**Supplementary Information**

For

# In silico switch from second to first row transition metals in olefin metathesis: from Ru to Fe and from Rh to Co

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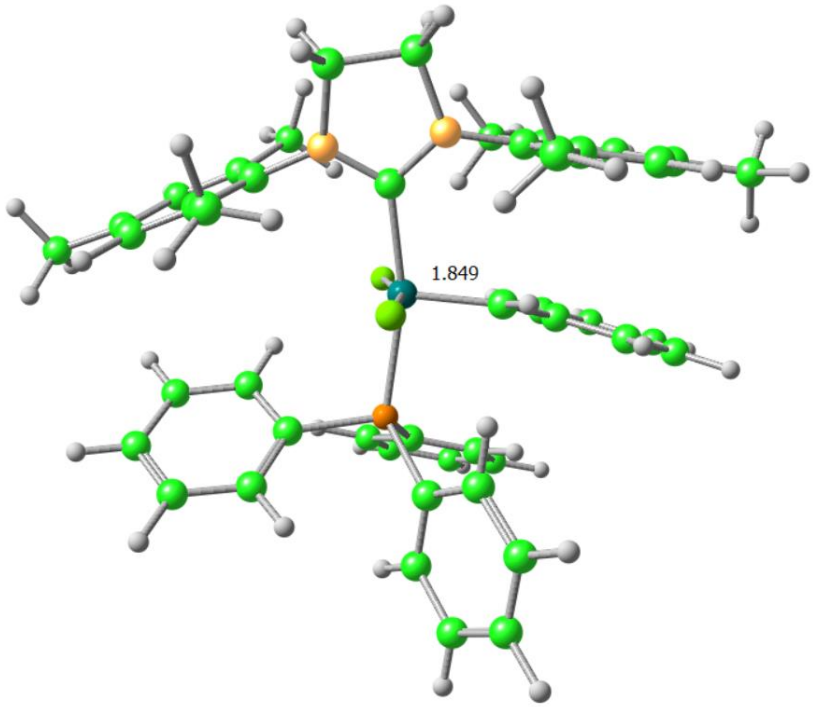
**Table S1**. 3D view, xyz coordinate data sets and absolute energies (a.u.) for the DFT optimized molecular systems.

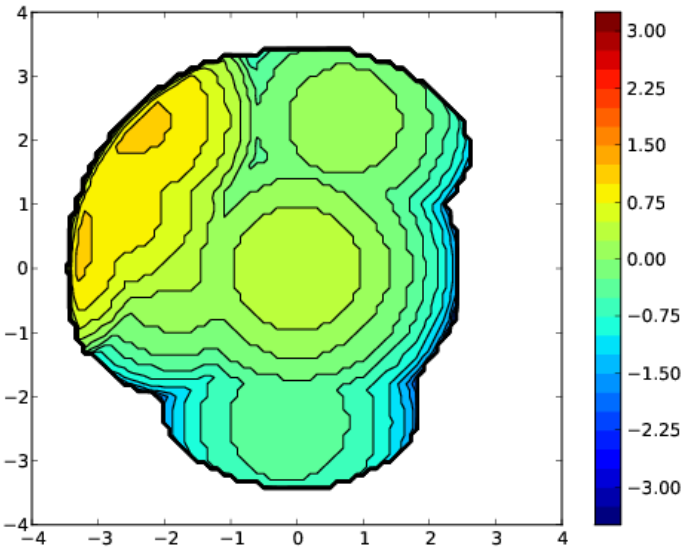
# Ru-Is




Zero-point correction= 0.783723 (Hartree/Particle)
Thermal correction to Energy= 0.836542
Thermal correction to Enthalpy= 0.837486
Thermal correction to Gibbs Free Energy= 0.694513
Sum of electronic and zero-point Energies= -3247.823550
Sum of electronic and thermal Energies= -3247.770731
Sum of electronic and thermal Enthalpies= -3247.769787
Sum of electronic and thermal Free Energies= -3247.912759

HOMO -0.14510 LUMO -0.09912

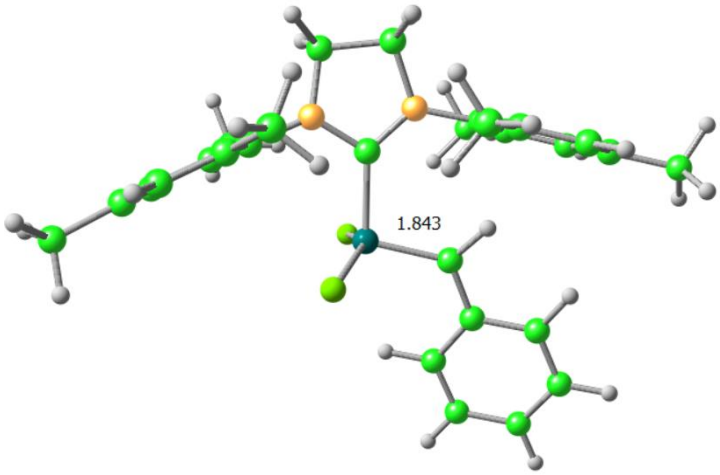
| | | | |
|---|---|---|---|
| Ru | -0.084471000 | -0.309513000 | -0.201522000 |
| Cl | -0.394197000 | -0.248227000 | 2.200296000 |
| Cl | -0.368042000 | -0.411051000 | -2.608349000 |
| P | -0.644277000 | 1.994568000 | -0.195983000 |
| N | -1.226538000 | -3.113586000 | -0.270629000 |
| N | 0.951643000 | -3.162455000 | -0.507673000 |
| C | -0.108441000 | -2.349055000 | -0.270161000 |
| C | -0.962608000 | -4.519255000 | -0.651386000 |
| H | -1.350060000 | -4.707520000 | -1.665643000 |
| H | -1.460234000 | -5.206016000 | 0.047662000 |
| C | 0.569897000 | -4.592055000 | -0.585891000 |
| H | 0.932962000 | -5.124366000 | 0.309559000 |
| H | 1.015720000 | -5.060981000 | -1.473842000 |
| C | -2.550619000 | -2.684823000 | 0.076528000 |
| C | -2.930708000 | -2.753494000 | 1.434283000 |
| C | -1.972063000 | -3.244689000 | 2.484202000 |
| H | -2.481058000 | -3.354196000 | 3.451362000 |
| H | -1.142506000 | -2.532209000 | 2.607658000 |
| H | -1.541580000 | -4.221466000 | 2.211878000 |
| C | -4.235374000 | -2.379395000 | 1.775620000 |
| H | -4.535919000 | -2.418568000 | 2.826496000 |
| C | -5.165425000 | -1.981327000 | 0.805858000 |
| C | -6.580605000 | -1.626435000 | 1.191954000 |
| H | -7.020948000 | -0.911295000 | 0.482123000 |
| H | -6.627198000 | -1.188518000 | 2.200101000 |
| H | -7.223482000 | -2.522336000 | 1.196561000 |
| C | -4.765627000 | -1.963914000 | -0.534141000 |
| H | -5.480789000 | -1.660775000 | -1.303821000 |
| C | -3.472354000 | -2.333416000 | -0.929266000 |
| C | -3.126040000 | -2.420813000 | -2.390403000 |
| H | -3.764984000 | -1.749326000 | -2.980018000 |
| H | -3.294415000 | -3.447190000 | -2.760446000 |
| H | -2.081715000 | -2.143781000 | -2.582854000 |
| C | 2.332323000 | -2.808759000 | -0.387248000 |
| C | 3.096399000 | -2.634360000 | -1.555952000 |
| C | 2.457342000 | -2.742218000 | -2.913781000 |
| H | 3.171709000 | -2.469040000 | -3.702458000 |
| H | 1.574556000 | -2.085767000 | -2.989669000 |
| H | 2.112504000 | -3.769622000 | -3.117407000 |
| C | 4.456620000 | -2.326836000 | -1.412887000 |
| H | 5.058981000 | -2.172776000 | -2.312589000 |
| C | 5.058775000 | -2.207715000 | -0.154126000 |
| C | 6.516896000 | -1.849588000 | -0.018588000 |
| H | 7.042027000 | -2.553035000 | 0.645818000 |
| H | 6.626576000 | -0.843082000 | 0.415818000 |
| H | 7.024649000 | -1.855279000 | -0.993361000 |
| C | 4.269278000 | -2.407360000 | 0.986822000 |
| H | 4.720822000 | -2.306388000 | 1.977345000 |
| C | 2.907952000 | -2.712794000 | 0.896703000 |
| C | 2.072846000 | -2.886626000 | 2.133976000 |
| H | 1.489708000 | -3.820422000 | 2.108846000 |
| H | 1.346411000 | -2.062998000 | 2.239226000 |
| H | 2.706616000 | -2.903003000 | 3.030704000 |
| C | 1.712239000 | 0.023017000 | -0.486214000 |
| C | 3.968101000 | 0.954420000 | -0.356637000 |
| C | 2.796456000 | 0.551685000 | 0.328109000 |
| C | 5.056788000 | 1.484826000 | 0.333048000 |
| C | 2.760211000 | 0.683191000 | 1.732786000 |
| C | 5.010271000 | 1.589749000 | 1.728962000 |
| H | 5.945596000 | 1.807486000 | -0.213497000 |
| C | 3.862420000 | 1.182478000 | 2.421692000 |
| H | 1.851749000 | 0.395783000 | 2.262455000 |
| H | 5.865988000 | 1.993368000 | 2.275135000 |
| H | 3.820207000 | 1.274075000 | 3.508958000 |
| C | -2.481697000 | 2.031296000 | -0.307653000 |
| C | -3.147260000 | 2.671385000 | -1.363740000 |
| C | -3.221681000 | 1.311899000 | 0.649517000 |
| C | -4.542124000 | 2.625190000 | -1.440421000 |
| H | -2.574653000 | 3.198524000 | -2.127509000 |
| C | -4.615890000 | 1.297838000 | 0.581429000 |
| H | -2.704321000 | 0.754879000 | 1.435161000 |
| C | -5.279811000 | 1.954061000 | -0.459583000 |
| H | -5.053469000 | 3.122125000 | -2.267735000 |
| H | -5.181506000 | 0.756544000 | 1.339611000 |
| H | -6.370493000 | 1.932468000 | -0.513958000 |




| South West | North West | North East | North West | **Total %V_Bur** |
|---|---|---|---|---|
| 46.5 | 61.0 | 42.6 | 34.5 | 46.2 |

| | | | |
|---|---|---|---|
| C | -0.041222000 | 3.154994000 | -1.497672000 |
| C | -0.372176000 | 4.519269000 | -1.407909000 |
| C | 0.802102000 | 2.711334000 | -2.522524000 |
| C | 0.127540000 | 5.424916000 | -2.345034000 |
| H | -1.008121000 | 4.870755000 | -0.592762000 |
| C | 1.306064000 | 3.624012000 | -3.456013000 |
| H | 1.032043000 | 1.648949000 | -2.604978000 |
| C | 0.970398000 | 4.977833000 | -3.370833000 |
| H | -0.132960000 | 6.482767000 | -2.269626000 |
| H | 1.961429000 | 3.270395000 | -4.254787000 |
| H | 1.365402000 | 5.687700000 | -4.100900000 |
| C | -0.188086000 | 2.955172000 | 1.313044000 |
| C | -1.064816000 | 3.175492000 | 2.382328000 |
| C | 1.138431000 | 3.409277000 | 1.399110000 |
| C | -0.620637000 | 3.849842000 | 3.523488000 |
| H | -2.096077000 | 2.827656000 | 2.324931000 |
| C | 1.579409000 | 4.077649000 | 2.542360000 |
| H | 1.826558000 | 3.243417000 | 0.568816000 |
| C | 0.701343000 | 4.298251000 | 3.608828000 |
| H | -1.311968000 | 4.020669000 | 4.351454000 |
| H | 2.614882000 | 4.419004000 | 2.599220000 |
| H | 1.046009000 | 4.820844000 | 4.503691000 |
| H | 4.002414000 | 0.846566000 | -1.442909000 |
| H | 2.037124000 | -0.128875000 | -1.533567000 |

