Supporting Information

Direct Nucleophilic Trifluoromethylation Using Fluoroform: A Theoretical Mechanistic Investigation and Insight into the Effect of Alkali Metal Cations

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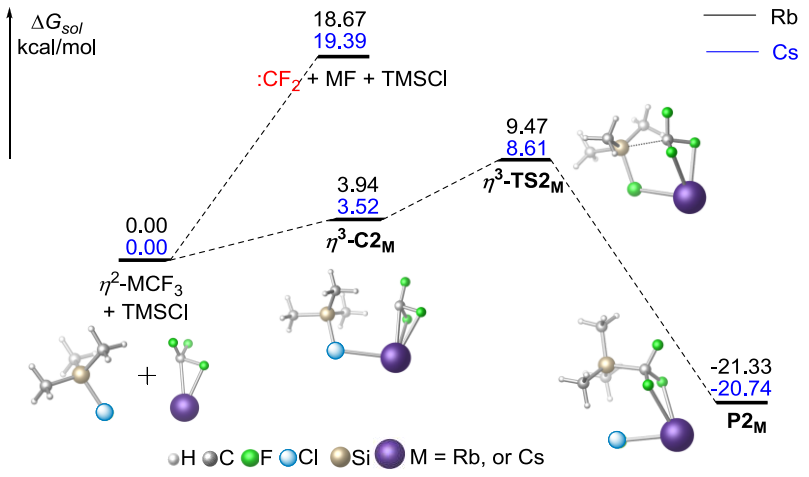

Figure *1S.* Energy profile (energies in kcal/mol) for the processes of decomposition of η^2-MCF_3 (M = Rb, Cs) and their trifluoromethylation with TMSCl.

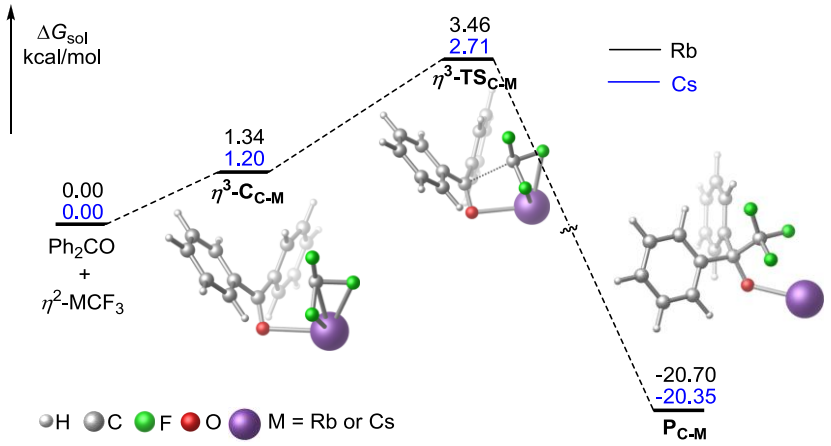

Figure *2S*. Energy profile (energies in kcal/mol) for the trifluoromethylation of benzophenone with η^2-MCF_3 (M = Rb, Cs).

Table *1S*. Orbital energies (a.u.) of HOMO and LUMO for M^+ (M = Li, Na, K, Rb, Cs)

	E_{HOMO}	E_{LUMO}	$(E_{LUMO}-E_{HOMO})/2$
Li^+	-2.28230	-0.09107	1.09562
Na^+	-1.39274	-0.09445	0.64915
K^+	-0.91133	-0.08208	0.41463
Rb^+	-0.77688	-0.08078	0.34805
Cs^+	-0.65791	-0.07679	0.29056

Table *2S*. Optimized Cartesian coordinates (Å) and total electronic energies (a.u.) of the stationary points as well as the imaginary frequency (cm^{-1}) of TSs.

Atoms	x	y	z
CF_3H, -338.234874987			
C	−0. 000099000	−0. 000215000	0. 340675000
H	−0. 000055000	−0. 000258000	1. 429290000
F	0. 949850000	−0. 809348000	−0. 128665000
F	−1. 176246000	−0. 417355000	−0. 128683000
F	0. 226468000	1. 226875000	−0. 128579000
$(TMS)_2NK$, -1473.19647054			
N	0. 000025000	0. 145152000	−0. 000750000

Si	-1.560397000	-0.477759000	-0.000188000
Si	1.560403000	-0.477891000	0.000025000
C	-2.007545000	-1.518438000	-1.516623000
H	-1.405596000	-2.431912000	-1.542123000
H	-3.061344000	-1.814199000	-1.518372000
H	-1.803879000	-0.968604000	-2.439938000
C	-2.008759000	-1.513245000	1.519464000
H	-1.805466000	-0.960531000	2.441146000
H	-3.062782000	-1.808251000	1.521373000
H	-1.407481000	-2.427056000	1.548404000
C	-2.784711000	0.995424000	-0.002842000
H	-3.822498000	0.650294000	-0.003156000
H	-2.670321000	1.623249000	0.890424000
H	-2.668864000	1.621011000	-0.897472000
C	2.008141000	-1.518342000	-1.516387000
H	1.406649000	-2.432094000	-1.542296000
H	1.804648000	-0.968427000	-2.439696000
H	3.062090000	-1.813598000	-1.517774000
C	2.007848000	-1.513503000	1.519854000
H	3.061987000	-1.808038000	1.523147000
H	1.802947000	-0.961051000	2.441336000
H	1.406914000	-2.427580000	1.547775000
C	2.784815000	0.995208000	-0.002542000
H	2.669827000	1.623708000	0.890172000
H	3.822586000	0.650030000	-0.001862000
H	2.669626000	1.620131000	-0.897722000
K	0.000104000	2.622808000	-0.000073000

η^2-C1$_K$, -1811.45370913

N	0.549142000	0.000619000	0.076344000
Si	1.102853000	-1.563486000	-0.206558000
Si	1.099296000	1.566607000	-0.203175000
C	0.365058000	-2.359278000	-1.761415000
H	0.604059000	-1.764555000	-2.648929000
H	0.758034000	-3.367684000	-1.923444000
H	-0.724613000	-2.442831000	-1.695580000
C	2.977242000	-1.773336000	-0.329362000
H	3.481019000	-1.352354000	0.545179000
H	3.252467000	-2.829864000	-0.404626000
H	3.373053000	-1.263613000	-1.212274000
C	0.539112000	-2.692117000	1.232474000
H	0.879595000	-3.720868000	1.084237000
H	0.951682000	-2.363499000	2.194838000
H	-0.554811000	-2.740032000	1.306676000

C	0.357204000	2.365367000	-1.754518000
H	0.595117000	1.773177000	-2.644025000
H	-0.732375000	2.448023000	-1.686520000
H	0.749133000	3.374483000	-1.914683000
C	2.973085000	1.779416000	-0.330526000
H	3.247214000	2.836676000	-0.399151000
H	3.480208000	1.352374000	0.539115000
H	3.366048000	1.276415000	-1.218570000
C	0.537184000	2.690477000	1.239966000
H	0.953885000	2.360894000	2.200174000
H	0.874335000	3.720488000	1.092743000
H	-0.556604000	2.735191000	1.317991000
C	-2.289199000	0.000149000	-0.790719000
H	-1.327992000	0.001871000	-1.297144000
F	-2.395951000	-1.077149000	0.018371000
F	-2.398291000	1.074695000	0.021569000
F	-3.338930000	0.000059000	-1.603530000
K	-0.889637000	-0.006571000	2.158040000

η^3-TS1$_K$, -1811.42939701, *i*972.6599

N	0.478598000	0.020440000	-0.118769000
Si	1.232625000	-1.520502000	-0.197203000
Si	1.017907000	1.652780000	-0.160754000
C	0.813981000	-2.386143000	-1.810590000
H	1.215291000	-1.829709000	-2.661797000
H	1.219077000	-3.401243000	-1.845873000
H	-0.270383000	-2.449826000	-1.941044000
C	3.100024000	-1.507883000	0.035004000
H	3.394477000	-1.060032000	0.987763000
H	3.472806000	-2.536700000	0.022726000
H	3.608998000	-0.962516000	-0.762853000
C	0.537640000	-2.625817000	1.190895000
H	0.964042000	-3.630963000	1.126925000
H	0.786435000	-2.250910000	2.191790000
H	-0.548462000	-2.746477000	1.101228000
C	0.296097000	2.531098000	-1.656062000
H	0.673225000	2.091630000	-2.583371000
H	-0.793930000	2.438416000	-1.666775000
H	0.544225000	3.596284000	-1.660017000
C	2.885531000	1.876583000	-0.147781000
H	3.126814000	2.943798000	-0.132209000
H	3.354177000	1.414467000	0.724368000
H	3.344414000	1.446963000	-1.041506000
C	0.344011000	2.569189000	1.367176000

H	0.701895000	2.132442000	2.307827000
H	0.667445000	3.613924000	1.368577000
H	-0.752552000	2.588718000	1.362437000
K	-1.182521000	-0.126125000	2.002967000
C	-2.090578000	-0.095743000	-0.828668000
H	-0.652229000	-0.039235000	-0.683502000
F	-2.936171000	-0.094605000	-1.864888000
F	-2.487400000	-1.209678000	-0.056211000
F	-2.550398000	0.957024000	-0.004251000

η^3-P1$_K$, -1811.43551162

N	-0.589504000	0.000022000	0.104351000
Si	-1.674438000	-1.357424000	0.238212000
Si	-0.854225000	1.727874000	0.046572000
C	-2.307312000	-1.596699000	1.986276000
H	-2.855970000	-0.711366000	2.320342000
H	-2.979313000	-2.456305000	2.059272000
H	-1.476723000	-1.753538000	2.679275000
C	-3.130489000	-1.171671000	-0.935638000
H	-2.813200000	-0.825347000	-1.923700000
H	-3.621082000	-2.140815000	-1.065818000
H	-3.879227000	-0.472045000	-0.558822000
C	-0.664997000	-2.867139000	-0.274191000
H	-1.169858000	-3.798668000	-0.005856000
H	-0.507710000	-2.900288000	-1.358781000
H	0.310646000	-2.864983000	0.223641000
C	-0.108476000	2.522019000	1.564282000
H	-0.598691000	2.162742000	2.472775000
H	0.953150000	2.267580000	1.629927000
H	-0.197723000	3.611302000	1.535525000
C	-2.686059000	2.115032000	-0.092603000
H	-2.833600000	3.197802000	-0.045277000
H	-3.111509000	1.764056000	-1.035832000
H	-3.257724000	1.669115000	0.726163000
C	0.005238000	2.423754000	-1.486538000
H	-0.346713000	1.939198000	-2.404940000
H	-0.197270000	3.492568000	-1.597475000
H	1.091759000	2.316774000	-1.402152000
K	1.364250000	-0.540296000	-1.781564000
C	2.365158000	-0.389083000	0.813499000
H	0.297389000	-0.212488000	0.610140000
F	3.204266000	-0.200306000	1.850400000
F	3.136930000	-1.251667000	-0.042429000
F	2.543475000	0.849372000	0.061290000

η^2-TS1$_K$, -1811.42680380, *i*1003.4229

N	0.465722000	0.009753000	0.076258000
Si	1.251869000	-1.502828000	-0.165574000
Si	1.041074000	1.619787000	-0.128478000
C	1.621546000	-1.860047000	-1.973814000
H	2.313834000	-1.115785000	-2.379031000
H	2.070984000	-2.847122000	-2.114950000
H	0.702908000	-1.815191000	-2.565670000
C	2.851270000	-1.670899000	0.819128000
H	2.695798000	-1.435816000	1.876625000
H	3.230210000	-2.695613000	0.758132000
H	3.634026000	-1.006489000	0.445641000
C	0.050533000	-2.824274000	0.469925000
H	0.384275000	-3.829823000	0.200211000
H	-0.033575000	-2.814901000	1.564235000
H	-0.946432000	-2.687829000	0.036920000
C	0.799126000	2.246248000	-1.882264000
H	1.371137000	1.638677000	-2.589212000
H	-0.254494000	2.182310000	-2.168173000
H	1.120345000	3.285818000	-1.992776000
C	2.848593000	1.825606000	0.352820000
H	3.130865000	2.882640000	0.347285000
H	3.051900000	1.424757000	1.349616000
H	3.503270000	1.307470000	-0.353706000
C	-0.009671000	2.720181000	1.010477000
H	0.190367000	2.528813000	2.072214000
H	0.194778000	3.781169000	0.844419000
H	-1.078448000	2.574527000	0.809397000
C	-2.152503000	-0.099543000	-0.728727000
H	-0.716648000	-0.054126000	-0.367952000
F	-2.583454000	-1.173974000	-1.436315000
F	-2.996534000	-0.134320000	0.431306000
F	-2.627610000	0.980669000	-1.400057000
K	-1.163755000	-0.109694000	2.160528000

