4	3	3.75	0.060	0.063	0.073	0.075	0.067	0.076	0.076	0.060	0.061	0.067	0.072
TS-4-5	3	3.75	0.053	0.056	0.053	0.069	0.059	0.059	0.072	0.053	0.054	0.051	0.064
5	3	3.75	0.050	0.053	0.050	0.052	0.054	0.061	0.063	0.052	0.054	0.055	0.049
TS-5-6	3	3.75	0.092	0.095	0.095	0.102	0.086	0.094	0.100	0.089	0.086	0.052	0.095
6	3	3.75	0.072	0.071	0.073	0.072	0.076	0.077	0.075	0.072	0.072	0.098	0.073
7	3	3.75	0.056	0.060	0.061	0.067	0.063	0.066	0.080	0.057	0.057	0.062	0.059
TS-7-8	3	3.75	0.051	0.053	0.053	0.059	0.058	0.055	0.067	0.051	0.052	0.055	0.051
8	3	3.75	0.059	0.062	0.056	0.060	0.064	0.072	0.074	0.062	0.065	0.063	0.057
TS-3-9	3	3.75	0.043	0.046	0.044	0.054	0.047	0.055	0.068	0.044	0.044	0.052	0.053
9	3	3.75	0.068	0.068	0.066	0.066	0.069	0.069	0.071	0.067	0.067	0.049	0.046



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