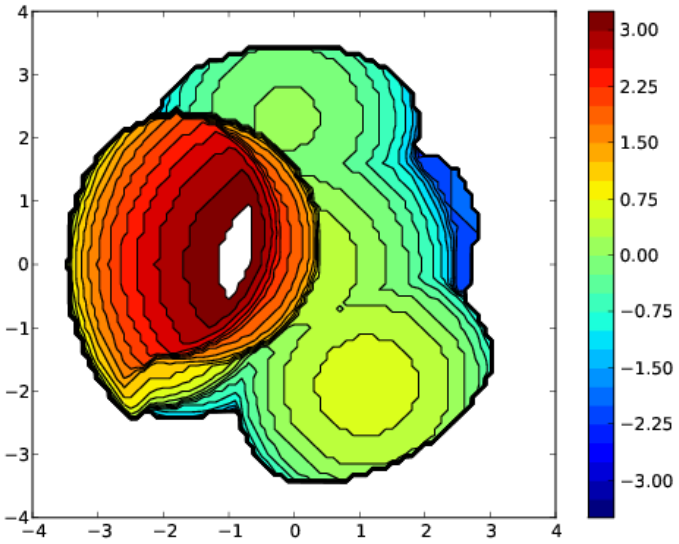
# Ru-IIs




Zero-point correction= 0.515313 (Hartree/Particle)
Thermal correction to Energy= 0.551205
Thermal correction to Enthalpy= 0.552149
Thermal correction to Gibbs Free Energy= 0.443808
Sum of electronic and zero-point Energies= -2211.395676
Sum of electronic and thermal Energies= -2211.359785
Sum of electronic and thermal Enthalpies= -2211.358840
Sum of electronic and thermal Free Energies= -2211.467182

HOMO -0.16947 LUMO -0.10489

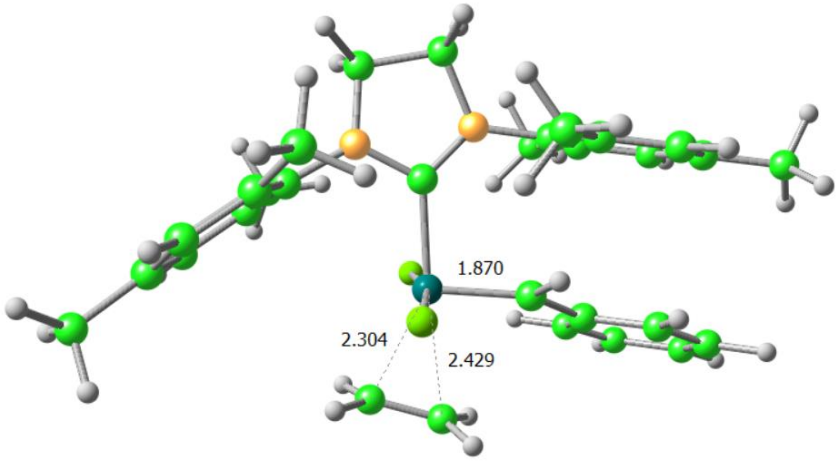
| | | | |
|---|---|---|---|
| Ru | -0.250257000 | 0.817996000 | 0.083916000 |
| Cl | -0.270299000 | 1.169360000 | 2.381304000 |
| Cl | -1.069621000 | 1.471492000 | -1.981355000 |
| N | -1.858030000 | -1.546344000 | 0.325285000 |
| N | 0.263804000 | -2.129778000 | 0.406246000 |
| C | -0.579047000 | -1.067107000 | 0.219886000 |
| C | -1.910590000 | -2.953803000 | 0.751640000 |
| H | -2.639189000 | -3.512738000 | 0.147432000 |
| H | -2.208375000 | -3.021707000 | 1.811829000 |
| C | -0.461146000 | -3.411468000 | 0.526941000 |
| H | -0.060349000 | -3.997220000 | 1.365759000 |
| H | -0.345462000 | -4.004089000 | -0.397116000 |
| C | -3.039497000 | -0.771761000 | 0.094358000 |
| C | -3.717601000 | -0.165722000 | 1.168751000 |
| C | -3.309471000 | -0.398013000 | 2.599341000 |
| H | -3.563570000 | 0.469156000 | 3.223756000 |
| H | -2.231119000 | -0.569304000 | 2.698152000 |
| H | -3.844752000 | -1.271393000 | 3.010097000 |
| C | -4.841449000 | 0.620196000 | 0.873452000 |
| H | -5.362946000 | 1.119106000 | 1.695246000 |
| C | -5.314181000 | 0.774038000 | -0.434319000 |
| C | -6.490062000 | 1.670629000 | -0.732343000 |
| H | -7.102006000 | 1.271666000 | -1.554674000 |
| H | -6.145188000 | 2.672594000 | -1.037065000 |
| H | -7.134466000 | 1.796266000 | 0.149384000 |
| C | -4.659188000 | 0.088353000 | -1.468179000 |
| H | -5.034081000 | 0.173738000 | -2.491704000 |
| C | -3.527119000 | -0.693452000 | -1.227570000 |
| C | -2.834557000 | -1.421168000 | -2.348206000 |
| H | -3.450490000 | -1.408160000 | -3.257414000 |
| H | -2.625498000 | -2.469794000 | -2.085837000 |
| H | -1.875520000 | -0.934538000 | -2.579894000 |
| C | 1.665684000 | -2.140428000 | 0.136509000 |
| C | 2.103973000 | -2.248653000 | -1.196658000 |
| C | 1.115181000 | -2.265442000 | -2.333141000 |
| H | 1.625167000 | -2.422204000 | -3.292768000 |
| H | 0.575427000 | -1.305118000 | -2.382251000 |
| H | 0.355332000 | -3.052865000 | -2.217896000 |
| C | 3.482918000 | -2.210798000 | -1.441994000 |
| H | 3.837739000 | -2.273915000 | -2.474511000 |
| C | 4.411444000 | -2.057766000 | -0.402192000 |
| C | 5.892978000 | -2.026205000 | -0.687104000 |
| H | 6.344300000 | -3.020454000 | -0.533845000 |
| H | 6.413719000 | -1.324941000 | -0.018675000 |
| H | 6.095674000 | -1.728880000 | -1.725833000 |
| C | 3.934285000 | -1.945274000 | 0.911494000 |
| H | 4.645418000 | -1.803164000 | 1.730026000 |




| South West | North West | North East | North West | **Total %V_Bur** |
|---|---|---|---|---|
| 72.9 | 82.5 | 37.8 | 53.6 | 61.7 |

| | | | |
|---|---|---|---|
| C | 2.565369000 | -1.986871000 | 1.206005000 |
| C | 2.058322000 | -1.793251000 | 2.609110000 |
| H | 1.394529000 | -2.615600000 | 2.918289000 |
| H | 1.469965000 | -0.864604000 | 2.683857000 |
| H | 2.892421000 | -1.738596000 | 3.321344000 |
| C | 1.561280000 | 0.862766000 | -0.252607000 |
| C | 3.708107000 | 2.008748000 | -0.600438000 |
| C | 2.359114000 | 2.069316000 | -0.174476000 |
| C | 4.520812000 | 3.139894000 | -0.560168000 |
| C | 1.859072000 | 3.303073000 | 0.307424000 |
| C | 4.005499000 | 4.354448000 | -0.089736000 |
| H | 5.559026000 | 3.078615000 | -0.893503000 |
| C | 2.674165000 | 4.430242000 | 0.344836000 |
| H | 0.830126000 | 3.364064000 | 0.670274000 |
| H | 4.641094000 | 5.241765000 | -0.056743000 |
| H | 2.276122000 | 5.375562000 | 0.718841000 |
| H | 4.098762000 | 1.053864000 | -0.961263000 |
| H | 2.111942000 | -0.017694000 | -0.599167000 |

# Ru-IIIs



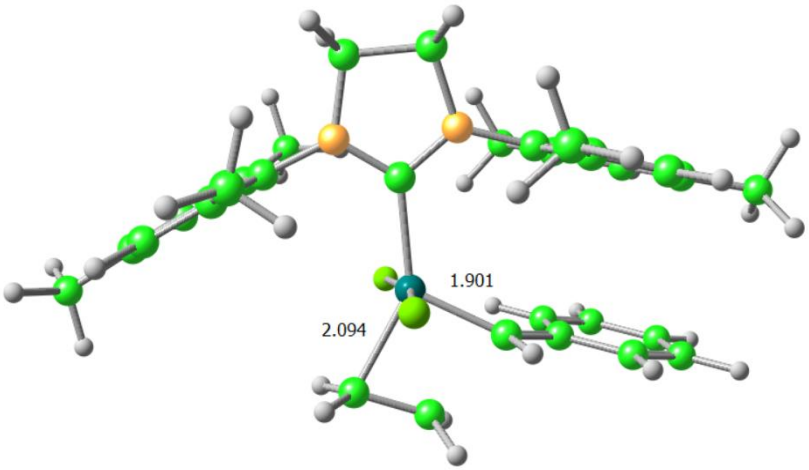

Zero-point correction= 0.569104 (Hartree/Particle)
Thermal correction to Energy= 0.608429
Thermal correction to Enthalpy= 0.609374
Thermal correction to Gibbs Free Energy= 0.495651
Sum of electronic and zero-point Energies= -2289.982941
Sum of electronic and thermal Energies= -2289.943615
Sum of electronic and thermal Enthalpies= -2289.942671
Sum of electronic and thermal Free Energies= -2290.056394