η^2-P1$_K$, -1811.43462805

N	-0.595416000	-0.073754000	-0.033542000
Si	-1.944242000	-1.160603000	0.225522000
Si	-0.617392000	1.683001000	-0.028424000
C	-2.923375000	-0.726960000	1.768515000
H	-3.368672000	0.269286000	1.689778000
H	-3.736057000	-1.439611000	1.935122000
H	-2.279255000	-0.734947000	2.651781000

C	-3.097805000	-1.125901000	-1.257997000
H	-2.554844000	-1.315846000	-2.188477000
H	-3.861973000	-1.902107000	-1.156832000
H	-3.612745000	-0.168608000	-1.360129000
C	-1.205668000	-2.879378000	0.394290000
H	-1.965517000	-3.607611000	0.689763000
H	-0.775875000	-3.227316000	-0.550598000
H	-0.412234000	-2.895688000	1.146461000
C	-0.459582000	2.373678000	1.701687000
H	-1.289468000	2.040717000	2.330788000
H	0.473833000	2.030217000	2.154383000
H	-0.457124000	3.467095000	1.695494000
C	-2.223748000	2.259641000	-0.813764000
H	-2.231507000	3.351575000	-0.874976000
H	-2.345709000	1.867771000	-1.827012000
H	-3.097389000	1.960843000	-0.227681000
C	0.822813000	2.284243000	-1.084170000
H	0.681948000	2.046474000	-2.145331000
H	0.908477000	3.372700000	-1.021971000
H	1.774595000	1.873578000	-0.730987000
C	2.462128000	-0.590564000	0.662352000
H	0.249278000	-0.416822000	0.450001000
F	3.324269000	-1.334867000	1.407422000
F	3.346124000	-0.128911000	-0.412164000
F	2.346867000	0.583162000	1.398456000
K	1.396164000	-0.790105000	-1.839635000

$(TMS)_2NH$, -873.857781526

N	0.000018000	-0.002247000	0.837277000
Si	-1.576195000	-0.009119000	0.093037000
Si	1.576197000	0.008678000	0.092977000
C	-2.054208000	1.694201000	-0.540341000
H	-1.331558000	2.058242000	-1.275540000
H	-3.037758000	1.675270000	-1.018771000
H	-2.090368000	2.418540000	0.277538000
C	-1.569719000	-1.198472000	-1.361967000
H	-1.310765000	-2.210210000	-1.039838000
H	-2.554967000	-1.233257000	-1.835311000
H	-0.851572000	-0.895968000	-2.129708000
C	-2.817390000	-0.563933000	1.385088000
H	-3.831202000	-0.570248000	0.976575000
H	-2.591111000	-1.572548000	1.739694000
H	-2.815936000	0.107016000	2.248693000
C	1.569996000	1.206505000	-1.354948000

H	0.851807000	0.908837000	-2.124524000
H	1.311220000	2.216317000	-1.026691000
H	2.555238000	1.244069000	-1.828090000
C	2.053815000	-1.691084000	-0.550080000
H	3.037189000	-1.669504000	-1.028761000
H	2.090306000	-2.419891000	0.263818000
H	1.330898000	-2.051116000	-1.286972000
C	2.817460000	0.555448000	1.388314000
H	2.815928000	-0.120960000	2.247643000
H	3.831261000	0.564171000	0.979813000
H	2.591432000	1.561845000	1.749323000
H	0.000081000	-0.004686000	1.849573000

η^2-KCF_3, -937.550186344

C	-0.756251000	-0.000007000	-0.305609000
F	-1.606112000	-1.068685000	-0.257376000
F	-0.236356000	-0.004349000	1.093869000
F	-1.600538000	1.073044000	-0.251900000
K	1.869714000	-0.000003000	-0.180404000

$TS[2\text{-}3]_K$, -937.549414603, *i*57.3016

C	-0.772274000	0.019789000	-0.345347000
F	-2.023148000	-0.453565000	-0.531673000
F	-0.313312000	-0.807149000	0.796716000
F	-0.984479000	1.223309000	0.335750000
K	1.816952000	0.011469000	-0.175530000

η^3-KCF_3, -937.550523238

C	-0.820723000	0.000042000	-0.415537000
F	-2.162646000	-0.000403000	-0.376058000
F	-0.488880000	-1.091869000	0.487952000
F	-0.489434000	1.092272000	0.487640000
K	1.746999000	-0.000013000	-0.152768000

$(CH_3)_3SiCl$, -869.473001795

Si	0.342899000	0.000512000	-0.000290000
C	0.887647000	-0.703118000	1.639471000
H	0.514973000	-1.721371000	1.769679000
H	1.979310000	-0.728905000	1.700519000
H	0.514648000	-0.096560000	2.467507000
C	0.887506000	-1.068239000	-1.428486000
H	0.514350000	-2.088425000	-1.316911000
H	0.514697000	-0.672558000	-2.375622000
H	1.979129000	-1.108797000	-1.482394000

C	0.885565000	1.772152000	-0.210714000
H	0.513982000	2.184318000	-1.151309000
H	0.509777000	2.394515000	0.604090000
H	1.977087000	1.840591000	-0.216315000
Cl	-1.751932000	-0.000868000	0.000187000

η^3-C2$_K$, -1807.04442525

Si	1.985291000	-0.402188000	-0.003702000
C	1.248299000	-1.059183000	1.569377000
H	1.591146000	-2.086648000	1.725525000
H	1.566490000	-0.464650000	2.429120000
H	0.157740000	-1.071126000	1.525326000
C	1.420953000	-1.265975000	-1.544170000
H	0.329658000	-1.263187000	-1.585226000
H	1.824407000	-0.785738000	-2.438144000
H	1.765101000	-2.304484000	-1.529512000
C	3.842742000	-0.258068000	0.101823000
H	4.254024000	0.203234000	-0.798401000
H	4.142977000	0.342185000	0.963317000
H	4.288768000	-1.251269000	0.208286000
Cl	1.348730000	1.644147000	-0.169688000
C	-1.883505000	-0.827647000	-0.179504000
F	-2.088202000	-2.164430000	-0.221488000
F	-2.149161000	-0.528193000	1.214904000
F	-3.107473000	-0.311800000	-0.728952000
K	-1.700537000	1.782466000	0.019522000

η^3-TS2$_K$, -1807.04012393, *i*85.4633

Si	-1.642061000	0.123447000	0.000189000
C	-1.425532000	0.996858000	1.642902000
H	-1.121585000	2.032875000	1.480064000
H	-2.356152000	0.978146000	2.215350000
H	-0.638494000	0.521473000	2.229961000
C	-1.425245000	0.996832000	-1.642495000
H	-0.637804000	0.521818000	-2.229305000
H	-2.355672000	0.977776000	-2.215245000
H	-1.121784000	2.032972000	-1.479488000
C	-3.416606000	-0.523511000	0.000027000
H	-3.630410000	-1.127771000	-0.884928000
H	-3.630718000	-1.127342000	0.885200000
H	-4.107705000	0.326903000	-0.000293000
Cl	-0.668183000	-1.827355000	0.000352000
C	0.976803000	1.068197000	0.000190000
F	0.932302000	2.423737000	0.000166000

F	1.882932000	0.807669000	1.090878000
F	1.881752000	0.807663000	-1.091515000
K	2.285205000	-1.441154000	-0.000497000

$P2_K$, -1807.08047612

Si	-1.826471000	0.563379000	-0.009030000
C	-3.006726000	0.127045000	-1.392278000
H	-3.517067000	-0.818930000	-1.199580000
H	-3.765938000	0.905549000	-1.501897000
H	-2.478168000	0.044264000	-2.345014000
C	-2.634266000	0.481823000	1.673405000
H	-1.897763000	0.644685000	2.463453000
H	-3.399678000	1.256361000	1.765899000
H	-3.112373000	-0.486217000	1.840206000
C	-0.872574000	2.121010000	-0.313136000
H	-0.141954000	2.316806000	0.474195000
H	-0.304392000	2.074524000	-1.244458000
H	-1.569524000	2.962541000	-0.371764000
Cl	2.550636000	1.715952000	0.018840000
C	-0.606523000	-0.960515000	0.011896000
F	-1.265156000	-2.137201000	0.054431000
F	0.213846000	-1.047196000	-1.077730000
F	0.247826000	-0.989932000	1.076560000
K	2.755185000	-1.000279000	-0.022820000

$(CH_3)_3SiCF_3$, -746.864819869

Si	1.256581000	-0.683653000	-0.043152000
C	2.401447000	-0.734248000	-1.517764000
H	3.126414000	0.081778000	-1.475704000
H	2.954375000	-1.676222000	-1.548204000
H	1.839876000	-0.642044000	-2.450118000
C	2.165422000	-0.698698000	1.587821000
H	1.469298000	-0.583564000	2.421636000
H	2.701511000	-1.641295000	1.723077000
H	2.892947000	0.114540000	1.637685000
C	-0.102726000	-1.960728000	-0.130696000
H	-0.814127000	-1.829920000	0.687731000
H	-0.650640000	-1.882410000	-1.072422000
H	0.308800000	-2.970756000	-0.061832000
C	0.364548000	1.034261000	-0.129605000
F	1.230162000	2.072886000	-0.090592000
F	-0.358905000	1.188241000	-1.261761000
F	-0.495983000	1.221613000	0.897246000

KCl, -1060.19605605

K	0.000000000	0.000000000	1.267504000
Cl	0.000000000	0.000000000	-1.416622000

K^+, -599.743189344

K	0.000000000	0.000000000	0.000000000

CF_3^-, -337.623798522

C	-0.000128000	0.000080000	0.548975000
F	-0.973270000	-0.790249000	-0.122006000
F	1.171192000	-0.447613000	-0.121959000
F	-0.197837000	1.237809000	-0.122018000

:CF_2, -237.693295140

C	0.000000000	0.000000000	0.596391000
F	0.000000000	1.023734000	-0.198797000
F	0.000000000	-1.023734000	-0.198797000

KF, -699.809211215

F	0.000000000	0.000000000	-1.486793000
K	0.000000000	0.000000000	0.704270000

$(TMS)_2NNa$, -1035.52893376

N	0.000002000	0.386464000	0.000790000
Si	1.566115000	-0.236797000	0.000133000
Si	-1.566109000	-0.236800000	0.000104000
C	2.002304000	-1.280228000	1.515278000
H	1.400407000	-2.193768000	1.536170000
H	3.055842000	-1.576329000	1.521077000
H	1.794846000	-0.731678000	2.438341000
C	2.006196000	-1.265837000	-1.523720000
H	1.798948000	-0.709292000	-2.442048000
H	3.060295000	-1.559894000	-1.530717000
H	1.405916000	-2.180180000	-1.553661000
C	2.762253000	1.254312000	0.008404000
H	3.811509000	0.945930000	0.008435000
H	2.623766000	1.880749000	-0.882758000
H	2.620898000	1.872432000	0.904838000
C	-2.007887000	-1.264284000	1.524501000
H	-1.407508000	-2.178517000	1.555982000
H	-1.801663000	-0.706799000	2.442485000
H	-3.061962000	-1.558443000	1.530665000
C	-2.000620000	-1.281772000	-1.514469000
H	-3.054168000	-1.577831000	-1.521046000

H	−1.792219000	−0.734140000	−2.437868000
H	−1.398785000	−2.195378000	−1.533872000
C	−2.762243000	1.254295000	−0.011088000
H	−2.620022000	1.871292000	−0.908153000
H	−3.811497000	0.945904000	−0.011715000
H	−2.624635000	1.881854000	0.879425000
Na	−0.000007000	2.539116000	0.000194000

η^2-C1$_{Na}$, -1373.78524077

N	−0.505116000	0.000048000	0.200831000
Si	−1.044651000	1.567427000	−0.120372000
Si	−1.045204000	−1.567123000	−0.120455000
C	−0.227736000	2.343189000	−1.643799000
H	−0.416250000	1.735528000	−2.534569000
H	−0.613042000	3.348174000	−1.841059000
H	0.856369000	2.430906000	−1.518209000
C	−2.909448000	1.769387000	−0.338388000
H	−3.455017000	1.351342000	0.512087000
H	−3.181871000	2.825050000	−0.431428000
H	−3.259970000	1.256123000	−1.238113000
C	−0.542432000	2.681783000	1.346680000
H	−0.854843000	3.719510000	1.198615000
H	−1.008008000	2.343384000	2.280600000
H	0.547028000	2.707293000	1.478794000
C	−0.228798000	−2.342960000	−1.644109000
H	−0.417450000	−1.735233000	−2.534803000
H	0.855328000	−2.430798000	−1.518781000
H	−0.614269000	−3.347892000	−1.841319000
C	−2.910106000	−1.768491000	−0.338106000
H	−3.182867000	−2.824047000	−0.431358000
H	−3.455366000	−1.350500000	0.512594000
H	−3.260666000	−1.254887000	−1.237621000
C	−0.543014000	−2.681762000	1.346402000
H	−1.008265000	−2.343294000	2.280463000
H	−0.855806000	−3.719373000	1.198336000
H	0.546469000	−2.707648000	1.478251000
C	2.412580000	−0.000267000	−0.477947000
H	1.517297000	−0.000126000	−1.092789000
F	3.546691000	−0.000274000	−1.163622000
F	2.425174000	1.074099000	0.342721000
F	2.425004000	−1.074848000	0.342439000
Na	0.743353000	−0.000381000	2.004349000

η^3-TS1$_{Na}$, -1373.75987129, *i*1103.9131

N	0.368627000	-0.000020000	-0.154433000
Si	1.023525000	-1.591777000	-0.155721000
Si	1.023410000	1.591774000	-0.155747000
C	0.192712000	-2.625913000	-1.482840000
H	0.401639000	-2.222856000	-2.477113000
H	0.536067000	-3.663810000	-1.458162000
H	-0.892447000	-2.627470000	-1.346982000
C	2.889958000	-1.693085000	-0.351595000
H	3.418619000	-1.195786000	0.465094000
H	3.199097000	-2.742846000	-0.356122000
H	3.224121000	-1.244789000	-1.290136000
C	0.608480000	-2.411885000	1.515525000
H	1.037799000	-3.415011000	1.588128000
H	1.015048000	-1.842505000	2.361893000
H	-0.474213000	-2.539073000	1.643563000
C	0.192814000	2.625882000	-1.483019000
H	0.402444000	2.223233000	-2.477307000
H	-0.892414000	2.626913000	-1.347719000
H	0.535684000	3.663928000	-1.457846000
C	2.889880000	1.693148000	-0.351341000
H	3.198966000	2.742923000	-0.355992000
H	3.418463000	1.196026000	0.465507000
H	3.224222000	1.244733000	-1.289761000
C	0.608073000	2.412038000	1.515358000
H	1.014526000	1.842806000	2.361882000
H	1.037367000	3.415183000	1.587880000
H	-0.474641000	2.539249000	1.643210000
C	-2.237226000	-0.000115000	-0.511752000
H	-0.819647000	-0.000087000	-0.633131000
F	-3.296569000	-0.000230000	-1.318330000
F	-2.463771000	-1.080246000	0.376365000
F	-2.463759000	1.080244000	0.376075000
Na	-0.927221000	0.000099000	1.800518000

η^3-P1$_{Na}$, -1373.76872411

N	0.467511000	-0.005869000	-0.317704000
Si	1.115480000	-1.624593000	-0.170937000
Si	1.082593000	1.622401000	-0.150855000
C	0.227182000	-2.706437000	-1.402878000
H	0.482556000	-2.426780000	-2.427864000
H	0.480082000	-3.760706000	-1.264147000
H	-0.853587000	-2.590700000	-1.282628000
C	2.973781000	-1.693109000	-0.404617000
H	3.518327000	-1.151013000	0.371274000

H	3.301361000	-2.736410000	-0.368863000
H	3.269379000	-1.285873000	-1.374282000
C	0.737109000	-2.254059000	1.578194000
H	1.235168000	-3.207841000	1.771698000
H	1.091097000	-1.559870000	2.351158000
H	-0.335566000	-2.440876000	1.709080000
C	0.340697000	2.664259000	-1.508276000
H	0.704141000	2.351266000	-2.489832000
H	-0.747143000	2.548986000	-1.500992000
H	0.574875000	3.723775000	-1.378020000
C	2.955989000	1.681498000	-0.151344000
H	3.281784000	2.725544000	-0.122112000
H	3.389589000	1.181421000	0.718223000
H	3.376876000	1.225273000	-1.049695000
C	0.505097000	2.319704000	1.517515000
H	0.822862000	1.696507000	2.363978000
H	0.935652000	3.309098000	1.694305000
H	-0.583081000	2.451694000	1.537215000
C	-2.501916000	-0.064096000	-0.711963000
H	-0.389715000	-0.015070000	-0.895988000
F	-3.822346000	-0.088836000	-0.943617000
F	-2.379888000	-1.144147000	0.294705000
F	-2.412051000	1.053862000	0.252504000
Na	-1.058257000	-0.008901000	1.597088000

η^1-C1$_{Na}$, -1373.78527417

N	-0.568111000	0.016446000	0.250241000
Si	-0.958997000	1.619539000	-0.118753000
Si	-1.192286000	-1.503554000	-0.144074000
C	-0.302811000	2.196667000	-1.796773000
H	-0.713563000	1.577148000	-2.599930000
H	-0.575569000	3.235592000	-2.005460000
H	0.788373000	2.127017000	-1.849277000
C	-2.801050000	2.032943000	-0.066264000
H	-3.238608000	1.747916000	0.894945000
H	-2.976801000	3.102524000	-0.215249000
H	-3.346091000	1.494550000	-0.846601000
C	-0.108078000	2.719659000	1.188313000
H	-0.253442000	3.785246000	0.990367000
H	-0.509316000	2.535816000	2.193844000
H	0.976931000	2.552183000	1.202684000
C	-0.407331000	-2.257297000	-1.692739000
H	-0.548679000	-1.594843000	-2.552451000
H	0.669226000	-2.414549000	-1.568840000

H	−0.850503000	−3.225926000	−1.942931000
C	−3.063971000	−1.581011000	−0.375658000
H	−3.414636000	−2.611796000	−0.481992000
H	−3.584464000	−1.127308000	0.472375000
H	−3.364144000	−1.035207000	−1.275105000
C	−0.744975000	−2.687809000	1.285881000
H	−1.210638000	−2.372468000	2.228243000
H	−1.080634000	−3.711681000	1.099258000
H	0.343189000	−2.745134000	1.427779000
C	2.491194000	−0.133268000	−0.393754000
H	1.453298000	−0.140732000	−0.729920000
F	3.102641000	1.021913000	−0.637584000
F	2.502831000	−0.296695000	0.970369000
F	3.223964000	−1.118801000	−0.897441000
Na	0.517094000	−0.101302000	2.152183000

η^2-TS1$_{Na}$, -1373.75988866, *i*921.7890

N	−0.349039000	−0.023169000	−0.223378000
Si	−1.454244000	−1.332987000	0.046825000
Si	−0.656015000	1.644447000	0.135756000
C	−2.300771000	−1.220690000	1.725161000
H	−2.880079000	−0.296959000	1.819359000
H	−2.986977000	−2.057433000	1.883023000
H	−1.562036000	−1.233619000	2.531384000
C	−2.794174000	−1.385139000	−1.278384000
H	−2.362822000	−1.497756000	−2.278059000
H	−3.470618000	−2.229462000	−1.116023000
H	−3.396366000	−0.472588000	−1.275521000
C	−0.460878000	−2.928264000	−0.035809000
H	−1.089598000	−3.797341000	0.176073000
H	−0.019994000	−3.079838000	−1.026810000
H	0.358123000	−2.919509000	0.688448000
C	−0.361941000	2.047842000	1.943992000
H	−1.050887000	1.489309000	2.583319000
H	0.657162000	1.771094000	2.228859000
H	−0.496892000	3.113271000	2.149802000
C	−2.385469000	2.187717000	−0.366958000
H	−2.518903000	3.258822000	−0.189620000
H	−2.574519000	1.995553000	−1.426878000
H	−3.153645000	1.662595000	0.207905000
C	0.599585000	2.641550000	−0.884223000
H	0.395641000	2.604005000	−1.963199000
H	0.576574000	3.700874000	−0.615410000
H	1.623937000	2.297609000	−0.692664000

C	2.253175000	-0.508407000	0.406770000
H	0.789052000	-0.312420000	0.215905000
F	2.808566000	-1.666427000	0.817915000
F	2.808377000	-0.361638000	-0.934713000
F	2.913822000	0.464409000	1.083630000
Na	1.006882000	0.079161000	-2.059740000

η^2-P1$_{Na}$, -1373.76830614

N	-0.495442000	-0.095682000	-0.037004000
Si	-1.865274000	-1.195054000	0.094131000
Si	-0.517164000	1.671915000	0.036277000
C	-2.807067000	-0.940079000	1.696060000
H	-3.212239000	0.073418000	1.765273000
H	-3.644117000	-1.638549000	1.780670000
H	-2.151933000	-1.095690000	2.557462000
C	-3.022788000	-0.965376000	-1.364830000
H	-2.478280000	-0.940064000	-2.313076000
H	-3.719616000	-1.807517000	-1.409089000
H	-3.615671000	-0.052101000	-1.292972000
C	-1.140245000	-2.924952000	0.043995000
H	-1.907241000	-3.677833000	0.244269000
H	-0.712233000	-3.155250000	-0.937034000
H	-0.346510000	-3.046668000	0.785994000
C	-0.251786000	2.246744000	1.793334000
H	-1.041683000	1.873341000	2.450510000
H	0.706597000	1.875037000	2.164647000
H	-0.243363000	3.337954000	1.859589000
C	-2.161753000	2.287087000	-0.627281000
H	-2.163577000	3.380733000	-0.617629000
H	-2.333382000	1.965785000	-1.657767000
H	-3.008484000	1.955024000	-0.020547000
C	0.860897000	2.308081000	-1.070186000
H	0.694699000	2.044459000	-2.121813000
H	0.909670000	3.399893000	-1.030598000
H	1.837214000	1.929427000	-0.752748000
C	2.661910000	-0.837187000	0.258872000
H	0.268413000	-0.440240000	0.555491000
F	3.762679000	-1.414580000	0.785475000
F	3.237664000	-0.070185000	-0.864172000
F	2.402977000	0.214729000	1.145441000
Na	1.229007000	-0.691183000	-1.596163000

η^2-NaCF$_3$, -499.881555903

C	-0.358742000	0.000228000	-0.305293000

F	−1.193311000	−1.067027000	−0.208702000
F	0.266059000	−0.003501000	1.055686000
F	−1.189846000	1.069967000	−0.204494000
Na	1.927849000	0.000334000	−0.359150000

TS[2-3]$_{Na}$, -499.878384616, *i*87.3442

C	−0.420225000	0.013198000	−0.385833000
F	−1.740060000	−0.193465000	−0.384976000
F	0.058445000	−0.994172000	0.581548000
F	−0.265521000	1.160557000	0.441836000
Na	1.822325000	0.014957000	−0.311879000

η^3-NaCF$_3$, -499.878619326

C	−0.452320000	0.000058000	−0.419166000
F	−1.780122000	−0.000800000	−0.301952000
F	−0.053607000	−1.091887000	0.462197000
F	−0.054941000	1.092598000	0.461703000
Na	1.791995000	0.000041000	−0.280231000

η^3-C2$_{Na}$, -1369.37563524

Si	1.837130000	−0.450539000	0.039099000
C	1.197633000	−1.111020000	1.649531000
H	1.507956000	−2.153826000	1.765551000
H	1.589798000	−0.544050000	2.496565000
H	0.105743000	−1.072455000	1.653679000
C	1.056007000	−1.197975000	−1.469086000
H	−0.030375000	−1.091270000	−1.445875000
H	1.441084000	−0.737161000	−2.381367000
H	1.289121000	−2.266532000	−1.505361000
C	3.697979000	−0.419192000	−0.053949000
H	4.039805000	0.062588000	−0.972262000
H	4.128815000	0.113496000	0.796213000
H	4.085185000	−1.442192000	−0.043558000
Cl	1.313491000	1.645790000	−0.001382000
C	−2.159937000	−0.507711000	0.190414000
F	−2.876491000	−1.641018000	0.165903000
F	−3.113858000	0.449928000	0.725057000
F	−2.229820000	−0.071737000	−1.200960000
Na	−1.361352000	1.658305000	0.000097000

η^3-TS2$_{Na}$, -1369.37176277, *i*65.0607

Si	−1.462866000	−0.363825000	0.001152000
C	−1.039605000	−1.181574000	−1.623687000
H	−0.507347000	−2.117233000	−1.441098000

H	-1.945212000	-1.386308000	-2.200440000
H	-0.377844000	-0.549375000	-2.217160000
C	-1.034898000	-1.171691000	1.629668000
H	-0.373052000	-0.535266000	2.218500000
H	-1.938810000	-1.374800000	2.209623000
H	-0.501324000	-2.107383000	1.451215000
C	-3.318003000	-0.044435000	0.001945000
H	-3.629182000	0.522752000	0.882389000
H	-3.630963000	0.507674000	-0.887516000
H	-3.854340000	-0.999267000	0.010626000
Cl	-0.846776000	1.736770000	-0.005818000
C	1.414140000	-0.688300000	-0.001924000
F	1.975681000	-1.911294000	-0.003309000
F	2.131003000	-0.035628000	-1.092916000
F	2.127102000	-0.039885000	1.094525000
Na	1.763593000	1.818629000	0.003264000