HOMO -0.15592 LUMO -0.11193

| | | | |
|---|---|---|---|
| Ru | -0.519262000 | 0.869355000 | -0.274135000 |
| Cl | -0.299535000 | 1.560874000 | 2.023918000 |
| Cl | -1.151183000 | 0.384022000 | -2.544193000 |
| N | -1.798206000 | -1.555469000 | 0.725195000 |
| N | 0.370930000 | -1.886598000 | 0.741067000 |
| C | -0.602215000 | -1.013931000 | 0.375485000 |
| C | -1.660953000 | -2.801827000 | 1.502492000 |
| H | -2.351519000 | -3.570455000 | 1.128470000 |
| H | -1.885120000 | -2.611456000 | 2.565227000 |
| C | -0.180750000 | -3.154467000 | 1.273392000 |
| H | 0.340292000 | -3.439813000 | 2.197334000 |
| H | -0.050083000 | -3.962425000 | 0.533453000 |
| C | -3.050542000 | -0.920236000 | 0.433805000 |
| C | -3.657356000 | -0.063628000 | 1.373408000 |
| C | -3.154478000 | 0.057469000 | 2.786876000 |
| H | -3.380282000 | 1.049931000 | 3.199473000 |
| H | -2.069534000 | -0.082488000 | 2.855507000 |
| H | -3.654882000 | -0.691570000 | 3.424913000 |
| C | -4.818475000 | 0.620125000 | 0.979712000 |
| H | -5.283033000 | 1.312122000 | 1.687833000 |
| C | -5.401379000 | 0.427630000 | -0.276952000 |
| C | -6.617581000 | 1.214079000 | -0.698792000 |
| H | -7.355802000 | 0.572758000 | -1.203446000 |
| H | -6.339726000 | 2.010164000 | -1.408947000 |
| H | -7.106381000 | 1.691201000 | 0.162237000 |
| C | -4.828848000 | -0.517851000 | -1.142215000 |
| H | -5.296678000 | -0.714438000 | -2.110697000 |
| C | -3.664449000 | -1.211065000 | -0.805074000 |
| C | -3.080693000 | -2.245004000 | -1.729081000 |
| H | -3.744497000 | -2.411590000 | -2.587855000 |
| H | -2.935105000 | -3.208153000 | -1.214359000 |
| H | -2.107116000 | -1.907039000 | -2.112267000 |
| C | 1.751113000 | -1.799895000 | 0.381752000 |
| C | 2.143118000 | -2.191380000 | -0.913787000 |
| C | 1.117549000 | -2.605289000 | -1.935445000 |
| H | 1.602745000 | -2.935221000 | -2.863616000 |
| H | 0.437324000 | -1.770287000 | -2.180071000 |
| H | 0.485036000 | -3.430037000 | -1.571873000 |
| C | 3.504077000 | -2.123331000 | -1.237191000 |
| H | 3.821836000 | -2.407826000 | -2.244279000 |
| C | 4.460356000 | -1.684812000 | -0.311321000 |
| C | 5.920569000 | -1.614794000 | -0.679932000 |
| H | 6.391273000 | -0.716980000 | -0.252973000 |
| H | 6.057543000 | -1.590306000 | -1.770301000 |
| H | 6.469168000 | -2.490221000 | -0.295005000 |
| C | 4.032465000 | -1.311342000 | 0.970026000 |
| H | 4.764290000 | -0.943425000 | 1.694205000 |
| C | 2.685466000 | -1.366471000 | 1.342711000 |
| C | 2.236665000 | -0.933142000 | 2.709790000 |
| H | 1.787269000 | -1.768891000 | 3.271049000 |
| H | 1.471551000 | -0.143724000 | 2.638778000 |
| H | 3.085425000 | -0.552244000 | 3.293367000 |
| C | 1.272560000 | 0.811950000 | -0.805857000 |
| C | 3.617970000 | 1.297588000 | -1.278131000 |

| | | | |
|---|---|---|---|
| C | 2.501847000 | 1.479651000 | -0.423705000 |
| C | 4.855378000 | 1.861080000 | -0.973855000 |
| C | 2.674106000 | 2.244116000 | 0.753394000 |
| C | 5.012361000 | 2.594121000 | 0.207898000 |
| H | 5.700835000 | 1.720481000 | -1.650235000 |
| C | 3.919927000 | 2.778740000 | 1.068411000 |
| H | 1.818156000 | 2.376134000 | 1.417062000 |
| H | 5.983735000 | 3.027131000 | 0.457336000 |
| H | 4.043977000 | 3.352718000 | 1.989212000 |
| C | -1.519688000 | 2.923388000 | -0.568770000 |
| C | -0.227576000 | 3.183864000 | -0.950822000 |
| H | -2.276273000 | 2.669862000 | -1.315886000 |
| H | -1.855760000 | 3.163610000 | 0.442041000 |
| H | 0.070654000 | 3.117917000 | -1.998087000 |
| H | 3.492325000 | 0.699222000 | -2.182408000 |
| H | 1.432834000 | 0.151093000 | -1.674625000 |
| H | 0.492937000 | 3.601855000 | -0.247108000 |

# Ru-III-IVs

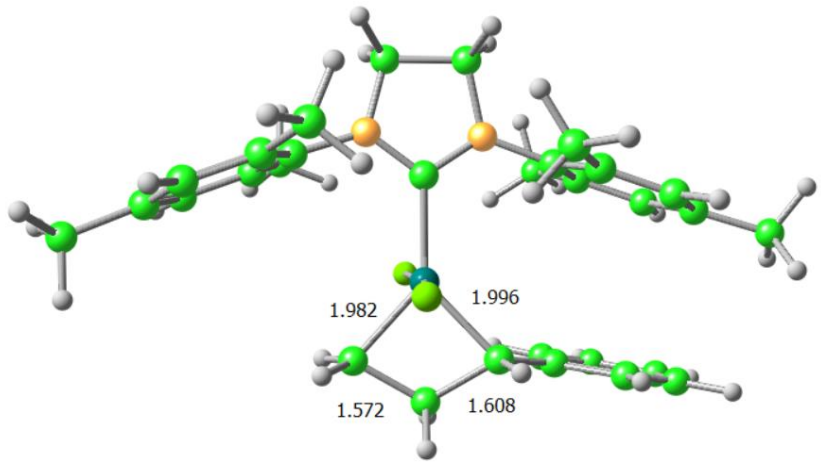



Zero-point correction= 0.570137 (Hartree/Particle)
Thermal correction to Energy= 0.608267
Thermal correction to Enthalpy= 0.609211
Thermal correction to Gibbs Free Energy= 0.499504
Sum of electronic and zero-point Energies= -2289.978294
Sum of electronic and thermal Energies= -2289.940164
Sum of electronic and thermal Enthalpies= -2289.939220
Sum of electronic and thermal Free Energies= -2290.048927

| | | | |
|---|---|---|---|
| Ru | 0.398764000 | -0.743570000 | -0.587993000 |
| Cl | 0.623833000 | -1.792731000 | 1.564165000 |
| Cl | 0.612332000 | 0.176430000 | -2.814771000 |
| N | 1.949595000 | 1.629538000 | 0.419161000 |
| N | -0.216175000 | 2.011396000 | 0.455057000 |
| C | 0.733180000 | 1.098578000 | 0.168780000 |
| C | 1.862464000 | 2.978297000 | 1.023541000 |
| H | 2.506399000 | 3.683167000 | 0.479189000 |
| H | 2.191948000 | 2.939496000 | 2.073795000 |
| C | 0.361769000 | 3.306516000 | 0.887011000 |
| H | -0.097965000 | 3.629117000 | 1.831971000 |
| H | 0.169429000 | 4.076359000 | 0.123590000 |
| C | 3.157625000 | 0.851608000 | 0.419630000 |
| C | 3.531704000 | 0.156864000 | 1.587693000 |
| C | 2.785053000 | 0.320059000 | 2.885765000 |
| H | 2.903102000 | -0.571964000 | 3.513973000 |
| H | 1.710181000 | 0.464833000 | 2.727482000 |
| H | 3.181230000 | 1.182903000 | 3.449429000 |
| C | 4.667453000 | -0.659633000 | 1.529207000 |
| H | 4.953059000 | -1.224886000 | 2.420636000 |
| C | 5.438264000 | -0.772150000 | 0.365120000 |
| C | 6.620605000 | -1.707716000 | 0.310588000 |
| H | 7.101103000 | -1.807145000 | 1.294713000 |
| H | 7.375229000 | -1.360661000 | -0.409864000 |
| H | 6.304439000 | -2.716378000 | -0.003524000 |
| C | 5.079355000 | -0.004097000 | -0.750454000 |
| H | 5.696110000 | -0.045173000 | -1.652521000 |
| C | 3.951780000 | 0.826918000 | -0.744834000 |
| C | 3.615108000 | 1.677987000 | -1.937728000 |
| H | 4.430527000 | 1.649333000 | -2.673252000 |
| H | 3.452136000 | 2.727396000 | -1.646379000 |
| H | 2.690087000 | 1.328601000 | -2.423451000 |
| C | -1.633626000 | 1.807694000 | 0.370622000 |
| C | -2.324073000 | 2.205747000 | -0.790557000 |
| C | -1.597821000 | 2.804775000 | -1.963653000 |
| H | -2.294986000 | 3.002795000 | -2.789007000 |
| H | -0.808688000 | 2.127925000 | -2.329023000 |
| H | -1.118595000 | 3.760970000 | -1.696709000 |
| C | -3.711239000 | 2.017317000 | -0.823940000 |
| H | -4.258074000 | 2.309767000 | -1.724931000 |
| C | -4.412175000 | 1.474594000 | 0.261594000 |
| C | -5.912362000 | 1.330208000 | 0.215176000 |
| H | -6.406327000 | 2.266010000 | 0.525917000 |
| H | -6.254960000 | 0.531329000 | 0.886994000 |
| H | -6.261030000 | 1.097260000 | -0.801432000 |
| C | -3.692049000 | 1.102704000 | 1.401993000 |
| H | -4.220617000 | 0.663938000 | 2.251828000 |
| C | -2.302942000 | 1.264417000 | 1.483329000 |
| C | -1.551899000 | 0.852937000 | 2.720022000 |
| H | -0.923302000 | 1.671886000 | 3.104907000 |
| H | -0.882606000 | 0.001184000 | 2.515314000 |
| H | -2.250277000 | 0.558596000 | 3.514823000 |
| C | -1.355684000 | -1.234184000 | -1.132125000 |
| C | -3.782020000 | -1.533635000 | -1.111340000 |

| | | | |
|---|---|---|---|
| C | -2.561870000 | -1.656802000 | -0.408599000 |
| C | -4.991836000 | -1.896111000 | -0.520036000 |
| C | -2.595010000 | -2.145405000 | 0.912338000 |
| C | -5.007474000 | -2.384346000 | 0.790139000 |
| H | -5.923255000 | -1.794566000 | -1.080386000 |
| C | -3.805574000 | -2.508424000 | 1.499499000 |
| H | -1.657538000 | -2.229430000 | 1.463494000 |
| H | -5.952543000 | -2.670233000 | 1.257284000 |
| H | -3.813493000 | -2.887640000 | 2.523657000 |
| C | -0.113465000 | -2.791478000 | -1.490474000 |
| C | 1.292037000 | -2.465333000 | -1.376205000 |
| H | -0.530227000 | -3.481529000 | -0.755592000 |
| H | -0.508997000 | -2.862719000 | -2.506865000 |
| H | 1.849845000 | -2.940680000 | -0.565244000 |
| H | -3.766146000 | -1.145894000 | -2.132506000 |
| H | -1.591928000 | -0.915344000 | -2.160938000 |
| H | 1.840717000 | -2.218400000 | -2.287510000 |

# Ru-IVs



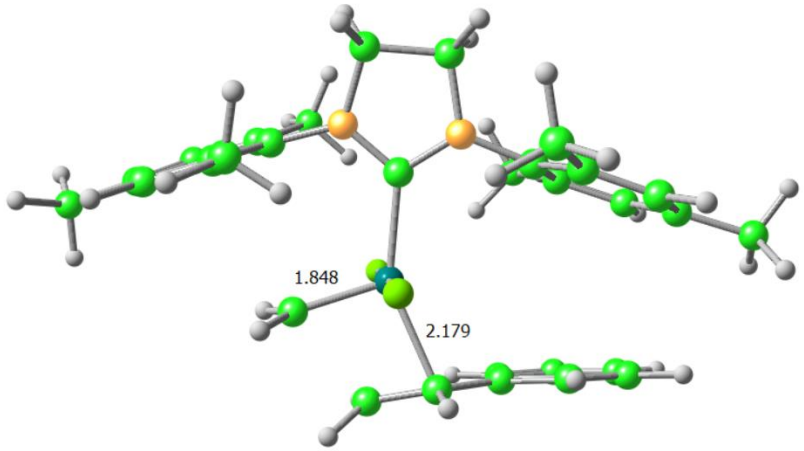

Zero-point correction= 0.571582 (Hartree/Particle)
Thermal correction to Energy= 0.609840
Thermal correction to Enthalpy= 0.610785
Thermal correction to Gibbs Free Energy= 0.500252
Sum of electronic and zero-point Energies= -2289.982838
Sum of electronic and thermal Energies= -2289.944579
Sum of electronic and thermal Enthalpies= -2289.943635
Sum of electronic and thermal Free Energies= -2290.054168