$P2_{Na}$, -1369.41535535

Si	1.490620000	-0.737097000	-0.013299000
C	2.689914000	-0.573572000	-1.436249000
H	3.398785000	0.240523000	-1.270784000
H	3.260121000	-1.498508000	-1.554261000
H	2.163368000	-0.387031000	-2.375061000
C	2.344340000	-0.828530000	1.643701000
H	1.618863000	-0.821608000	2.460037000
H	2.920670000	-1.754237000	1.717943000
H	3.033011000	0.007442000	1.784986000
C	0.184671000	-2.026694000	-0.273808000
H	-0.580491000	-2.012398000	0.506009000
H	-0.340950000	-1.887734000	-1.221150000
H	0.651144000	-3.016178000	-0.285593000
Cl	-3.227284000	-1.025650000	0.030741000
C	0.604932000	1.003921000	0.026767000
F	1.452837000	2.039571000	0.094674000
F	-0.188097000	1.248227000	-1.069044000
F	-0.259924000	1.164976000	1.077677000
Na	-2.374169000	1.214493000	-0.071889000

NaCl, -622.528625170

Na	0.000000000	0.000000000	-1.436666000
Cl	0.000000000	0.000000000	0.929607000

Na^+, -162.050222488

Na	0.000000000	0.000000000	0.000000000

NaF, -262.140278332

F	0.000000000	0.000000000	-1.064739000
Na	0.000000000	0.000000000	0.871150000

$(TMS)_2NLi$, -880.798954619

N	0.014333000	0.743299000	-0.060290000
Si	1.573401000	0.056601000	-0.015455000
Si	-1.495386000	-0.023287000	-0.006109000
C	2.121424000	-0.345678000	1.748405000
H	1.434180000	-1.062029000	2.208807000
H	3.126767000	-0.776272000	1.779761000
H	2.120815000	0.555168000	2.369201000
C	1.684803000	-1.552205000	-1.003116000
H	1.374080000	-1.398329000	-2.040491000
H	2.702721000	-1.952698000	-1.009608000
H	1.033131000	-2.319645000	-0.571732000
C	2.832708000	1.271259000	-0.729345000
H	3.847463000	0.864382000	-0.701959000
H	2.595786000	1.512558000	-1.769550000
H	2.841186000	2.205751000	-0.158578000
C	-1.797419000	-1.132907000	1.487373000
H	-1.134550000	-2.003259000	1.449948000
H	-1.588633000	-0.602679000	2.420357000
H	-2.825903000	-1.503971000	1.523032000
C	-1.980000000	-0.997947000	-1.545078000
H	-2.995674000	-1.397574000	-1.469251000
H	-1.923263000	-0.372001000	-2.439794000
H	-1.298765000	-1.840754000	-1.691458000
C	-2.762273000	1.426502000	0.119991000
H	-2.747980000	2.099282000	-0.751694000
H	-3.782234000	1.036468000	0.153313000
H	-2.649899000	2.021489000	1.038317000
Li	-0.639080000	2.416826000	-0.028028000

η^1-$C1_{Li}$, -1219.05566844

N	-0.424231000	-0.025093000	-0.407431000
Si	-1.251733000	-1.462774000	-0.008959000
Si	-0.853088000	1.566603000	0.012726000
C	-1.997376000	-1.426157000	1.728269000
H	-2.734970000	-0.623701000	1.832204000
H	-2.502672000	-2.367412000	1.963885000
H	-1.223658000	-1.263488000	2.484746000
C	-2.656768000	-1.848607000	-1.210358000

H	−2.279810000	−1.955125000	−2.231931000
H	−3.178757000	−2.773242000	−0.947278000
H	−3.390947000	−1.037134000	−1.212926000
C	−0.047569000	−2.924072000	−0.067270000
H	−0.575303000	−3.876246000	0.038865000
H	0.495158000	−2.958613000	−1.018019000
H	0.692312000	−2.879648000	0.738921000
C	−0.464053000	2.047295000	1.792580000
H	−1.058053000	1.444039000	2.485193000
H	0.591141000	1.876875000	2.024470000
H	−0.688364000	3.099778000	1.989405000
C	−2.644580000	2.040398000	−0.337380000
H	−2.842311000	3.090987000	−0.105325000
H	−2.896649000	1.868388000	−1.387576000
H	−3.327281000	1.434726000	0.266614000
C	0.242847000	2.681817000	−1.104373000
H	0.034862000	2.561740000	−2.178430000
H	0.049450000	3.736664000	−0.894597000
H	1.318154000	2.539172000	−0.928451000
C	2.617165000	−0.353568000	0.172845000
H	1.642690000	−0.677290000	0.531803000
F	3.570977000	−1.261653000	0.293346000
F	2.507548000	−0.078596000	−1.176175000
F	3.014252000	0.774194000	0.747484000
Li	0.726372000	0.424478000	−1.760022000

η^2-TS1$_{Li}$, -1219.02776517, *i*948.6121

N	−0.271393000	−0.026168000	−0.300255000
Si	−1.366766000	−1.348364000	0.002233000
Si	−0.592432000	1.650178000	0.037918000
C	−2.148023000	−1.216433000	1.709759000
H	−2.754450000	−0.310864000	1.808177000
H	−2.798382000	−2.070942000	1.916527000
H	−1.376090000	−1.186894000	2.483990000
C	−2.742248000	−1.404870000	−1.280349000
H	−2.338948000	−1.510781000	−2.291694000
H	−3.404069000	−2.256721000	−1.098382000
H	−3.354117000	−0.499425000	−1.256007000
C	−0.360979000	−2.931648000	−0.095008000
H	−0.982832000	−3.806712000	0.112168000
H	0.080653000	−3.068343000	−1.086977000
H	0.458503000	−2.922842000	0.628761000
C	−0.192428000	2.100562000	1.812011000
H	−0.842952000	1.559752000	2.504640000

H	0.841943000	1.833222000	2.046309000
H	-0.317947000	3.170870000	1.996722000
C	-2.350575000	2.156604000	-0.385451000
H	-2.491142000	3.227194000	-0.210856000
H	-2.583768000	1.953210000	-1.434106000
H	-3.082606000	1.625569000	0.229083000
C	0.595062000	2.606234000	-1.097781000
H	0.378862000	2.458809000	-2.166043000
H	0.512728000	3.683398000	-0.932575000
H	1.642956000	2.345358000	-0.903907000
C	2.318077000	-0.507754000	0.218288000
H	0.853514000	-0.320212000	0.175979000
F	2.979507000	-1.654005000	0.421486000
F	2.534170000	-0.288788000	-1.247629000
F	3.097398000	0.461792000	0.740201000
Li	0.891226000	0.188987000	-1.832492000

η^2-P1$_{Li}$, -1219.04189349

N	-0.364949000	-0.185001000	-0.233954000
Si	-0.735005000	1.553946000	-0.034112000
Si	-1.552558000	-1.497766000	-0.163646000
C	-2.440438000	1.952811000	-0.713923000
H	-3.242818000	1.405543000	-0.212478000
H	-2.644846000	3.019830000	-0.586001000
H	-2.495354000	1.732558000	-1.783427000
C	-0.680054000	1.931044000	1.800198000
H	0.335673000	1.812373000	2.188501000
H	-0.978876000	2.966436000	1.985607000
H	-1.356498000	1.289849000	2.371956000
C	0.562818000	2.502824000	-0.976676000
H	0.425786000	3.577981000	-0.832639000
H	1.564587000	2.235485000	-0.633631000
H	0.500243000	2.301969000	-2.049747000
C	-2.670605000	-1.527806000	-1.666286000
H	-3.318898000	-0.649672000	-1.705198000
H	-2.084690000	-1.555412000	-2.589035000
H	-3.308686000	-2.415825000	-1.652934000
C	-2.555305000	-1.262943000	1.402350000
H	-3.275692000	-2.079008000	1.506151000
H	-1.922868000	-1.270621000	2.294734000
H	-3.120128000	-0.327649000	1.400623000
C	-0.573924000	-3.094975000	-0.067941000
H	0.017548000	-3.164755000	0.850629000
H	-1.238973000	-3.962402000	-0.088212000

H	0.118369000	-3.188101000	-0.909220000
C	2.978996000	-0.401002000	0.367483000
H	0.268165000	-0.308671000	-1.027228000
F	3.202832000	0.237455000	-0.815256000
F	2.363538000	0.756538000	1.175944000
F	4.197947000	-0.480003000	0.929116000
Li	1.131704000	-0.592538000	1.064283000

η^2-$LiCF_3$, -345.147826110

C	0.114690000	0.000055000	0.418789000
F	0.800839000	-1.061148000	-0.030310000
F	-1.102116000	-0.001434000	-0.576775000
F	0.798775000	1.062342000	-0.031274000
Li	-1.721877000	0.000608000	1.077497000

$TS[2\text{-}3]_{Li}$, -345.138534248, *i*131.2352

C	0.162883000	0.010541000	0.476578000
F	1.400658000	-0.129144000	0.046774000
F	-0.582037000	-1.033003000	-0.304285000
F	-0.343725000	1.137730000	-0.284179000
Li	-1.750455000	0.052167000	0.671911000

η^3-$LiCF_3$, -345.141757456

C	0.398066000	-0.000075000	0.616721000
F	1.336364000	-0.000134000	-0.316520000
F	-0.510983000	-1.117098000	0.038468000
F	-0.510624000	1.117195000	0.038494000
Li	-1.740403000	0.000261000	-0.514768000

η^3-$C2_{Li}$, -1214.64395106

Si	-1.603648000	-0.424576000	0.000540000
C	-0.909728000	-1.146402000	-1.559272000
H	-1.278008000	-2.170310000	-1.675372000
H	-1.218457000	-0.572272000	-2.435363000
H	0.180695000	-1.179455000	-1.513625000
C	-0.909215000	-1.143284000	1.561529000
H	0.181505000	-1.169406000	1.518644000
H	-1.224076000	-0.572348000	2.437506000
H	-1.270831000	-2.169842000	1.675267000
C	-3.462484000	-0.310834000	0.000784000
H	-3.826829000	0.215553000	0.885265000
H	-3.827712000	0.209143000	-0.887102000
H	-3.891391000	-1.317116000	0.004696000
Cl	-1.009712000	1.665890000	-0.001530000

C	2.291980000	-0.627057000	0.001953000
F	3.622721000	-0.672463000	0.000367000
F	2.067600000	0.386217000	-1.102424000
F	2.070295000	0.392013000	1.100789000
Li	1.294140000	1.587853000	-0.003340000

η^3-TS2$_{Li}$, -1214.63745119, *i*92.2107

Si	1.209506000	-0.416116000	-0.000042000
C	0.769950000	-1.201692000	1.637399000
H	0.168339000	-2.097369000	1.467737000
H	1.670108000	-1.469499000	2.195769000
H	0.169082000	-0.521267000	2.242840000
C	0.769722000	-1.202146000	-1.637204000
H	0.168732000	-0.521901000	-2.242724000
H	1.669795000	-1.470077000	-2.195653000
H	0.168152000	-2.097785000	-1.467193000
C	3.080992000	-0.194246000	-0.000190000
H	3.427835000	0.343484000	-0.885694000
H	3.427927000	0.343807000	0.885083000
H	3.556777000	-1.181199000	-0.000032000
Cl	0.760464000	1.752205000	-0.000314000
C	-1.536433000	-0.381630000	0.000140000
F	-2.464773000	-1.337012000	0.000319000
F	-2.005414000	0.494681000	1.088742000
F	-2.005652000	0.494490000	-1.088498000
Li	-1.503525000	1.906265000	-0.000052000

P2$_{Li}$, -1214.68415338

Si	1.258155000	-0.726251000	-0.042050000
C	2.416420000	-0.721466000	-1.505951000
H	3.170608000	0.063225000	-1.416146000
H	2.934877000	-1.680882000	-1.577732000
H	1.871039000	-0.569719000	-2.440343000
C	2.142549000	-0.695649000	1.599358000
H	1.430158000	-0.606931000	2.422428000
H	2.704205000	-1.622169000	1.742242000
H	2.847413000	0.136683000	1.660254000
C	-0.102603000	-1.981601000	-0.155378000
H	-0.856410000	-1.846621000	0.624325000
H	-0.624176000	-1.921103000	-1.113381000
H	0.318408000	-2.986683000	-0.061221000
Cl	-3.353935000	-0.504320000	0.570974000
C	0.404346000	1.031757000	-0.129566000
F	1.244246000	2.051830000	-0.311134000

F	-0.545468000	1.142919000	-1.121095000
F	-0.324766000	1.342442000	0.998739000
Li	-2.199863000	1.152800000	0.175630000

LiCl, -467.794756581

Cl	0.000000000	0.000000000	0.303030000
Li	0.000000000	0.000000000	-1.717170000

Li^+, -7.28119827131

Li	0.000000000	0.000000000	0.000000000

LiF, -107.419975174

F	0.000000000	0.000000000	-1.064739000
Na	0.000000000	0.000000000	0.871150000

C, -2342.69040054

Si	-2.770456000	0.392314000	-0.487330000
C	-4.606725000	0.401025000	-0.811039000
H	-5.176676000	0.420203000	0.120103000
H	-4.879512000	1.282506000	-1.398441000
H	-4.903361000	-0.485510000	-1.375686000
C	-2.255059000	1.804931000	0.621495000
H	-2.740868000	1.749820000	1.599373000
H	-1.168677000	1.805314000	0.737141000
H	-2.525645000	2.763145000	0.168300000
C	-1.738923000	0.280666000	-2.018471000
H	-0.685448000	0.209383000	-1.731185000
H	-2.006589000	-0.585681000	-2.626967000
H	-1.879498000	1.185049000	-2.619279000
Cl	-2.439699000	-1.359141000	0.682699000
N	1.135483000	0.008942000	0.023713000
Si	1.769516000	1.557357000	-0.128350000
Si	1.571686000	-1.548789000	-0.444039000
C	3.609708000	1.676555000	-0.552537000
H	3.812669000	1.274329000	-1.548953000
H	3.949626000	2.716914000	-0.539079000
H	4.218142000	1.111998000	0.159325000
C	0.877962000	2.648591000	-1.399165000
H	-0.190592000	2.746495000	-1.186307000
H	1.305984000	3.655478000	-1.427898000
H	0.972785000	2.217006000	-2.400682000
C	1.596767000	2.486494000	1.541423000
H	2.000251000	3.500747000	1.466063000

H	0.559630000	2.600410000	1.881361000
H	2.167819000	1.981111000	2.330276000
C	3.390861000	-1.787089000	-0.908759000
H	3.653054000	-1.199526000	-1.793025000
H	4.053858000	-1.472544000	-0.097861000
H	3.603198000	-2.837359000	-1.131891000
C	0.554049000	-2.284379000	-1.860229000
H	0.905450000	-3.291440000	-2.105677000
H	-0.501728000	-2.356527000	-1.581716000
H	0.622010000	-1.674828000	-2.766058000
C	1.261738000	-2.773453000	1.000804000
H	0.197858000	-2.850495000	1.259305000
H	1.572563000	-3.781380000	0.711189000
H	1.838775000	-2.519707000	1.899490000
K	0.032565000	-0.287078000	2.283254000

TS, -2342.66980081, *i*108.1951

Si	1.738279000	-0.635306000	-0.555117000
C	3.616547000	-0.835204000	-0.924075000
H	4.206063000	-0.999099000	-0.018446000
H	3.781616000	-1.684018000	-1.598016000
H	4.018901000	0.055431000	-1.416055000
C	1.569395000	-2.165285000	0.550191000
H	2.261789000	-2.030174000	1.388485000
H	0.586321000	-2.433915000	0.926219000
H	1.948598000	-3.024729000	-0.012052000
C	1.213079000	-0.564714000	-2.370968000
H	0.161228000	-0.375035000	-2.559890000
H	1.816925000	0.193585000	-2.876727000
H	1.493584000	-1.530705000	-2.807925000
Cl	2.256385000	1.036424000	0.851003000
N	-0.455516000	0.022847000	-0.101044000
Si	-1.615666000	-1.245337000	-0.177957000
Si	-0.777841000	1.690693000	-0.434878000
C	-3.387546000	-0.831716000	-0.693567000
H	-3.462011000	-0.420892000	-1.701229000
H	-3.953505000	-1.768991000	-0.677056000
H	-3.881896000	-0.139833000	-0.008150000
C	-1.155054000	-2.674464000	-1.328683000
H	-0.157073000	-3.089560000	-1.187619000
H	-1.876199000	-3.486603000	-1.192209000
H	-1.230761000	-2.345547000	-2.369124000
C	-1.955294000	-2.002936000	1.560921000
H	-2.687819000	-2.807049000	1.442965000

H	-1.110158000	-2.450320000	2.093955000
H	-2.435874000	-1.263830000	2.216494000
C	-2.434808000	2.115647000	-1.246031000
H	-2.565336000	1.610209000	-2.206121000
H	-3.310198000	1.907295000	-0.629958000
H	-2.421995000	3.192124000	-1.446822000
C	0.443861000	2.525457000	-1.610923000
H	0.251494000	3.603244000	-1.589068000
H	1.497293000	2.375574000	-1.377588000
H	0.265337000	2.187366000	-2.635654000
C	-0.828333000	2.714638000	1.179263000
H	0.132144000	2.763125000	1.699928000
H	-1.107182000	3.746613000	0.946550000
H	-1.602196000	2.341553000	1.864081000
K	0.047005000	0.056096000	2.506624000

$(TMS)_3N$, -1282.50918651

N	0.016820000	0.016234000	0.040097000
Si	-0.894730000	-1.493879000	0.001340000
Si	-0.882025000	1.531256000	-0.057590000
C	-1.819786000	-1.780495000	1.613235000
H	-2.615266000	-1.059432000	1.799334000
H	-2.266888000	-2.778974000	1.611453000
H	-1.118882000	-1.731519000	2.451954000
C	-2.059645000	-1.518042000	-1.479460000
H	-1.467110000	-1.494062000	-2.399260000
H	-2.640950000	-2.444964000	-1.484524000
H	-2.763238000	-0.685412000	-1.518839000
C	0.198443000	-3.010133000	-0.227576000
H	-0.440367000	-3.882911000	-0.057846000
H	0.593784000	-3.087019000	-1.241325000
H	1.031887000	-3.080193000	0.473739000
C	-2.639766000	1.355171000	0.602226000
H	-3.233736000	0.545511000	0.179223000
H	-2.630286000	1.240389000	1.689249000
H	-3.158469000	2.293201000	0.379354000
C	-0.968298000	2.100083000	-1.847388000
H	-1.489004000	3.057725000	-1.937549000
H	0.032008000	2.220516000	-2.272237000
H	-1.499278000	1.365863000	-2.459271000
C	-0.151073000	2.902819000	1.008988000
H	0.587300000	3.512983000	0.488987000
H	-0.966863000	3.563262000	1.317516000
H	0.308847000	2.505035000	1.917762000

Si	1.778653000	-0.016996000	0.051879000
C	2.472922000	-1.049866000	-1.368192000
H	2.623361000	-2.096537000	-1.102020000
H	1.814093000	-1.013163000	-2.240559000
H	3.442630000	-0.644316000	-1.669518000
C	2.532453000	1.696239000	-0.162735000
H	2.106201000	2.259581000	-0.996701000
H	2.463791000	2.306864000	0.737680000
H	3.595036000	1.550112000	-0.379325000
C	2.403394000	-0.678663000	1.698004000
H	3.495305000	-0.746180000	1.701169000
H	2.106482000	-0.005939000	2.507564000
H	2.006693000	-1.669326000	1.931033000

C1, -2220.08279093

N	-0.831998000	0.078112000	0.082182000
Si	-0.214187000	1.640678000	0.724109000
Si	-1.914817000	0.157304000	-1.309434000
C	0.865131000	2.534270000	-0.524658000
H	1.331597000	1.856280000	-1.241943000
H	0.321116000	3.309993000	-1.067301000
H	1.689951000	3.009797000	0.013909000
C	-1.705415000	2.712148000	1.171447000
H	-2.292520000	2.242868000	1.966533000
H	-1.360984000	3.681437000	1.545148000
H	-2.378188000	2.906186000	0.333483000
C	0.753816000	1.427055000	2.315174000
H	0.941937000	2.439242000	2.689375000
H	0.229168000	0.886935000	3.105873000
H	1.719388000	0.955559000	2.127151000
C	-1.702034000	1.718526000	-2.331399000
H	-1.932947000	2.643128000	-1.801933000
H	-0.694998000	1.810233000	-2.743854000
H	-2.397079000	1.641033000	-3.174111000
C	-3.717331000	0.059419000	-0.785788000
H	-4.370479000	0.111416000	-1.661658000
H	-3.967180000	-0.851255000	-0.237886000
H	-3.957636000	0.909748000	-0.140730000
C	-1.532554000	-1.220485000	-2.555730000
H	-1.423228000	-2.221622000	-2.136489000
H	-2.360178000	-1.270739000	-3.270014000
H	-0.646045000	-0.977350000	-3.153040000
Si	-1.054547000	-1.220115000	1.269080000
C	-2.279537000	-0.734812000	2.605896000

H	-1.942649000	0.129218000	3.182477000
H	-3.253394000	-0.488656000	2.174074000
H	-2.420546000	-1.564961000	3.304160000
C	-1.728513000	-2.784996000	0.445735000
H	-2.653062000	-2.659807000	-0.120101000
H	-0.997791000	-3.274707000	-0.205642000
H	-1.934419000	-3.493131000	1.255217000
C	0.602302000	-1.735891000	2.010851000
H	0.627239000	-1.537523000	3.085239000
H	0.763149000	-2.811229000	1.883888000
H	1.456406000	-1.201016000	1.582468000
C	3.176152000	0.090039000	-0.015685000
F	3.706726000	-1.250532000	-0.035953000
F	3.253182000	0.355397000	-1.439727000
F	4.222664000	0.804370000	0.457033000
K	1.329570000	-1.389091000	-1.173125000

TS1, -2220.07154249, *i*66.3969

N	-0.529366000	0.106541000	0.074139000
Si	0.686840000	1.263261000	0.847015000
Si	-1.632131000	0.815927000	-1.102894000
C	1.680355000	2.518335000	-0.176751000
H	1.929869000	2.202947000	-1.188241000
H	1.172265000	3.483776000	-0.217760000
H	2.629652000	2.661402000	0.348842000
C	-0.545429000	2.534640000	1.632392000
H	-1.278571000	2.093777000	2.312730000
H	0.046053000	3.251720000	2.215040000
H	-1.093559000	3.123864000	0.889856000
C	1.517777000	0.623538000	2.428521000
H	1.102725000	1.102773000	3.319257000
H	1.461646000	-0.457303000	2.564191000
H	2.581869000	0.870291000	2.371250000
C	-0.932656000	2.307475000	-1.997204000
H	-0.809802000	3.185267000	-1.363316000
H	0.030426000	2.091951000	-2.465070000
H	-1.640825000	2.565782000	-2.791646000
C	-3.287274000	1.322768000	-0.361898000
H	-3.944092000	1.715031000	-1.144114000
H	-3.817708000	0.512069000	0.141073000
H	-3.131804000	2.117267000	0.372338000
C	-1.943390000	-0.408127000	-2.528415000
H	-2.216832000	-1.423589000	-2.235385000
H	-2.774933000	-0.026827000	-3.128859000

H	-1.083589000	-0.439464000	-3.208857000
Si	-1.170739000	-1.139322000	1.145425000
C	-1.876494000	-0.484529000	2.753602000
H	-1.112642000	0.003510000	3.362456000
H	-2.678803000	0.235469000	2.574760000
H	-2.288179000	-1.318723000	3.329815000
C	-2.542982000	-2.150962000	0.308834000
H	-3.379617000	-1.584160000	-0.099871000
H	-2.165875000	-2.805207000	-0.484243000
H	-2.942786000	-2.815980000	1.081740000
C	0.118593000	-2.476065000	1.540441000
H	0.039359000	-2.745164000	2.597820000
H	-0.080164000	-3.398701000	0.981458000
H	1.151818000	-2.179093000	1.364306000
C	2.448283000	-0.124930000	-0.218110000
F	2.665466000	-1.529178000	-0.060396000
F	2.337998000	-0.086581000	-1.649913000
F	3.690096000	0.369350000	-0.013331000
K	0.608491000	-1.930620000	-1.539363000

P1, -2220.07546677

N	-0.484859000	0.025929000	0.059226000
Si	0.767058000	1.216948000	0.831568000
Si	-1.622333000	0.755789000	-1.065344000
C	1.602240000	2.726473000	-0.015211000
H	1.856447000	2.586335000	-1.066958000
H	1.014925000	3.640226000	0.088406000
H	2.550278000	2.877187000	0.513529000
C	-0.570235000	2.299279000	1.766308000
H	-1.233312000	1.741882000	2.432775000
H	-0.038844000	3.035559000	2.382312000
H	-1.204729000	2.878772000	1.085622000
C	1.636141000	0.597802000	2.414717000
H	2.081082000	1.482757000	2.881956000
H	0.922808000	0.198302000	3.141620000
H	2.432199000	-0.134175000	2.265890000
C	-0.994827000	2.335198000	-1.855028000
H	-0.866684000	3.158026000	-1.152667000
H	-0.042591000	2.176895000	-2.366612000
H	-1.731629000	2.642335000	-2.604698000
C	-3.313702000	1.100368000	-0.311232000
H	-3.953881000	1.593658000	-1.048832000
H	-3.833258000	0.201066000	0.027625000
H	-3.213089000	1.769800000	0.546699000