HOMO -0.15441 LUMO -0.09965

| | | | |
|---|---|---|---|
| Ru | 0.313890000 | -0.810268000 | -0.365801000 |
| Cl | 0.220977000 | -1.626098000 | 1.895371000 |
| Cl | 0.747885000 | -0.144269000 | -2.639285000 |
| N | 1.981835000 | 1.437926000 | 0.740756000 |
| N | -0.169756000 | 1.903228000 | 0.705794000 |
| C | 0.765644000 | 0.994601000 | 0.370416000 |
| C | 1.898928000 | 2.710722000 | 1.496485000 |
| H | 2.616842000 | 3.438147000 | 1.093361000 |
| H | 2.135198000 | 2.529800000 | 2.556775000 |
| C | 0.429673000 | 3.127970000 | 1.286635000 |
| H | -0.078809000 | 3.390308000 | 2.224150000 |
| H | 0.322836000 | 3.968254000 | 0.581303000 |
| C | 3.220048000 | 0.769471000 | 0.455393000 |
| C | 3.806749000 | -0.072469000 | 1.419550000 |
| C | 3.234077000 | -0.207132000 | 2.804491000 |
| H | 3.677930000 | -1.066249000 | 3.325233000 |
| H | 2.145260000 | -0.353400000 | 2.780704000 |
| H | 3.454010000 | 0.692448000 | 3.404441000 |
| C | 4.979577000 | -0.752486000 | 1.064002000 |
| H | 5.435416000 | -1.426284000 | 1.794855000 |
| C | 5.583149000 | -0.585518000 | -0.188833000 |
| C | 6.813399000 | -1.373005000 | -0.566148000 |
| H | 7.474970000 | -0.793526000 | -1.226518000 |
| H | 6.536504000 | -2.293624000 | -1.106376000 |
| H | 7.387462000 | -1.672782000 | 0.322278000 |
| C | 5.014150000 | 0.327060000 | -1.087785000 |
| H | 5.496042000 | 0.504029000 | -2.053227000 |
| C | 3.841740000 | 1.027512000 | -0.783299000 |
| C | 3.271454000 | 2.035632000 | -1.743334000 |
| H | 3.963451000 | 2.205505000 | -2.579016000 |
| H | 3.087702000 | 3.003205000 | -1.249739000 |
| H | 2.315114000 | 1.679109000 | -2.155767000 |
| C | -1.567604000 | 1.809813000 | 0.383964000 |
| C | -2.009637000 | 2.252402000 | -0.879971000 |
| C | -1.050176000 | 2.771364000 | -1.915516000 |
| H | -1.591378000 | 3.306525000 | -2.707449000 |
| H | -0.486492000 | 1.942966000 | -2.376596000 |
| H | -0.309246000 | 3.460218000 | -1.482788000 |
| C | -3.382391000 | 2.192381000 | -1.150406000 |
| H | -3.739005000 | 2.529255000 | -2.127988000 |
| C | -4.304673000 | 1.736146000 | -0.200148000 |
| C | -5.782394000 | 1.738937000 | -0.500168000 |
| H | -6.209818000 | 2.744330000 | -0.350027000 |
| H | -6.322476000 | 1.044460000 | 0.157649000 |
| H | -5.981229000 | 1.451919000 | -1.543163000 |
| C | -3.829121000 | 1.321289000 | 1.048706000 |
| H | -4.535339000 | 0.952752000 | 1.796735000 |
| C | -2.467669000 | 1.362515000 | 1.372238000 |
| C | -1.992792000 | 0.953447000 | 2.738378000 |
| H | -1.522338000 | 1.797193000 | 3.269987000 |
| H | -1.247133000 | 0.145996000 | 2.675519000 |
| H | -2.836242000 | 0.602251000 | 3.347655000 |
| C | -1.293778000 | -1.687551000 | -1.159012000 |
| C | -3.735398000 | -1.436159000 | -1.249579000 |
| C | -2.608568000 | -1.829637000 | -0.498797000 |

| | | | |
|---|---|---|---|
| C | -5.025619000 | -1.569693000 | -0.735825000 |
| C | -2.813885000 | -2.339563000 | 0.797942000 |
| C | -5.215197000 | -2.077143000 | 0.552398000 |
| H | -5.883989000 | -1.272493000 | -1.341115000 |
| C | -4.102845000 | -2.456237000 | 1.315722000 |
| H | -1.950283000 | -2.605506000 | 1.407840000 |
| H | -6.223010000 | -2.177802000 | 0.961203000 |
| H | -4.242039000 | -2.847463000 | 2.325936000 |
| C | -0.224445000 | -2.885623000 | -1.080462000 |
| C | 1.271490000 | -2.489678000 | -0.801131000 |
| H | -0.564396000 | -3.597288000 | -0.322153000 |
| H | -0.238477000 | -3.286728000 | -2.102639000 |
| H | 1.695387000 | -3.005340000 | 0.066097000 |
| H | -3.585790000 | -1.028453000 | -2.251885000 |
| H | -1.409405000 | -1.364111000 | -2.200918000 |
| H | 1.903086000 | -2.453885000 | -1.693855000 |

# Ru-IV-Vs

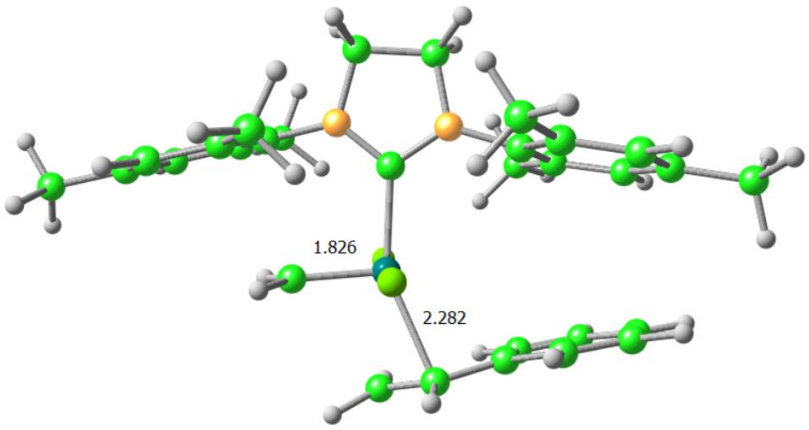



Zero-point correction= 0.568831 (Hartree/Particle)
Thermal correction to Energy= 0.607087
Thermal correction to Enthalpy= 0.608031
Thermal correction to Gibbs Free Energy= 0.496426
Sum of electronic and zero-point Energies= -2289.970958
Sum of electronic and thermal Energies= -2289.932702
Sum of electronic and thermal Enthalpies= -2289.931758
Sum of electronic and thermal Free Energies= -2290.043362

| | | | |
|---|---|---|---|
| Ru | 0.313642000 | -0.762669000 | -0.594964000 |
| Cl | 0.677358000 | -1.858109000 | 1.532209000 |
| Cl | 0.039482000 | 0.328324000 | -2.739069000 |
| N | 1.824349000 | 1.608406000 | 0.488941000 |
| N | -0.333021000 | 2.011376000 | 0.403525000 |
| C | 0.617512000 | 1.075245000 | 0.185302000 |
| C | 1.731946000 | 3.050732000 | 0.810879000 |
| H | 2.114657000 | 3.645385000 | -0.034685000 |
| H | 2.326303000 | 3.284801000 | 1.704282000 |
| C | 0.222586000 | 3.239586000 | 1.019268000 |
| H | -0.057212000 | 3.278168000 | 2.085623000 |
| H | -0.173269000 | 4.133179000 | 0.519234000 |
| C | 3.082975000 | 0.928776000 | 0.425184000 |
| C | 3.581211000 | 0.341576000 | 1.603551000 |
| C | 2.832950000 | 0.458991000 | 2.903828000 |
| H | 3.409942000 | 0.011904000 | 3.724411000 |
| H | 1.868700000 | -0.067528000 | 2.832224000 |
| H | 2.629698000 | 1.509962000 | 3.164073000 |
| C | 4.785951000 | -0.366840000 | 1.526193000 |
| H | 5.175875000 | -0.841156000 | 2.431040000 |
| C | 5.495581000 | -0.488015000 | 0.323417000 |
| C | 6.761644000 | -1.306406000 | 0.256722000 |
| H | 7.341782000 | -1.224519000 | 1.187525000 |
| H | 7.402411000 | -0.989365000 | -0.578479000 |
| H | 6.530176000 | -2.374419000 | 0.109191000 |
| C | 4.995222000 | 0.157455000 | -0.815100000 |
| H | 5.554402000 | 0.102472000 | -1.753465000 |
| C | 3.797471000 | 0.886068000 | -0.787722000 |
| C | 3.301762000 | 1.606245000 | -2.012409000 |
| H | 3.931792000 | 1.370505000 | -2.880799000 |
| H | 3.333489000 | 2.698907000 | -1.868223000 |
| H | 2.262507000 | 1.334800000 | -2.255917000 |
| C | -1.751189000 | 1.791932000 | 0.378313000 |
| C | -2.502804000 | 2.354537000 | -0.672615000 |
| C | -1.836770000 | 3.118093000 | -1.785149000 |
| H | -2.562276000 | 3.365349000 | -2.571881000 |
| H | -1.022229000 | 2.527032000 | -2.229457000 |
| H | -1.408036000 | 4.066630000 | -1.419640000 |
| C | -3.894064000 | 2.197841000 | -0.642998000 |
| H | -4.486864000 | 2.617771000 | -1.460672000 |
| C | -4.541064000 | 1.539248000 | 0.410356000 |
| C | -6.045333000 | 1.429756000 | 0.444310000 |
| H | -6.494066000 | 2.311065000 | 0.932034000 |
| H | -6.368527000 | 0.542901000 | 1.008132000 |
| H | -6.467221000 | 1.368374000 | -0.569720000 |
| C | -3.763636000 | 1.014464000 | 1.448307000 |
| H | -4.252697000 | 0.495662000 | 2.276729000 |
| C | -2.368329000 | 1.133078000 | 1.462891000 |
| C | -1.573807000 | 0.582305000 | 2.614457000 |
| H | -2.236940000 | 0.339673000 | 3.455553000 |
| H | -0.816011000 | 1.297337000 | 2.970140000 |
| H | -1.028827000 | -0.332708000 | 2.330852000 |
| C | -1.021513000 | -2.212358000 | -1.523671000 |
| C | -3.353844000 | -1.596775000 | -1.067502000 |
| C | -2.200802000 | -2.287015000 | -0.639836000 |

| | | | |
|---|---|---|---|
| C | -4.543776000 | -1.681169000 | -0.346028000 |
| C | -2.259633000 | -3.029539000 | 0.556301000 |
| C | -4.594840000 | -2.429792000 | 0.832853000 |
| H | -5.430025000 | -1.153254000 | -0.700339000 |
| C | -3.444903000 | -3.091048000 | 1.285912000 |
| H | -1.367173000 | -3.533188000 | 0.926210000 |
| H | -5.524692000 | -2.496005000 | 1.401962000 |
| H | -3.476059000 | -3.667709000 | 2.212673000 |
| C | 0.194616000 | -2.938733000 | -1.407626000 |
| C | 1.887806000 | -1.529322000 | -1.185312000 |
| H | 0.380779000 | -3.592153000 | -0.554951000 |
| H | 0.700079000 | -3.190065000 | -2.342567000 |
| H | 2.528351000 | -2.110033000 | -0.503762000 |
| H | -3.299613000 | -0.993218000 | -1.976352000 |
| H | -1.248519000 | -1.822194000 | -2.519428000 |
| H | 2.245943000 | -1.382539000 | -2.216212000 |