C	-1.900077000	-0.370602000	-2.583495000
H	-2.160299000	-1.410511000	-2.369725000
H	-2.741732000	0.040362000	-3.149317000
H	-1.045276000	-0.332195000	-3.270162000
Si	-1.076278000	-1.266352000	1.089835000
C	-2.015055000	-0.741526000	2.628947000
H	-1.365688000	-0.279465000	3.374228000
H	-2.809403000	-0.030867000	2.389953000
H	-2.472622000	-1.625391000	3.083952000
C	-2.281445000	-2.396561000	0.138489000
H	-3.155641000	-1.885083000	-0.267751000
H	-1.833597000	-2.976662000	-0.676844000
H	-2.645595000	-3.134634000	0.860417000
C	0.281771000	-2.462422000	1.628142000
H	-0.152093000	-3.136230000	2.374244000
H	0.662038000	-3.097794000	0.821394000
H	1.141478000	-1.966744000	2.075863000
C	2.226033000	0.120613000	-0.323838000
F	2.343126000	-1.265874000	-0.100571000
F	1.978192000	0.131087000	-1.719433000
F	3.501106000	0.546592000	-0.234297000
K	0.519150000	-1.951091000	-1.726291000

TS2, -2220.06239866, *i*82.4798

N	-0.568350000	0.022405000	0.097345000
Si	1.534373000	1.007416000	1.019918000
Si	-1.440767000	1.177475000	-0.827629000
C	3.117550000	2.088270000	1.092501000
H	3.135638000	2.842749000	0.298470000
H	3.145314000	2.624097000	2.045554000
H	4.038538000	1.507900000	1.004611000
C	0.322453000	2.281517000	1.721022000
H	-0.650625000	1.862647000	1.963317000
H	0.789447000	2.650637000	2.640947000
H	0.190484000	3.144687000	1.066616000
C	1.890165000	-0.340688000	2.285845000
H	2.297253000	0.165269000	3.167024000
H	1.029083000	-0.923079000	2.606131000
H	2.654843000	-1.032756000	1.924357000
C	-0.424880000	2.661664000	-1.447716000
H	0.641205000	2.612049000	-1.221286000
H	-0.511390000	2.740174000	-2.535410000
H	-0.809163000	3.592331000	-1.021622000
C	-2.951178000	1.938668000	0.026143000

H	-3.460128000	2.624381000	-0.658856000
H	-3.684364000	1.200181000	0.358893000
H	-2.643523000	2.518887000	0.900827000
C	-2.119238000	0.391837000	-2.441010000
H	-2.704440000	-0.518574000	-2.267986000
H	-2.789756000	1.101118000	-2.935297000
H	-1.322684000	0.186362000	-3.168182000
Si	-1.366210000	-1.094629000	1.113374000
C	-1.813263000	-0.466907000	2.835312000
H	-0.951504000	-0.078132000	3.382657000
H	-2.543930000	0.344465000	2.753525000
H	-2.266887000	-1.262341000	3.434273000
C	-3.003645000	-1.767627000	0.391131000
H	-3.744158000	-0.991639000	0.184942000
H	-2.863017000	-2.332080000	-0.539803000
H	-3.449338000	-2.466041000	1.107427000
C	-0.322091000	-2.694999000	1.263189000
H	-0.342284000	-3.085540000	2.284866000
H	-0.724999000	-3.498281000	0.632810000
H	0.728287000	-2.535620000	1.006401000
C	2.067776000	0.160901000	-0.732504000
F	2.057549000	-1.221089000	-0.616686000
F	1.348306000	0.371981000	-1.881527000
F	3.333772000	0.439836000	-1.090147000
K	-0.159633000	-1.856758000	-1.780031000

P2, -2220.08192115

N	1.640210000	-0.003422000	-0.188811000
Si	-2.735286000	0.327779000	1.060934000
Si	2.476852000	-1.194043000	0.660151000
C	-4.287374000	-0.291724000	1.895235000
H	-4.267503000	-1.377984000	2.010639000
H	-4.380820000	0.146281000	2.892235000
H	-5.178598000	-0.025201000	1.323124000
C	-1.169162000	-0.211906000	1.898757000
H	-0.292013000	-0.074152000	1.252568000
H	-1.002254000	0.367615000	2.811276000
H	-1.230177000	-1.268350000	2.175464000
C	-2.824224000	2.141070000	0.627908000
H	-2.808398000	2.752693000	1.533618000
H	-1.974105000	2.439153000	0.010049000
H	-3.743306000	2.368915000	0.082302000
C	2.395561000	-1.053610000	2.547252000
H	1.365360000	-1.086218000	2.911752000

H	2.953338000	-1.857867000	3.037147000
H	2.830017000	-0.102998000	2.873034000
C	4.315196000	-1.337568000	0.228358000
H	4.787004000	-2.186332000	0.733420000
H	4.455117000	-1.464243000	-0.849510000
H	4.855422000	-0.432791000	0.521582000
C	1.709368000	-2.887640000	0.218393000
H	1.904187000	-3.172445000	-0.824084000
H	2.129121000	-3.688781000	0.833284000
H	0.625547000	-2.889613000	0.386664000
Si	1.777416000	1.671566000	-0.281727000
C	1.031082000	2.602587000	1.195265000
H	-0.036828000	2.397914000	1.311175000
H	1.523399000	2.293621000	2.123008000
H	1.155663000	3.685507000	1.094474000
C	3.543525000	2.330116000	-0.461319000
H	4.120855000	2.134286000	0.447860000
H	4.061669000	1.839262000	-1.290370000
H	3.560606000	3.409952000	-0.638109000
C	0.818345000	2.274390000	-1.817113000
H	0.822862000	3.365472000	-1.896688000
H	1.267130000	1.890105000	-2.741456000
H	-0.232694000	1.962204000	-1.788067000
C	-2.731341000	-0.565901000	-0.680945000
F	-2.097361000	0.170228000	-1.649028000
F	-2.055918000	-1.755278000	-0.685123000
F	-3.949459000	-0.834434000	-1.174146000
K	0.298663000	-1.035875000	-2.051237000

η^2-$RbCF_3$, -361.663721128

C	-1.334382000	0.000292000	-0.298423000
F	-2.193469000	-1.070129000	-0.287371000
F	-0.886833000	-0.005425000	1.114503000
F	-2.188443000	1.074947000	-0.280372000
Rb	1.497973000	0.000100000	-0.084603000

RbF, -123.913508468

F	0.000000000	0.000000000	-1.948959000
Rb	0.000000000	0.000000000	0.474071000

η^3-$C2_{Rb}$, -1231.15922860

Si	2.348874000	0.289017000	0.003495000
C	1.920388000	1.239978000	-1.529777000
H	2.410397000	2.217949000	-1.504533000

H	2.253475000	0.713261000	-2.426677000
H	0.839871000	1.394860000	-1.569020000
C	1.685951000	1.006493000	1.583097000
H	0.602267000	1.129938000	1.539349000
H	1.945981000	0.375755000	2.436666000
H	2.127460000	1.994420000	1.746503000
C	4.171929000	-0.094153000	0.120611000
H	4.389988000	-0.734596000	0.977722000
H	4.526311000	-0.595994000	-0.782232000
H	4.739174000	0.834031000	0.236752000
Cl	1.444185000	-1.648534000	-0.201714000
C	-1.421109000	1.438375000	-0.185428000
F	-1.418764000	2.795554000	-0.182053000
F	-2.701054000	1.145110000	-0.772092000
F	-1.763253000	1.147547000	1.197194000
Rb	-1.796368000	-1.369969000	0.016411000

η^3-TS2$_{Rb}$, -1231.15540752, *i*85.9929

Si	-2.044957000	-0.161391000	0.000036000
C	-2.026070000	0.739323000	1.641232000
H	-2.003626000	1.818523000	1.476186000
H	-2.909434000	0.482304000	2.231428000
H	-1.130883000	0.486635000	2.210620000
C	-2.026088000	0.739393000	-1.641122000
H	-1.130881000	0.486782000	-2.210513000
H	-2.909432000	0.482350000	-2.231337000
H	-2.003710000	1.818588000	-1.476033000
C	-3.630802000	-1.188720000	0.000017000
H	-3.699836000	-1.825639000	-0.885250000
H	-3.699837000	-1.825679000	0.885257000
H	-4.497272000	-0.517985000	0.000031000
Cl	-0.648463000	-1.824528000	-0.000012000
C	0.293935000	1.425238000	0.000016000
F	-0.151718000	2.713213000	-0.000041000
F	1.229685000	1.449606000	1.091506000
F	1.229454000	1.449420000	-1.091678000
Rb	2.356906000	-0.781918000	0.000010000

P2$_{Rb}$, -1231.19754820

Si	-2.009599000	0.516102000	-0.121648000
C	-2.290347000	0.941098000	1.666899000
H	-1.919101000	1.944532000	1.890466000
H	-3.362995000	0.924858000	1.880001000
H	-1.793182000	0.213722000	2.311420000

C	-2.778310000	1.809452000	-1.243571000
H	-2.535201000	1.630097000	-2.293203000
H	-3.866756000	1.783548000	-1.141619000
H	-2.442533000	2.816567000	-0.986217000
C	-2.476058000	-1.201732000	-0.659145000
H	-2.222340000	-1.365666000	-1.709476000
H	-1.963574000	-1.939144000	-0.038396000
H	-3.555333000	-1.339377000	-0.548347000
Cl	-0.343804000	-1.992449000	2.073079000
C	-0.083221000	0.735050000	-0.483167000
F	0.173827000	1.675364000	-1.417031000
F	0.659356000	1.111070000	0.603334000
F	0.545850000	-0.389687000	-0.939898000
Rb	2.370292000	-1.157890000	1.156871000

η^2-$CsCF_3$, -357.716781494

C	-1.735173000	0.000175000	-0.299564000
F	-2.597493000	-1.070938000	-0.298816000
F	-1.312299000	-0.004899000	1.119455000
F	-2.592591000	1.075481000	-0.292410000
Cs	1.253318000	0.000039000	-0.053758000

CsF, -119.966850897

F	0.000000000	0.000000000	-2.165100000
Cs	0.000000000	0.000000000	0.354289000

η^3-$C2_{Cs}$, -1227.21219004

Si	2.626754000	0.048597000	0.070138000
C	2.500624000	1.318256000	-1.274075000
H	3.084792000	2.202023000	-1.000014000
H	2.887887000	0.930408000	-2.218928000
H	1.458379000	1.619203000	-1.395791000
C	1.930656000	0.569545000	1.714014000
H	0.916454000	0.960907000	1.610833000
H	1.934223000	-0.266093000	2.418523000
H	2.552561000	1.364750000	2.136395000
C	4.357915000	-0.631867000	0.243482000
H	4.396275000	-1.441802000	0.974922000
H	4.724173000	-1.015113000	-0.711369000
H	5.038251000	0.158145000	0.574724000
Cl	1.482558000	-1.653914000	-0.549990000
C	-0.831230000	1.799805000	-0.196269000
F	-0.489820000	3.116300000	-0.239594000
F	-2.113053000	1.806514000	-0.840020000

F	−1.292355000	1.668128000	1.173905000
Cs	−1.848396000	−0.995076000	0.040128000

η^3-TS$_{Cs}$, -1227.20848184, *i*83.8788

Si	2.380179000	−0.314056000	0.000182000
C	2.474612000	0.577923000	−1.643625000
H	2.595467000	1.650704000	−1.478716000
H	3.315013000	0.206600000	−2.235524000
H	1.551608000	0.445212000	−2.208973000
C	2.473504000	0.577290000	1.644406000
H	1.550898000	0.442398000	2.209911000
H	3.314725000	0.207166000	2.235901000
H	2.592221000	1.650400000	1.480181000
C	3.842578000	−1.512563000	0.000495000
H	3.840771000	−2.153537000	0.885566000
H	3.841087000	−2.153618000	−0.884516000
H	4.778333000	−0.942298000	0.000642000
Cl	0.809932000	−1.808997000	−0.000805000
C	0.258855000	1.530295000	−0.000066000
F	0.858889000	2.756591000	−0.000310000
F	−0.664919000	1.670391000	−1.090875000
F	−0.665046000	1.670899000	1.090550000
Cs	−2.264165000	−0.474944000	0.000093000

P$_{Cs}$, -1227.25030912

Si	−2.577919000	0.291380000	0.000266000
C	−4.134828000	−0.759833000	−0.000394000
H	−4.188582000	−1.400318000	0.882920000
H	−5.016173000	−0.112535000	−0.000079000
H	−4.188400000	−1.399108000	−0.884604000
C	−2.432942000	1.252412000	1.585685000
H	−1.502606000	1.823116000	1.597283000
H	−3.273451000	1.947514000	1.667133000
H	−2.464664000	0.584231000	2.450082000
C	−2.433252000	1.253501000	−1.584543000
H	−1.503104000	1.824456000	−1.596270000
H	−2.465210000	0.585680000	−2.449224000
H	−3.274081000	1.948303000	−1.665343000
Cl	0.568832000	2.263561000	−0.000237000
C	−1.151757000	−1.069784000	−0.000151000
F	−1.633658000	−2.332609000	−0.000073000
F	−0.315164000	−1.018521000	−1.078848000
F	−0.314542000	−1.018595000	1.078134000
Cs	2.465162000	−0.238026000	0.000035000