# Ru-Vs



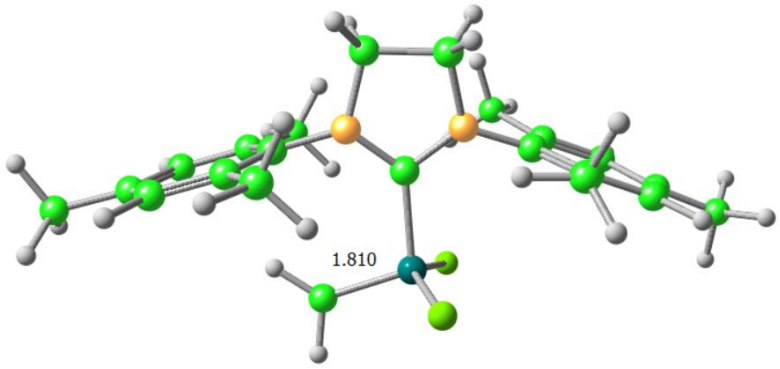

Zero-point correction= 0.568552 (Hartree/Particle)
Thermal correction to Energy= 0.606854
Thermal correction to Enthalpy= 0.607798
Thermal correction to Gibbs Free Energy= 0.497332
Sum of electronic and zero-point Energies= -2289.975253
Sum of electronic and thermal Energies= -2289.936952
Sum of electronic and thermal Enthalpies= -2289.936008
Sum of electronic and thermal Free Energies= -2290.046474

HOMO -0.15757 LUMO -0.09886

| | | | |
|---|---|---|---|
| Ru | -0.328903000 | -1.057938000 | 0.328535000 |
| Cl | -0.521192000 | -1.640268000 | -2.020612000 |
| Cl | -0.116878000 | -0.394310000 | 2.660194000 |
| N | -1.794616000 | 1.473053000 | -0.497735000 |
| N | 0.374260000 | 1.783587000 | -0.447266000 |
| C | -0.603161000 | 0.876953000 | -0.225468000 |
| C | -1.656367000 | 2.901949000 | -0.856803000 |
| H | -2.080527000 | 3.530704000 | -0.057242000 |
| H | -2.196357000 | 3.115039000 | -1.789683000 |
| C | -0.137951000 | 3.062892000 | -0.993429000 |
| H | 0.186875000 | 3.173219000 | -2.040309000 |
| H | 0.263532000 | 3.906834000 | -0.415397000 |
| C | -3.104022000 | 0.933671000 | -0.298170000 |
| C | -3.819175000 | 0.442048000 | -1.412404000 |
| C | -3.208631000 | 0.446520000 | -2.785731000 |
| H | -3.874501000 | -0.044727000 | -3.507773000 |
| H | -2.241234000 | -0.080101000 | -2.782777000 |
| H | -3.029942000 | 1.475025000 | -3.141105000 |
| C | -5.105833000 | -0.061489000 | -1.195801000 |
| H | -5.658825000 | -0.471059000 | -2.045828000 |
| C | -5.701793000 | -0.052528000 | 0.074847000 |
| C | -7.094789000 | -0.597927000 | 0.271576000 |
| H | -7.849300000 | 0.083197000 | -0.155101000 |
| H | -7.327192000 | -0.727951000 | 1.337654000 |
| H | -7.216738000 | -1.570940000 | -0.227749000 |
| C | -4.988635000 | 0.503812000 | 1.143036000 |
| H | -5.448127000 | 0.541973000 | 2.134527000 |
| C | -3.695978000 | 1.022161000 | 0.980692000 |
| C | -2.960896000 | 1.639375000 | 2.137309000 |
| H | -3.595600000 | 1.656692000 | 3.033324000 |
| H | -2.662165000 | 2.676528000 | 1.915846000 |
| H | -2.039630000 | 1.081706000 | 2.375316000 |
| C | 1.794263000 | 1.654045000 | -0.279873000 |
| C | 2.369629000 | 2.149775000 | 0.906927000 |
| C | 1.515021000 | 2.632597000 | 2.046141000 |
| H | 2.136605000 | 3.077330000 | 2.834994000 |
| H | 0.936128000 | 1.798621000 | 2.475744000 |
| H | 0.787804000 | 3.392679000 | 1.717821000 |
| C | 3.767815000 | 2.199358000 | 0.989089000 |
| H | 4.226438000 | 2.581284000 | 1.905526000 |
| C | 4.584048000 | 1.808666000 | -0.078161000 |
| C | 6.086433000 | 1.864097000 | 0.032478000 |
| H | 6.547400000 | 2.194135000 | -0.910299000 |
| H | 6.500056000 | 0.867607000 | 0.263251000 |
| H | 6.407203000 | 2.547234000 | 0.831602000 |
| C | 3.974408000 | 1.334299000 | -1.245899000 |
| H | 4.596697000 | 1.027678000 | -2.090748000 |
| C | 2.583553000 | 1.249284000 | -1.375756000 |
| C | 1.961918000 | 0.777020000 | -2.660272000 |
| H | 1.311559000 | 1.548436000 | -3.104370000 |
| H | 1.327448000 | -0.109940000 | -2.506580000 |
| H | 2.739284000 | 0.529726000 | -3.395624000 |
| C | 0.954196000 | -2.767459000 | 1.127572000 |
| C | 3.142279000 | -1.635762000 | 1.324411000 |
| C | 2.224645000 | -2.337831000 | 0.513932000 |
| C | 4.411401000 | -1.320367000 | 0.846865000 |

| | | | |
|---|---|---|---|
| C | 2.586409000 | -2.647787000 | -0.813200000 |
| C | 4.774465000 | -1.670329000 | -0.457817000 |
| H | 5.115047000 | -0.789920000 | 1.490205000 |
| C | 3.852238000 | -2.314389000 | -1.290994000 |
| H | 1.871799000 | -3.148934000 | -1.466181000 |
| H | 5.770840000 | -1.426649000 | -0.832654000 |
| H | 4.124934000 | -2.565880000 | -2.317840000 |
| C | -0.076813000 | -3.427968000 | 0.485669000 |
| C | -2.087755000 | -1.446507000 | 0.627167000 |
| H | -0.038172000 | -3.709924000 | -0.565511000 |
| H | -0.872918000 | -3.872367000 | 1.082866000 |
| H | -2.736267000 | -1.837223000 | -0.173726000 |
| H | 2.838409000 | -1.352643000 | 2.334219000 |
| H | 0.918476000 | -2.673583000 | 2.214426000 |
| H | -2.523126000 | -1.392253000 | 1.638150000 |

# Ru-VIs



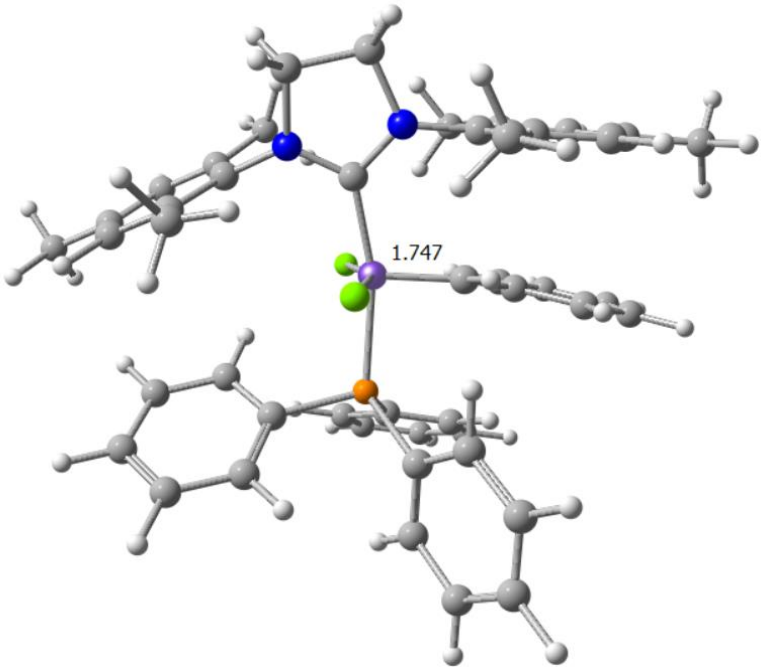

Zero-point correction= 0.435869 (Hartree/Particle)
Thermal correction to Energy= 0.467654
Thermal correction to Enthalpy= 0.468598
Thermal correction to Gibbs Free Energy= 0.370159
Sum of electronic and zero-point Energies= -1980.311308
Sum of electronic and thermal Energies= -1980.279523
Sum of electronic and thermal Enthalpies= -1980.278579
Sum of electronic and thermal Free Energies= -1980.377017

HOMO -0.17438 LUMO -0.09416

| | | | |
|---|---|---|---|
| Ru | -0.103097000 | 0.400806000 | -1.327125000 |
| Cl | -1.119323000 | -1.520722000 | -2.126155000 |
| Cl | -0.322772000 | 2.691586000 | -1.047452000 |
| N | 1.214538000 | -0.060251000 | 1.323008000 |
| N | -0.984637000 | -0.067490000 | 1.385965000 |
| C | 0.093738000 | 0.026076000 | 0.548400000 |
| C | 0.904721000 | -0.356778000 | 2.736389000 |
| H | 1.495148000 | 0.290599000 | 3.399418000 |
| H | 1.150020000 | -1.408001000 | 2.966902000 |
| C | -0.603376000 | -0.077912000 | 2.809007000 |
| H | -1.161421000 | -0.853786000 | 3.351415000 |
| H | -0.827168000 | 0.900379000 | 3.267358000 |
| C | 2.558274000 | -0.182917000 | 0.858427000 |
| C | 3.027989000 | -1.440929000 | 0.437754000 |
| C | 2.102705000 | -2.628120000 | 0.374305000 |
| H | 2.650665000 | -3.535362000 | 0.087670000 |
| H | 1.306933000 | -2.455940000 | -0.368828000 |
| H | 1.605895000 | -2.821108000 | 1.337232000 |
| C | 4.352051000 | -1.530735000 | -0.010641000 |
| H | 4.728693000 | -2.498137000 | -0.354416000 |
| C | 5.194695000 | -0.410084000 | -0.050421000 |
| C | 6.626157000 | -0.537975000 | -0.509860000 |
| H | 7.297521000 | -0.715377000 | 0.346775000 |
| H | 6.970236000 | 0.378077000 | -1.011325000 |
| H | 6.751104000 | -1.379941000 | -1.205528000 |
| C | 4.683062000 | 0.828816000 | 0.362081000 |
| H | 5.321089000 | 1.715671000 | 0.313645000 |
| C | 3.366791000 | 0.966554000 | 0.821236000 |
| C | 2.799359000 | 2.309374000 | 1.195627000 |
| H | 3.573747000 | 3.086855000 | 1.152596000 |
| H | 2.374990000 | 2.303643000 | 2.211794000 |
| H | 1.981773000 | 2.588463000 | 0.511479000 |
| C | -2.352210000 | -0.136710000 | 0.967302000 |
| C | -3.134829000 | 1.029354000 | 0.885292000 |
| C | -2.627383000 | 2.368045000 | 1.352514000 |
| H | -2.980130000 | 3.173670000 | 0.694508000 |
| H | -1.532903000 | 2.413340000 | 1.362742000 |
| H | -3.001988000 | 2.577132000 | 2.369138000 |
| C | -4.451078000 | 0.901921000 | 0.415200000 |
| H | -5.062751000 | 1.803406000 | 0.318015000 |
| C | -4.999940000 | -0.339273000 | 0.078786000 |
| C | -6.397193000 | -0.444242000 | -0.479537000 |
| H | -6.914295000 | -1.339548000 | -0.103783000 |
| H | -6.370008000 | -0.519431000 | -1.579138000 |
| H | -7.000925000 | 0.437689000 | -0.222563000 |
| C | -4.216052000 | -1.489704000 | 0.260258000 |
| H | -4.641783000 | -2.471417000 | 0.035629000 |
| C | -2.896902000 | -1.413614000 | 0.710025000 |
| C | -2.075131000 | -2.656848000 | 0.923787000 |
| H | -1.695838000 | -2.716954000 | 1.956803000 |
| H | -1.210899000 | -2.672833000 | 0.245548000 |
| H | -2.675697000 | -3.555345000 | 0.729537000 |
| C | 1.572392000 | 0.247556000 | -1.994306000 |
| H | 2.500650000 | -0.068450000 | -1.507945000 |

| | | | | |
|---|---|---|---|---|
| | H | 1.642904000 | 0.505592000 | -3.072409000 |

# Fe-I



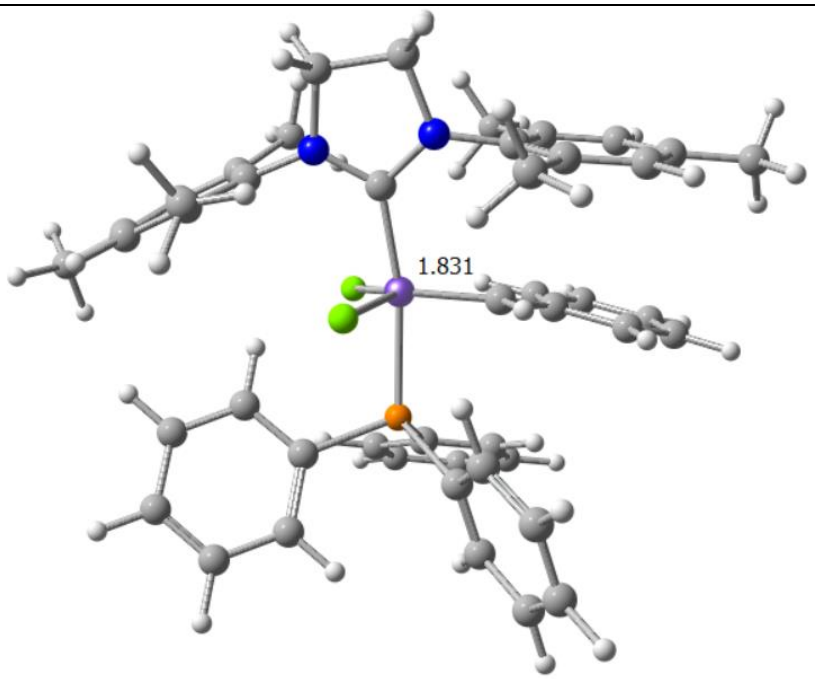

Zero-point correction= 0.783700 (Hartree/Particle)
Thermal correction to Energy= 0.836367
Thermal correction to Enthalpy= 0.837311
Thermal correction to Gibbs Free Energy= 0.695621
Sum of electronic and zero-point Energies= -3276.780768
Sum of electronic and thermal Energies= -3276.728101
Sum of electronic and thermal Enthalpies= -3276.727156
Sum of electronic and thermal Free Energies= -3276.868847

HOMO -0.14028 LUMO -0.09888

| | | | |
|---|---|---|---|
| Fe | -0.087142000 | -0.315704000 | -0.218941000 |
| Cl | -0.620307000 | -0.333176000 | 2.002531000 |
| Cl | -0.423931000 | -0.277070000 | -2.504745000 |
| P | -0.479650000 | 1.922315000 | -0.215725000 |
| N | -1.389104000 | -2.940998000 | -0.408813000 |
| N | 0.779707000 | -3.088134000 | -0.679862000 |
| C | -0.231762000 | -2.235159000 | -0.376177000 |
| C | -1.200694000 | -4.324758000 | -0.902635000 |
| H | -1.594078000 | -4.405081000 | -1.929202000 |
| H | -1.740802000 | -5.036157000 | -0.262593000 |
| C | 0.323728000 | -4.487681000 | -0.845400000 |
| H | 0.658271000 | -5.093670000 | 0.013957000 |
| H | 0.743387000 | -4.923179000 | -1.762472000 |
| C | -2.683642000 | -2.521098000 | 0.046694000 |
| C | -3.005721000 | -2.759488000 | 1.403732000 |
| C | -2.014460000 | -3.399360000 | 2.337684000 |
| H | -2.491331000 | -3.648414000 | 3.295402000 |
| H | -1.180800000 | -2.707931000 | 2.530481000 |
| H | -1.591950000 | -4.324454000 | 1.914884000 |
| C | -4.273056000 | -2.391250000 | 1.859227000 |
| H | -4.521974000 | -2.554882000 | 2.911721000 |
| C | -5.232287000 | -1.831660000 | 1.000322000 |
| C | -6.589817000 | -1.431140000 | 1.524170000 |
| H | -7.210743000 | -0.991970000 | 0.730589000 |
| H | -6.502317000 | -0.692322000 | 2.337237000 |
| H | -7.131755000 | -2.297628000 | 1.935592000 |
| C | -4.899544000 | -1.665268000 | -0.344570000 |
| H | -5.637112000 | -1.244131000 | -1.033145000 |
| C | -3.637822000 | -2.016705000 | -0.852393000 |
| C | -3.379516000 | -1.891340000 | -2.329259000 |
| H | -3.752415000 | -0.927708000 | -2.705830000 |
| H | -3.910400000 | -2.688967000 | -2.876211000 |
| H | -2.311745000 | -1.936467000 | -2.568598000 |
| C | 2.179189000 | -2.825073000 | -0.543688000 |
| C | 2.957049000 | -2.630260000 | -1.699674000 |
| C | 2.320017000 | -2.625935000 | -3.062785000 |
| H | 3.046406000 | -2.327663000 | -3.831197000 |
| H | 1.460211000 | -1.936681000 | -3.095173000 |
| H | 1.940995000 | -3.625530000 | -3.333650000 |
| C | 4.331122000 | -2.404966000 | -1.536953000 |
| H | 4.944501000 | -2.230920000 | -2.425579000 |
| C | 4.933665000 | -2.388758000 | -0.272594000 |
| C | 6.407487000 | -2.113416000 | -0.115192000 |
| H | 6.909371000 | -2.922522000 | 0.438158000 |
| H | 6.567036000 | -1.181772000 | 0.450799000 |
| H | 6.902843000 | -2.008879000 | -1.090633000 |
| C | 4.130509000 | -2.612384000 | 0.854471000 |
| H | 4.580652000 | -2.583703000 | 1.850324000 |
| C | 2.755643000 | -2.836560000 | 0.744202000 |
| C | 1.899564000 | -3.021070000 | 1.965058000 |
| H | 1.312768000 | -3.952127000 | 1.918560000 |
| H | 1.176290000 | -2.194379000 | 2.060293000 |
| H | 2.516421000 | -3.049400000 | 2.872873000 |
| C | 1.635371000 | -0.047576000 | -0.337001000 |
| C | 3.919757000 | 0.770700000 | -0.033750000 |
| C | 2.696343000 | 0.373015000 | 0.561093000 |
| C | 4.994874000 | 1.195920000 | 0.743621000 |
| C | 2.596517000 | 0.412839000 | 1.969928000 |
| C | 4.883080000 | 1.205728000 | 2.139792000 |
| H | 5.923498000 | 1.513359000 | 0.264168000 |
| C | 3.682699000 | 0.809891000 | 2.744733000 |
| H | 1.649590000 | 0.137438000 | 2.433407000 |
| H | 5.726912000 | 1.528245000 | 2.754026000 |
| H | 3.587701000 | 0.831431000 | 3.832405000 |
| C | -2.288709000 | 2.106187000 | -0.524819000 |
| C | -2.773286000 | 2.813985000 | -1.635790000 |
| C | -3.193319000 | 1.441503000 | 0.322883000 |
| C | -4.148334000 | 2.893303000 | -1.870558000 |
| H | -2.075430000 | 3.295301000 | -2.321173000 |
| C | -4.567257000 | 1.550552000 | 0.097018000 |
| H | -2.820741000 | 0.821147000 | 1.141676000 |
| C | -5.049487000 | 2.277149000 | -0.995524000 |
| H | -4.515673000 | 3.443248000 | -2.739751000 |
| H | -5.260219000 | 1.046485000 | 0.771041000 |
| H | -6.124485000 | 2.351016000 | -1.174035000 |
| C | 0.326624000 | 3.069245000 | -1.420234000 |
| C | 0.098228000 | 4.451341000 | -1.290518000 |
| C | 1.199032000 | 2.604532000 | -2.411103000 |
| C | 0.731780000 | 5.353189000 | -2.146926000 |
| H | -0.567161000 | 4.818863000 | -0.506932000 |
| C | 1.838191000 | 3.511765000 | -3.263194000 |
| H | 1.346589000 | 1.532053000 | -2.532537000 |
| C | 1.606875000 | 4.884045000 | -3.134528000 |
| H | 0.548368000 | 6.424211000 | -2.038263000 |

| | | | | |
|---|---|---|---|---|
| H | 2.516198000 | 3.140025000 | -4.034430000 |
| H | 2.107061000 | 5.589633000 | -3.801502000 |
| C | -0.120048000 | 2.832221000 | 1.351387000 |
| C | -1.079677000 | 3.046225000 | 2.348869000 |
| C | 1.205673000 | 3.244347000 | 1.567378000 |
| C | -0.719078000 | 3.671437000 | 3.545711000 |
| H | -2.110757000 | 2.731615000 | 2.190336000 |
| C | 1.563879000 | 3.861563000 | 2.767272000 |
| H | 1.959626000 | 3.088034000 | 0.794546000 |
| C | 0.602870000 | 4.075055000 | 3.760840000 |
| H | -1.475446000 | 3.837939000 | 4.315698000 |
| H | 2.599478000 | 4.169397000 | 2.924545000 |
| H | 0.882439000 | 4.557877000 | 4.699715000 |
| H | 4.004446000 | 0.740722000 | -1.122017000 |
| H | 2.001036000 | -0.128797000 | -1.375720000 |

# Fe-It



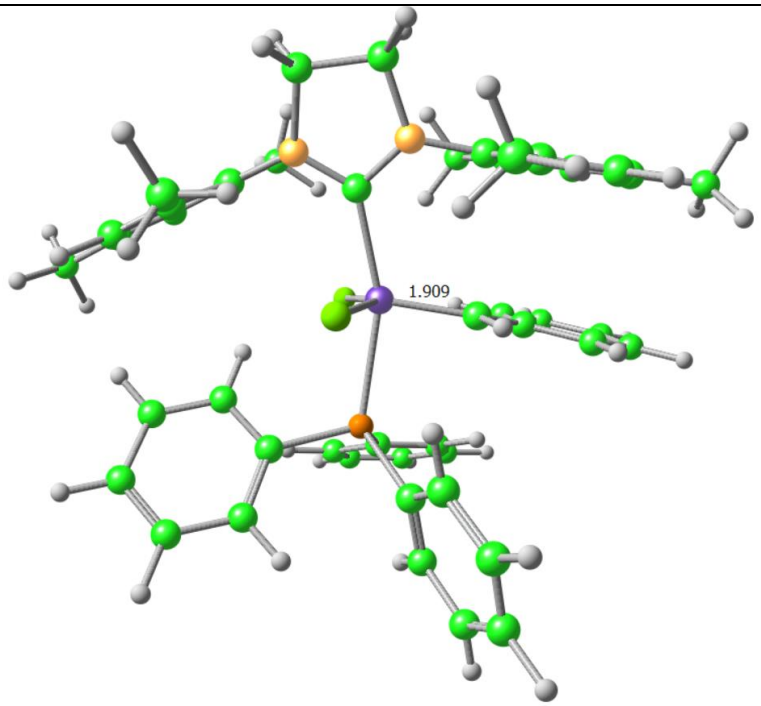

Zero-point correction= 0.782279 (Hartree/Particle)
Thermal correction to Energy= 0.835490
Thermal correction to Enthalpy= 0.836435
Thermal correction to Gibbs Free Energy= 0.692352
Sum of electronic and zero-point Energies= -3276.774042
Sum of electronic and thermal Energies= -3276.720831
Sum of electronic and thermal Enthalpies= -3276.719887
Sum of electronic and thermal Free Energies= -3276.863969