Ph_2CO, -576.535647165

C	2.659593000	-1.514143000	-0.718568000
C	1.420226000	-0.885970000	-0.659097000
C	1.295067000	0.353470000	-0.029119000
C	2.419488000	0.959508000	0.534857000
C	3.650568000	0.320722000	0.494228000
C	3.771566000	-0.916719000	-0.134303000
H	2.757278000	-2.468960000	-1.221175000
H	0.555728000	-1.347568000	-1.122071000
H	2.307045000	1.933206000	0.997137000
H	4.518178000	0.787624000	0.944797000
H	4.734540000	-1.412341000	-0.173858000
C	0.000008000	1.108931000	0.000126000
C	-1.295057000	0.353486000	0.029218000
C	-1.420310000	-0.885906000	0.659271000
C	-2.419392000	0.959493000	-0.534958000
C	-2.659693000	-1.514059000	0.718629000
H	-0.555876000	-1.347471000	1.122396000
C	-3.650485000	0.320721000	-0.494447000
H	-2.306881000	1.933162000	-0.997282000
C	-3.771581000	-0.916668000	0.134166000
H	-2.757457000	-2.468830000	1.221305000
H	-4.518030000	0.787601000	-0.945163000
H	-4.734566000	-1.412275000	0.173633000
O	0.000007000	2.319832000	0.000034000

η^3-$C_{C\text{-}Li}$, -921.717485323

C	2.700906000	-2.580536000	0.379009000
C	1.473255000	-2.089147000	-0.049246000
C	1.362242000	-0.757875000	-0.456009000
C	2.476287000	0.084356000	-0.417162000
C	3.692307000	-0.404741000	0.034527000
C	3.806212000	-1.737618000	0.425607000
H	2.793091000	-3.617110000	0.679400000
H	0.607742000	-2.740447000	-0.087650000
H	2.359989000	1.122044000	-0.705314000
H	4.552445000	0.251360000	0.088611000
H	4.759937000	-2.118577000	0.771839000
C	0.083099000	-0.217409000	-0.973861000
C	-1.205893000	-0.730566000	-0.446796000
C	-1.348306000	-1.053894000	0.903845000
C	-2.300616000	-0.815194000	-1.308542000
C	-2.584723000	-1.462825000	1.385400000

H	-0.505605000	-0.930882000	1.573509000
C	-3.528121000	-1.249630000	-0.828045000
H	-2.172705000	-0.551742000	-2.352136000
C	-3.669826000	-1.569322000	0.519706000
H	-2.705442000	-1.688737000	2.437750000
H	-4.374651000	-1.333437000	-1.498703000
H	-4.631795000	-1.895032000	0.898253000
O	0.088729000	0.638859000	-1.858982000
C	-0.075225000	2.228960000	0.828377000
F	-0.216698000	3.222132000	1.709662000
F	0.773918000	2.923744000	-0.214534000
F	-1.338340000	2.388774000	0.041141000
Li	-0.388405000	2.391381000	-1.524929000

η^3-$TS_{C\text{-}Li}$, -921.713086666, *i*149.2793

C	2.626533000	-2.426834000	0.532322000
C	1.399672000	-1.866351000	0.186213000
C	1.346123000	-0.582833000	-0.356065000
C	2.531071000	0.128905000	-0.561165000
C	3.748774000	-0.425162000	-0.202378000
C	3.798808000	-1.706453000	0.346283000
H	2.662813000	-3.428205000	0.944144000
H	0.490188000	-2.438722000	0.319762000
H	2.476688000	1.123580000	-0.985209000
H	4.662989000	0.137535000	-0.348403000
H	4.752286000	-2.140692000	0.623314000
C	0.059187000	0.025588000	-0.811549000
C	-1.239395000	-0.556544000	-0.342129000
C	-1.477728000	-0.867189000	0.997990000
C	-2.228095000	-0.794543000	-1.293627000
C	-2.694855000	-1.412417000	1.377073000
H	-0.715733000	-0.642525000	1.736313000
C	-3.446576000	-1.349777000	-0.912904000
H	-2.029430000	-0.550468000	-2.330685000
C	-3.680486000	-1.658328000	0.421110000
H	-2.883707000	-1.636696000	2.420103000
H	-4.210772000	-1.537384000	-1.657885000
H	-4.631048000	-2.083202000	0.721780000
O	0.062089000	0.761456000	-1.819282000
C	-0.031307000	1.912850000	0.682881000
F	-0.021441000	2.470557000	1.893576000
F	0.834193000	2.797397000	-0.082630000
F	-1.280836000	2.409673000	0.116811000
Li	-0.376198000	2.493672000	-1.541039000

$P_{C\text{-}Li}$, -921.757569254

C	-2.509834000	-1.779864000	-1.295665000
C	-1.383173000	-1.005814000	-1.044883000
C	-1.254851000	-0.322610000	0.164386000
C	-2.257568000	-0.427401000	1.122320000
C	-3.381424000	-1.210113000	0.873837000
C	-3.511960000	-1.884743000	-0.335184000
H	-2.601856000	-2.308110000	-2.237483000
H	-0.596766000	-0.945092000	-1.789497000
H	-2.126855000	0.106025000	2.055397000
H	-4.156706000	-1.294403000	1.626922000
H	-4.387359000	-2.493810000	-0.528634000
C	-0.027076000	0.550699000	0.476272000
C	1.263116000	-0.249631000	0.173629000
C	1.986416000	-0.249725000	-1.020083000
C	1.706126000	-1.062245000	1.221999000
C	3.127767000	-1.040509000	-1.154612000
H	1.682004000	0.359340000	-1.860278000
C	2.834865000	-1.857140000	1.082751000
H	1.140757000	-1.053649000	2.146168000
C	3.554990000	-1.847524000	-0.109692000
H	3.680307000	-1.021349000	-2.086945000
H	3.153582000	-2.487404000	1.905148000
H	4.439108000	-2.464188000	-0.220764000
O	-0.015810000	1.021244000	1.759680000
C	-0.131937000	1.816604000	-0.403848000
F	-0.044531000	1.677001000	-1.725402000
F	-1.238809000	2.509546000	-0.157052000
F	0.913484000	2.675717000	-0.044716000
Li	1.045409000	2.364135000	1.916568000

η^3-$C_{C\text{-}Na}$, -1076.44689306

C	3.089309000	-2.316899000	0.338086000
C	1.793005000	-1.993402000	-0.048611000
C	1.489503000	-0.688215000	-0.437001000
C	2.479200000	0.296720000	-0.420536000
C	3.764026000	-0.025017000	-0.012307000
C	4.071067000	-1.332972000	0.360474000
H	3.329912000	-3.333476000	0.624894000
H	1.022640000	-2.755805000	-0.066129000
H	2.211515000	1.311465000	-0.688584000
H	4.527526000	0.742525000	0.025858000
H	5.077941000	-1.582587000	0.674524000

C	0.133104000	-0.329681000	-0.924271000
C	-1.057268000	-1.025884000	-0.363338000
C	-1.128916000	-1.339915000	0.994478000
C	-2.132359000	-1.308293000	-1.206396000
C	-2.276581000	-1.933504000	1.502341000
H	-0.307200000	-1.064601000	1.644739000
C	-3.269724000	-1.923349000	-0.698814000
H	-2.058198000	-1.057092000	-2.258558000
C	-3.342170000	-2.231549000	0.656629000
H	-2.345542000	-2.154541000	2.560456000
H	-4.098641000	-2.159958000	-1.355107000
H	-4.233981000	-2.699615000	1.056798000
O	-0.004601000	0.497602000	-1.820442000
C	-0.210540000	1.933091000	1.032646000
F	-0.291571000	2.703839000	2.135619000
F	0.422388000	2.891860000	0.090541000
F	-1.581322000	2.087141000	0.502463000
Na	-0.949505000	2.449139000	-1.532113000

η^3-TS$_{C\text{-}Na}$, -1076.44452833, *i*130.2175

C	2.781616000	-2.519024000	0.249682000
C	1.523317000	-1.994283000	-0.036911000
C	1.390805000	-0.655922000	-0.402779000
C	2.527628000	0.151462000	-0.486485000
C	3.775966000	-0.368302000	-0.187012000
C	3.906077000	-1.707796000	0.180746000
H	2.878551000	-3.561978000	0.526643000
H	0.650029000	-2.633754000	0.008101000
H	2.408823000	1.192269000	-0.760417000
H	4.652054000	0.267776000	-0.233266000
H	4.883702000	-2.113935000	0.412792000
C	0.068778000	-0.080384000	-0.803495000
C	-1.190785000	-0.753301000	-0.344331000
C	-1.361190000	-1.198883000	0.967580000
C	-2.209649000	-0.940751000	-1.274971000
C	-2.541566000	-1.824177000	1.339855000
H	-0.576712000	-1.014551000	1.693150000
C	-3.391419000	-1.575934000	-0.902490000
H	-2.060914000	-0.596872000	-2.292071000
C	-3.558252000	-2.016534000	0.404379000
H	-2.677292000	-2.153625000	2.362988000
H	-4.177818000	-1.726388000	-1.632797000
H	-4.479287000	-2.505764000	0.699131000
O	0.017818000	0.734009000	-1.735219000

C	-0.039745000	1.649829000	0.985027000
F	0.058085000	1.951217000	2.291621000
F	0.752150000	2.703243000	0.372471000
F	-1.343271000	2.187134000	0.649947000
Na	-0.630532000	2.764037000	-1.351057000

$P_{C\text{-}Na}$, -1076.48734679

C	-2.969512000	-1.602794000	-1.095321000
C	-1.728164000	-0.988998000	-0.969614000
C	-1.439686000	-0.212690000	0.152879000
C	-2.397653000	-0.061383000	1.149398000
C	-3.639258000	-0.678317000	1.024579000
C	-3.928221000	-1.447881000	-0.097428000
H	-3.188266000	-2.205797000	-1.969116000
H	-0.978778000	-1.124075000	-1.743099000
H	-2.133423000	0.538346000	2.012038000
H	-4.382861000	-0.557763000	1.804331000
H	-4.894891000	-1.928685000	-0.194983000
C	-0.082011000	0.489122000	0.346651000
C	1.064728000	-0.504503000	0.013433000
C	1.986598000	-0.405901000	-1.030722000
C	1.218031000	-1.545768000	0.939783000
C	3.035176000	-1.324767000	-1.141835000
H	1.900042000	0.372498000	-1.778535000
C	2.251352000	-2.462719000	0.822925000
H	0.504354000	-1.612762000	1.754020000
C	3.170796000	-2.352979000	-0.221632000
H	3.738747000	-1.232322000	-1.961351000
H	2.341800000	-3.268088000	1.542885000
H	3.979219000	-3.068329000	-0.316037000
O	0.091868000	0.991241000	1.594999000
C	-0.046377000	1.690377000	-0.625279000
F	-0.138227000	1.397585000	-1.932035000
F	-0.986748000	2.585194000	-0.356506000
F	1.158750000	2.358620000	-0.485092000
Na	2.100030000	1.594513000	1.585968000

η^3-$C_{C\text{-}K}$, -1514.11456033

C	3.052143000	-2.350298000	0.426150000
C	1.741782000	-2.061598000	0.060152000
C	1.446673000	-0.851948000	-0.569587000
C	2.463816000	0.070494000	-0.825469000
C	3.764255000	-0.211916000	-0.439513000
C	4.059816000	-1.423829000	0.182584000

H	3.283485000	-3.293606000	0.905790000
H	0.954485000	-2.782523000	0.248351000
H	2.207403000	1.013758000	-1.291554000
H	4.548503000	0.515030000	-0.612081000
H	5.078065000	-1.642676000	0.482740000
C	0.070424000	-0.524037000	-1.021134000
C	-1.108003000	-1.122753000	-0.312526000
C	-1.143251000	-1.254001000	1.077620000
C	-2.215512000	-1.496315000	-1.076761000
C	-2.281023000	-1.760837000	1.692375000
H	-0.297348000	-0.911675000	1.662293000
C	-3.348455000	-2.015497000	-0.457956000
H	-2.168343000	-1.392978000	-2.155638000
C	-3.380055000	-2.146639000	0.926881000
H	-2.315533000	-1.846162000	2.771754000
H	-4.199753000	-2.322716000	-1.054000000
H	-4.262466000	-2.547646000	1.411678000
O	-0.124531000	0.189214000	-1.995457000
C	0.208305000	1.846936000	0.908769000
F	1.140212000	1.926278000	1.888211000
F	0.742501000	2.746090000	-0.087020000
F	-0.834793000	2.706877000	1.416281000
K	-1.644685000	2.057773000	-0.989075000