HOMO -0.14389 LUMO -0.11407

| | | | |
|---|---|---|---|
| Fe | -0.138346000 | -0.342779000 | -0.202659000 |
| Cl | -1.100112000 | -0.183356000 | 1.924496000 |
| Cl | -1.033920000 | -0.249458000 | -2.389122000 |
| P | -0.318011000 | 1.954577000 | -0.238711000 |
| N | -1.490132000 | -3.000056000 | -0.324778000 |
| N | 0.669478000 | -3.135077000 | -0.648652000 |
| C | -0.338490000 | -2.284556000 | -0.324879000 |
| C | -1.303570000 | -4.401278000 | -0.767246000 |
| H | -1.772002000 | -4.542102000 | -1.754294000 |
| H | -1.779490000 | -5.090642000 | -0.055492000 |
| C | 0.224544000 | -4.537975000 | -0.815731000 |
| H | 0.626265000 | -5.158289000 | 0.002717000 |
| H | 0.590120000 | -4.944982000 | -1.769059000 |
| C | -2.794141000 | -2.557285000 | 0.079326000 |
| C | -3.123585000 | -2.648385000 | 1.449556000 |
| C | -2.164937000 | -3.258122000 | 2.437394000 |
| H | -2.617738000 | -3.299570000 | 3.437136000 |
| H | -1.248196000 | -2.656491000 | 2.502054000 |
| H | -1.886726000 | -4.284630000 | 2.147404000 |
| C | -4.370994000 | -2.176495000 | 1.863105000 |
| H | -4.620379000 | -2.210464000 | 2.927196000 |
| C | -5.301288000 | -1.655439000 | 0.950926000 |
| C | -6.608445000 | -1.075993000 | 1.432480000 |
| H | -7.335706000 | -0.988005000 | 0.612701000 |
| H | -6.456130000 | -0.068667000 | 1.854935000 |
| H | -7.056468000 | -1.694365000 | 2.224885000 |
| C | -4.982725000 | -1.685617000 | -0.409254000 |
| H | -5.718054000 | -1.341309000 | -1.142380000 |
| C | -3.744362000 | -2.157467000 | -0.875502000 |
| C | -3.518284000 | -2.295771000 | -2.357555000 |
| H | -3.876463000 | -1.405570000 | -2.892298000 |
| H | -4.078955000 | -3.167594000 | -2.737400000 |
| H | -2.457462000 | -2.407058000 | -2.603347000 |
| C | 2.067704000 | -2.868840000 | -0.536960000 |
| C | 2.810779000 | -2.606605000 | -1.702275000 |
| C | 2.116779000 | -2.482526000 | -3.032483000 |
| H | 2.805249000 | -2.099200000 | -3.797897000 |
| H | 1.244924000 | -1.811424000 | -2.964622000 |
| H | 1.738577000 | -3.457245000 | -3.382451000 |
| C | 4.194250000 | -2.422631000 | -1.570102000 |
| H | 4.784813000 | -2.199703000 | -2.463254000 |
| C | 4.833597000 | -2.502136000 | -0.326287000 |
| C | 6.319569000 | -2.282625000 | -0.199448000 |
| H | 6.822273000 | -3.174837000 | 0.206333000 |
| H | 6.530654000 | -1.447150000 | 0.486506000 |
| H | 6.775375000 | -2.049899000 | -1.171936000 |
| C | 4.057929000 | -2.764938000 | 0.813640000 |
| H | 4.538117000 | -2.792577000 | 1.795414000 |
| C | 2.677172000 | -2.953627000 | 0.732264000 |
| C | 1.837268000 | -3.158990000 | 1.962630000 |
| H | 1.277950000 | -4.107473000 | 1.927512000 |
| H | 1.089750000 | -2.354600000 | 2.058681000 |
| H | 2.461033000 | -3.162292000 | 2.865890000 |
| C | 1.667995000 | -0.107569000 | -0.384937000 |
| C | 3.979354000 | 0.634734000 | 0.091997000 |
| C | 2.702096000 | 0.230874000 | 0.555126000 |
| C | 4.990785000 | 0.968928000 | 0.989864000 |
| C | 2.475651000 | 0.180750000 | 1.953042000 |
| C | 4.755551000 | 0.883121000 | 2.369012000 |
| H | 5.965850000 | 1.293417000 | 0.619988000 |
| C | 3.496207000 | 0.489490000 | 2.845013000 |
| H | 1.475381000 | -0.079804000 | 2.306824000 |
| H | 5.550790000 | 1.136785000 | 3.073651000 |
| H | 3.306865000 | 0.449838000 | 3.919467000 |
| C | -2.072945000 | 2.450939000 | -0.562619000 |
| C | -2.380689000 | 3.706200000 | -1.106631000 |
| C | -3.108046000 | 1.554005000 | -0.254874000 |
| C | -3.713267000 | 4.069566000 | -1.322643000 |
| H | -1.581299000 | 4.398402000 | -1.374692000 |
| C | -4.437206000 | 1.923227000 | -0.471384000 |

| | | | |
|---|---|---|---|
| H | -2.878519000 | 0.572218000 | 0.159436000 |
| C | -4.744448000 | 3.179407000 | -1.004091000 |
| H | -3.943975000 | 5.048062000 | -1.749626000 |
| H | -5.230271000 | 1.212339000 | -0.232787000 |
| H | -5.785020000 | 3.463456000 | -1.176565000 |
| C | 0.670857000 | 2.923060000 | -1.471917000 |
| C | 0.990613000 | 4.272439000 | -1.237653000 |
| C | 1.106728000 | 2.313421000 | -2.658806000 |
| C | 1.739445000 | 4.994824000 | -2.170817000 |
| H | 0.665802000 | 4.756105000 | -0.315665000 |
| C | 1.858380000 | 3.038745000 | -3.587388000 |
| H | 0.815745000 | 1.281803000 | -2.864109000 |
| C | 2.179953000 | 4.378400000 | -3.346556000 |
| H | 1.981451000 | 6.041628000 | -1.974525000 |
| H | 2.188286000 | 2.552839000 | -4.508311000 |
| H | 2.767569000 | 4.942473000 | -4.074209000 |
| C | 0.098520000 | 2.818617000 | 1.336638000 |
| C | -0.904312000 | 3.103419000 | 2.275402000 |
| C | 1.437144000 | 3.109101000 | 1.645958000 |
| C | -0.571678000 | 3.683161000 | 3.501881000 |
| H | -1.942705000 | 2.865849000 | 2.044534000 |
| C | 1.765858000 | 3.688753000 | 2.873630000 |
| H | 2.225304000 | 2.892482000 | 0.924541000 |
| C | 0.762889000 | 3.975462000 | 3.805097000 |
| H | -1.359154000 | 3.901570000 | 4.226172000 |
| H | 2.810954000 | 3.907749000 | 3.101565000 |
| H | 1.019977000 | 4.427234000 | 4.765714000 |
| H | 4.152716000 | 0.686599000 | -0.984664000 |
| H | 1.998028000 | -0.052178000 | -1.434866000 |

# Fe-Iq



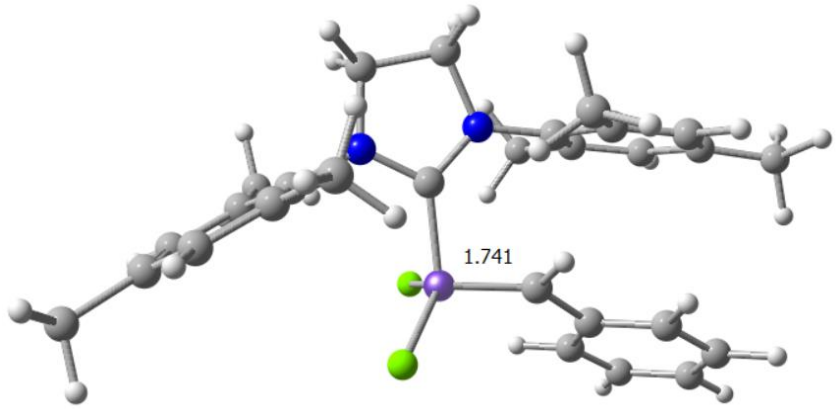

Zero-point correction= 0.780249 (Hartree/Particle)
Thermal correction to Energy= 0.834485
Thermal correction to Enthalpy= 0.835429
Thermal correction to Gibbs Free Energy= 0.686013
Sum of electronic and zero-point Energies= -3276.755559
Sum of electronic and thermal Energies= -3276.701324
Sum of electronic and thermal Enthalpies= -3276.700379
Sum of electronic and thermal Free Energies= -3276.849795

HOMO -0.20422 LUMO -0.09114

| | | | |
|---|---|---|---|
| Fe | 0.037615000 | -0.342269000 | -0.190020000 |
| Cl | -0.677282000 | -0.266494000 | 2.033146000 |
| Cl | -0.754840000 | -0.350681000 | -2.410050000 |
| P | -0.601955000 | 2.105279000 | -0.250673000 |
| N | -1.252766000 | -3.278504000 | -0.308115000 |
| N | 0.900564000 | -3.257310000 | -0.637548000 |
| C | -0.159926000 | -2.497559000 | -0.299475000 |
| C | -0.977946000 | -4.672350000 | -0.750099000 |
| H | -1.452044000 | -4.849225000 | -1.728126000 |
| H | -1.390270000 | -5.389961000 | -0.026608000 |
| C | 0.557772000 | -4.694128000 | -0.823123000 |
| H | 1.018947000 | -5.290546000 | -0.019042000 |
| H | 0.938563000 | -5.059082000 | -1.786973000 |
| C | -2.564728000 | -2.884543000 | 0.116163000 |
| C | -2.857584000 | -2.944514000 | 1.495523000 |
| C | -1.835257000 | -3.439395000 | 2.483193000 |
| H | -2.278272000 | -3.531390000 | 3.483953000 |
| H | -0.991798000 | -2.736720000 | 2.545294000 |
| H | -1.436164000 | -4.424644000 | 2.193452000 |
| C | -4.126119000 | -2.540378000 | 1.919089000 |
| H | -4.355724000 | -2.560816000 | 2.988150000 |
| C | -5.107279000 | -2.117861000 | 1.009049000 |
| C | -6.458965000 | -1.658886000 | 1.499993000 |
| H | -7.142993000 | -1.460164000 | 0.662859000 |
| H | -6.372402000 | -0.734451000 | 2.094295000 |
| H | -6.927452000 | -2.415204000 | 2.148929000 |
| C | -4.800447000 | -2.133079000 | -0.354459000 |
| H | -5.559396000 | -1.827243000 | -1.079984000 |
| C | -3.539332000 | -2.527067000 | -0.829461000 |
| C | -3.283297000 | -2.604287000 | -2.310635000 |
| H | -3.813956000 | -1.800539000 | -2.839065000 |
| H | -3.648229000 | -3.565464000 | -2.712562000 |
| H | -2.218017000 | -2.498911000 | -2.545245000 |
| C | 2.274535000 | -2.860265000 | -0.552471000 |
| C | 2.977917000 | -2.562782000 | -1.734635000 |
| C | 2.270615000 | -2.551291000 | -3.063560000 |
| H | 2.951819000 | -2.231047000 | -3.863682000 |
| H | 1.403040000 | -1.871858000 | -3.042197000 |
| H | 1.886896000 | -3.549592000 | -3.330082000 |
| C | 4.334270000 | -2.230518000 | -1.625802000 |
| H | 4.889801000 | -1.981316000 | -2.534688000 |
| C | 4.989772000 | -2.194893000 | -0.387366000 |
| C | 6.456759000 | -1.856793000 | -0.300094000 |
| H | 7.077734000 | -2.762378000 | -0.402800000 |
| H | 6.699842000 | -1.392634000 | 0.665951000 |
| H | 6.754641000 | -1.161523000 | -1.098415000 |
| C | 4.253034000 | -2.485294000 | 0.767840000 |
| H | 4.738891000 | -2.421821000 | 1.744963000 |
| C | 2.895678000 | -2.820028000 | 0.710171000 |
| C | 2.100350000 | -3.052396000 | 1.965619000 |
| H | 1.547753000 | -4.004370000 | 1.935532000 |
| H | 1.351250000 | -2.254958000 | 2.102079000 |
| H | 2.756306000 | -3.062545000 | 2.846103000 |
| C | 1.869043000 | 0.155976000 | -0.396328000 |
| C | 4.179154000 | 0.986023000 | -0.035287000 |
| C | 2.928698000 | 0.551413000 | 0.482439000 |