η^3-$TS_{C\text{-}K}$, -1514.11341293, *i*100.7155

C	3.142457000	-2.155529000	0.327778000
C	1.819967000	-1.831302000	0.034152000
C	1.516747000	-0.604448000	-0.552926000
C	2.545530000	0.290686000	-0.855638000
C	3.858125000	-0.028378000	-0.550707000
C	4.159475000	-1.254006000	0.043186000
H	3.373447000	-3.112478000	0.780381000
H	1.032168000	-2.543633000	0.248006000
H	2.288949000	1.241323000	-1.307426000
H	4.650608000	0.678083000	-0.766964000
H	5.187007000	-1.502041000	0.283078000
C	0.123578000	-0.225418000	-0.936641000
C	-1.047372000	-0.965801000	-0.335969000
C	-1.139293000	-1.272864000	1.024113000
C	-2.085941000	-1.331556000	-1.193535000
C	-2.255483000	-1.935487000	1.513228000
H	-0.347085000	-0.952944000	1.691608000
C	-3.205713000	-1.999597000	-0.701116000
H	-1.994561000	-1.105249000	-2.250564000

C	-3.291303000	-2.300209000	0.652540000
H	-2.327192000	-2.157324000	2.571249000
H	-4.002095000	-2.291822000	-1.375593000
H	-4.161930000	-2.815883000	1.040518000
O	-0.078523000	0.489945000	-1.920024000
C	0.153432000	1.535403000	0.942611000
F	1.060484000	1.438104000	1.940259000
F	0.520490000	2.740697000	0.287117000
F	-1.018709000	1.989158000	1.630037000
K	-1.784039000	2.084306000	-0.880909000

$P_{C\text{-}K}$, -1514.15445623

C	3.008478000	-2.012058000	0.607568000
C	1.737132000	-1.453409000	0.677448000
C	1.378067000	-0.404256000	-0.169812000
C	2.304916000	0.065431000	-1.094883000
C	3.576431000	-0.495669000	-1.169533000
C	3.933483000	-1.533862000	-0.316656000
H	3.274389000	-2.829167000	1.268309000
H	1.019035000	-1.848991000	1.387095000
H	1.992584000	0.863215000	-1.756721000
H	4.288468000	-0.124103000	-1.898260000
H	4.922098000	-1.974430000	-0.376020000
C	-0.022666000	0.258382000	-0.147713000
C	-1.103953000	-0.848555000	-0.158917000
C	-1.641873000	-1.481982000	0.961542000
C	-1.544179000	-1.241116000	-1.424030000
C	-2.598992000	-2.485822000	0.816242000
H	-1.334678000	-1.202148000	1.961336000
C	-2.486999000	-2.249974000	-1.569776000
H	-1.131476000	-0.726076000	-2.282921000
C	-3.021884000	-2.877197000	-0.447180000
H	-3.013099000	-2.959516000	1.699043000
H	-2.809792000	-2.546575000	-2.561496000
H	-3.762967000	-3.660306000	-0.558199000
O	-0.203431000	1.144743000	-1.150239000
C	-0.113722000	1.079610000	1.164226000
F	0.129403000	0.450456000	2.317901000
F	0.735482000	2.137147000	1.126034000
F	-1.347896000	1.652628000	1.289598000
K	-0.941866000	3.356365000	-0.876485000

η^3-$C_{C\text{-}Rb}$, -938.229133353

C	-3.933008000	1.523408000	0.134632000

C	-2.572666000	1.610048000	-0.144968000
C	-1.891701000	0.495328000	-0.632887000
C	-2.568425000	-0.710656000	-0.825061000
C	-3.918034000	-0.799003000	-0.523937000
C	-4.602387000	0.319429000	-0.049762000
H	-4.465558000	2.392533000	0.501634000
H	-2.047012000	2.546857000	0.001833000
H	-2.009401000	-1.573325000	-1.167847000
H	-4.437340000	-1.741631000	-0.646433000
H	-5.658437000	0.248011000	0.183451000
C	-0.454538000	0.568815000	-1.003996000
C	0.449089000	1.523119000	-0.276285000
C	0.357323000	1.712197000	1.103999000
C	1.446851000	2.174392000	-1.004274000
C	1.264738000	2.544765000	1.747207000
H	-0.393318000	1.163882000	1.660963000
C	2.346529000	3.017592000	-0.358653000
H	1.496022000	2.023155000	-2.077600000
C	2.255994000	3.199574000	1.018270000
H	1.205455000	2.676452000	2.820882000
H	3.108458000	3.537835000	-0.927291000
H	2.957791000	3.851988000	1.524758000
O	-0.001051000	-0.084834000	-1.929744000
C	-0.062962000	-1.591327000	1.082155000
F	-1.066324000	-1.914914000	1.940701000
F	-0.067196000	-2.724849000	0.189012000
F	1.105705000	-1.939955000	1.852848000
Rb	2.210845000	-1.317721000	-0.645354000

η^3-$TS_{C\text{-}Rb}$, -938.228390601, *i*90.9587

C	-3.897386000	1.471758000	0.086702000
C	-2.520688000	1.483452000	-0.126675000
C	-1.880698000	0.344481000	-0.610576000
C	-2.628002000	-0.801936000	-0.890328000
C	-3.994330000	-0.815304000	-0.666209000
C	-4.632880000	0.323709000	-0.175274000
H	-4.391149000	2.361141000	0.459780000
H	-1.955211000	2.386252000	0.070861000
H	-2.109883000	-1.679425000	-1.258264000
H	-4.565633000	-1.713916000	-0.866595000
H	-5.701933000	0.312270000	0.002029000
C	-0.417190000	0.314421000	-0.910923000
C	0.493320000	1.364001000	-0.317894000
C	0.430883000	1.766029000	1.018514000

C	1.454694000	1.927022000	-1.158366000
C	1.321479000	2.714812000	1.501779000
H	-0.292857000	1.299270000	1.677046000
C	2.347506000	2.880902000	-0.672589000
H	1.480279000	1.621116000	-2.199065000
C	2.282236000	3.273609000	0.658950000
H	1.276728000	3.010904000	2.543157000
H	3.082082000	3.322491000	-1.336221000
H	2.975713000	4.012895000	1.042786000
O	0.015490000	-0.385758000	-1.823919000
C	-0.140026000	-1.268516000	1.138316000
F	-1.146397000	-1.361528000	2.043096000
F	-0.084389000	-2.581900000	0.596258000
F	1.023627000	-1.309953000	1.974086000
Rb	2.233213000	-1.471274000	-0.549126000

$P_{C\text{-}Rb}$, -938.269967053

C	-3.951893000	1.150157000	0.377982000
C	-2.615237000	0.842427000	0.608293000
C	-1.935350000	-0.022884000	-0.248555000
C	-2.600520000	-0.569686000	-1.340139000
C	-3.937553000	-0.260350000	-1.572981000
C	-4.616066000	0.598621000	-0.714581000
H	-4.474452000	1.824329000	1.047013000
H	-2.097303000	1.283557000	1.454032000
H	-2.032289000	-1.226931000	-1.987879000
H	-4.450614000	-0.689776000	-2.426309000
H	-5.656891000	0.841245000	-0.896630000
C	-0.449451000	-0.399717000	-0.055778000
C	0.365158000	0.898089000	0.226404000
C	1.074406000	1.216037000	1.385780000
C	0.488463000	1.751204000	-0.879002000
C	1.903297000	2.343137000	1.428217000
H	0.996166000	0.598179000	2.271724000
C	1.300721000	2.874626000	-0.835293000
H	-0.062735000	1.496004000	-1.778275000
C	2.024273000	3.171850000	0.322453000
H	2.445117000	2.571154000	2.339501000
H	1.368171000	3.526447000	-1.699277000
H	2.660269000	4.048593000	0.360921000
O	0.084264000	-1.052988000	-1.104381000
C	-0.373991000	-1.343944000	1.166757000
F	-0.806801000	-0.821601000	2.332835000
F	-1.051416000	-2.470348000	0.973788000

F	0.926960000	-1.717977000	1.398377000
Rb	2.674438000	-0.925864000	-0.848976000

η^3-$C_{C\text{-}Cs}$, -934.283160425

C	-4.336538000	1.100204000	0.171947000
C	-2.991982000	1.334473000	-0.100764000
C	-2.217556000	0.337313000	-0.691872000
C	-2.790566000	-0.896303000	-1.005842000
C	-4.124540000	-1.132612000	-0.718812000
C	-4.899741000	-0.132920000	-0.131213000
H	-4.938934000	1.878001000	0.625627000
H	-2.551978000	2.297018000	0.133334000
H	-2.162675000	-1.663677000	-1.442169000
H	-4.562670000	-2.098747000	-0.938037000
H	-5.942813000	-0.321204000	0.095468000
C	-0.792101000	0.567811000	-1.045503000
C	0.003199000	1.596160000	-0.288664000
C	-0.075880000	1.717601000	1.099578000
C	0.916916000	2.373342000	-1.004334000
C	0.767410000	2.601152000	1.763581000
H	-0.758686000	1.081277000	1.650052000
C	1.746743000	3.269848000	-0.338842000
H	0.961870000	2.267041000	-2.083200000
C	1.676360000	3.377609000	1.047949000
H	0.722321000	2.674913000	2.843427000
H	2.441305000	3.885111000	-0.898973000
H	2.327363000	4.068570000	1.570939000
O	-0.259426000	-0.005708000	-1.981394000
C	-0.238284000	-1.469301000	1.101376000
F	-1.302983000	-1.787019000	1.891568000
F	0.171634000	-2.754866000	0.624530000
F	0.799067000	-1.263640000	2.084119000
Cs	2.248549000	-0.902530000	-0.477432000

η^3-$TS_{C\text{-}Cs}$, -934.282425798, *i*90.1315

C	-4.361348000	0.922262000	-0.056009000
C	-2.996193000	1.145082000	-0.221593000
C	-2.165564000	0.107873000	-0.639819000
C	-2.710236000	-1.151395000	-0.899638000
C	-4.065206000	-1.374534000	-0.722391000
C	-4.895330000	-0.335793000	-0.299869000
H	-5.003913000	1.734101000	0.263517000
H	-2.587420000	2.132343000	-0.041970000
H	-2.045841000	-1.946322000	-1.216644000

H	-4.480105000	-2.358810000	-0.904852000
H	-5.955709000	-0.511609000	-0.160824000
C	-0.707991000	0.311619000	-0.901473000
C	-0.007236000	1.516355000	-0.317183000
C	-0.170249000	1.928841000	1.007254000
C	0.860911000	2.220739000	-1.152444000
C	0.534292000	3.024798000	1.486196000
H	-0.822015000	1.360012000	1.660827000
C	1.564186000	3.323814000	-0.672315000
H	0.964483000	1.900463000	-2.183887000
C	1.403653000	3.724059000	0.649164000
H	0.415045000	3.329265000	2.519117000
H	2.225996000	3.874288000	-1.331163000
H	1.950759000	4.579445000	1.028299000
O	-0.140293000	-0.320388000	-1.789797000
C	-0.257845000	-1.123188000	1.216836000
F	-1.323471000	-1.259150000	2.049857000
F	0.015971000	-2.460154000	0.836485000
F	0.816267000	-0.908584000	2.136262000
Cs	2.340493000	-1.005859000	-0.388687000

$P_{C\text{-}Cs}$, -934.325219288

C	-4.359651000	0.929680000	0.056790000
C	-3.025895000	0.762731000	0.412761000
C	-2.214838000	-0.124128000	-0.295257000
C	-2.746509000	-0.833953000	-1.365668000
C	-4.080994000	-0.665944000	-1.724290000
C	-4.890259000	0.214775000	-1.013885000
H	-4.984354000	1.620378000	0.611648000
H	-2.612629000	1.328562000	1.241659000
H	-2.080650000	-1.504546000	-1.896170000
H	-4.490976000	-1.222856000	-2.559548000
H	-5.929320000	0.346956000	-1.293095000
C	-0.726856000	-0.354076000	0.049239000
C	-0.036861000	1.026323000	0.251616000
C	0.554018000	1.511257000	1.418445000
C	0.109356000	1.775473000	-0.924287000
C	1.294261000	2.698752000	1.402877000
H	0.451782000	0.977484000	2.354870000
C	0.833975000	2.957869000	-0.940080000
H	-0.350069000	1.392333000	-1.829776000
C	1.442919000	3.422221000	0.228516000
H	1.745514000	3.056759000	2.321706000
H	0.921669000	3.525164000	-1.860158000

H	2.011248000	4.344989000	0.221380000
O	-0.056221000	-1.061153000	-0.878823000
C	-0.688600000	-1.164259000	1.365836000
F	-1.268141000	-0.568585000	2.429852000
F	-1.259255000	-2.357744000	1.234963000
F	0.606080000	-1.401128000	1.745066000
Cs	2.623182000	-0.715804000	-0.591028000