| | | | |
|---|---|---|---|
| C | 5.227289000 | 1.329444000 | 0.812704000 |
| C | 2.775368000 | 0.490024000 | 1.893402000 |
| C | 5.055514000 | 1.247229000 | 2.202426000 |
| H | 6.181840000 | 1.661774000 | 0.399059000 |
| C | 3.826181000 | 0.831968000 | 2.736784000 |
| H | 1.805881000 | 0.186225000 | 2.293608000 |
| H | 5.877876000 | 1.516275000 | 2.869292000 |
| H | 3.690343000 | 0.784841000 | 3.819302000 |
| C | -2.411802000 | 2.272857000 | -0.556021000 |
| C | -2.946230000 | 3.295364000 | -1.353460000 |
| C | -3.265817000 | 1.306991000 | 0.004234000 |
| C | -4.325605000 | 3.364686000 | -1.571155000 |
| H | -2.284394000 | 4.032261000 | -1.811536000 |
| C | -4.643592000 | 1.390548000 | -0.206647000 |
| H | -2.849843000 | 0.494501000 | 0.604980000 |
| C | -5.177054000 | 2.416347000 | -0.994656000 |
| H | -4.734436000 | 4.161173000 | -2.196961000 |
| H | -5.296555000 | 0.635803000 | 0.232642000 |
| H | -6.254361000 | 2.471955000 | -1.166151000 |
| C | 0.182277000 | 3.258342000 | -1.465142000 |
| C | 0.277394000 | 4.635567000 | -1.198059000 |
| C | 0.694042000 | 2.753123000 | -2.670555000 |
| C | 0.877831000 | 5.492654000 | -2.124369000 |
| H | -0.111247000 | 5.033313000 | -0.259142000 |
| C | 1.292091000 | 3.615245000 | -3.594416000 |
| H | 0.597920000 | 1.687137000 | -2.886010000 |
| C | 1.388123000 | 4.984333000 | -3.324195000 |
| H | 0.947470000 | 6.560739000 | -1.906622000 |
| H | 1.684556000 | 3.212524000 | -4.530826000 |
| H | 1.858169000 | 5.655097000 | -4.046744000 |
| C | -0.307849000 | 2.978261000 | 1.341128000 |
| C | -1.343397000 | 3.268181000 | 2.240154000 |
| C | 1.021920000 | 3.257280000 | 1.701482000 |
| C | -1.051642000 | 3.839292000 | 3.481955000 |
| H | -2.375785000 | 3.042124000 | 1.969443000 |
| C | 1.308435000 | 3.826708000 | 2.942869000 |
| H | 1.833240000 | 3.027060000 | 1.009477000 |
| C | 0.272308000 | 4.118754000 | 3.837610000 |
| H | -1.864170000 | 4.064090000 | 4.176316000 |
| H | 2.345843000 | 4.034306000 | 3.213476000 |
| H | 0.496658000 | 4.560468000 | 4.810837000 |
| H | 4.301864000 | 1.040049000 | -1.119257000 |
| H | 2.146949000 | 0.285698000 | -1.457397000 |

# Fe-II



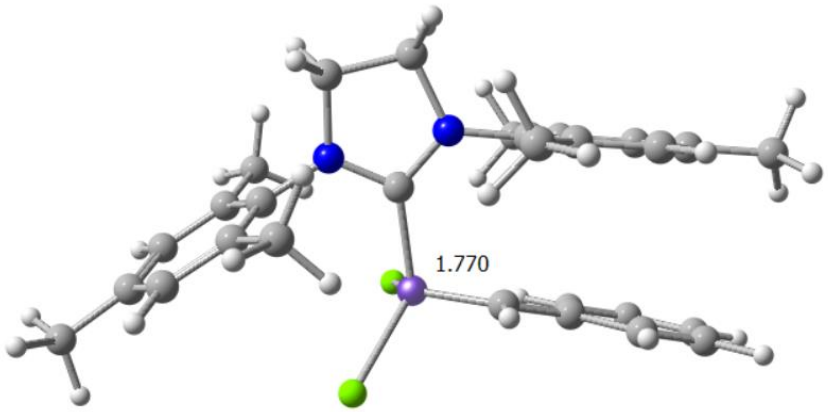

Zero-point correction= 0.515376 (Hartree/Particle)
Thermal correction to Energy= 0.552002
Thermal correction to Enthalpy= 0.552947
Thermal correction to Gibbs Free Energy= 0.442430
Sum of electronic and zero-point Energies= -2240.359671
Sum of electronic and thermal Energies= -2240.323044
Sum of electronic and thermal Enthalpies= -2240.322099
Sum of electronic and thermal Free Energies= -2240.432616

HOMO -0.15759 LUMO -0.11765

| | | | |
|---|---|---|---|
| Fe | 0.439586000 | -0.995542000 | -0.141878000 |
| Cl | 0.377217000 | -1.590162000 | 1.968086000 |
| Cl | 1.515257000 | -1.801854000 | -1.846410000 |
| N | 1.882328000 | 1.338073000 | 0.444411000 |
| N | -0.272000000 | 1.776696000 | 0.452075000 |
| C | 0.654102000 | 0.802950000 | 0.214291000 |
| C | 1.821848000 | 2.710722000 | 0.984274000 |
| H | 2.524724000 | 3.361771000 | 0.445834000 |
| H | 2.090926000 | 2.709669000 | 2.053095000 |
| C | 0.349074000 | 3.085734000 | 0.754087000 |
| H | -0.124906000 | 3.532918000 | 1.638728000 |
| H | 0.218718000 | 3.775416000 | -0.096603000 |
| C | 3.130532000 | 0.684439000 | 0.186330000 |
| C | 3.847008000 | 0.091954000 | 1.242211000 |
| C | 3.360113000 | 0.166063000 | 2.665173000 |
| H | 3.865513000 | -0.585271000 | 3.286732000 |
| H | 2.278006000 | -0.012749000 | 2.730481000 |
| H | 3.575177000 | 1.155463000 | 3.104034000 |
| C | 5.053322000 | -0.551137000 | 0.933212000 |
| H | 5.610623000 | -1.035965000 | 1.739713000 |
| C | 5.558191000 | -0.591510000 | -0.371883000 |
| C | 6.828375000 | -1.341512000 | -0.687501000 |
| H | 7.394430000 | -0.852048000 | -1.493595000 |
| H | 6.599125000 | -2.366494000 | -1.022925000 |
| H | 7.479773000 | -1.420187000 | 0.194661000 |
| C | 4.842646000 | 0.059610000 | -1.386375000 |
| H | 5.231906000 | 0.052430000 | -2.408119000 |
| C | 3.631150000 | 0.707623000 | -1.130368000 |
| C | 2.870594000 | 1.390963000 | -2.235431000 |
| H | 3.489389000 | 1.471948000 | -3.139125000 |
| H | 2.547785000 | 2.402651000 | -1.944630000 |
| H | 1.969834000 | 0.812035000 | -2.491194000 |
| C | -1.685222000 | 1.700479000 | 0.242410000 |
| C | -2.212856000 | 2.060403000 | -1.013328000 |
| C | -1.308345000 | 2.465963000 | -2.149089000 |
| H | -1.836921000 | 2.403088000 | -3.109738000 |
| H | -0.414934000 | 1.826353000 | -2.203853000 |
| H | -0.955849000 | 3.504631000 | -2.036006000 |
| C | -3.599200000 | 1.988258000 | -1.194945000 |
| H | -4.018152000 | 2.241448000 | -2.173124000 |
| C | -4.456530000 | 1.578227000 | -0.165517000 |
| C | -5.937670000 | 1.432451000 | -0.400969000 |

| | | | |
|---|---|---|---|
| H | -6.520401000 | 1.803148000 | 0.455253000 |
| H | -6.196738000 | 0.369414000 | -0.537698000 |
| H | -6.259903000 | 1.976077000 | -1.300218000 |
| C | -3.899958000 | 1.264560000 | 1.081404000 |
| H | -4.556309000 | 0.951959000 | 1.897981000 |
| C | -2.522077000 | 1.328782000 | 1.313736000 |
| C | -1.947495000 | 0.985350000 | 2.658053000 |
| H | -1.291490000 | 1.786517000 | 3.033762000 |
| H | -1.329552000 | 0.076492000 | 2.597489000 |
| H | -2.747313000 | 0.821301000 | 3.392322000 |
| C | -1.193908000 | -0.890176000 | -0.735260000 |
| C | -3.496611000 | -1.448654000 | -1.360143000 |
| C | -2.396293000 | -1.649087000 | -0.485501000 |
| C | -4.711597000 | -2.093220000 | -1.145437000 |
| C | -2.565419000 | -2.529533000 | 0.610572000 |
| C | -4.864694000 | -2.945303000 | -0.044220000 |
| H | -5.542655000 | -1.934581000 | -1.836184000 |
| C | -3.787947000 | -3.158287000 | 0.828614000 |
| H | -1.725517000 | -2.687809000 | 1.287387000 |
| H | -5.818663000 | -3.447522000 | 0.130571000 |
| H | -3.905803000 | -3.826785000 | 1.684105000 |
| H | -3.376717000 | -0.768503000 | -2.205365000 |
| H | -1.294485000 | -0.188506000 | -1.579228000 |

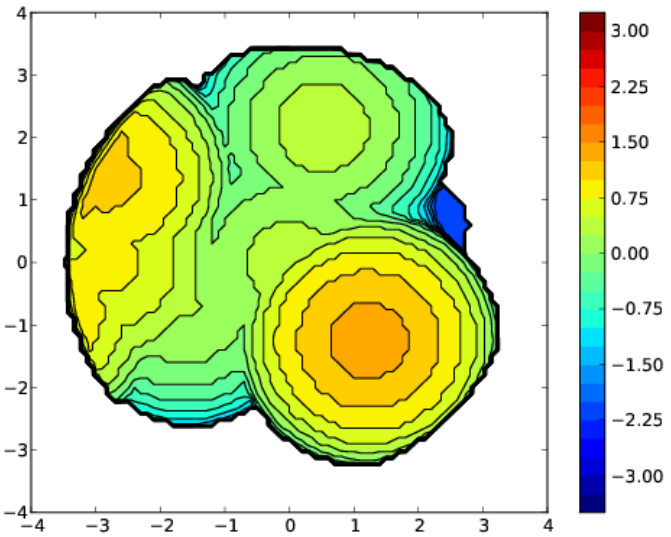
# Fe-IIt




Zero-point correction= 0.514763 (Hartree/Particle)
Thermal correction to Energy= 0.550537
Thermal correction to Enthalpy= 0.551482
Thermal correction to Gibbs Free Energy= 0.445401
Sum of electronic and zero-point Energies= -2240.368140
Sum of electronic and thermal Energies= -2240.332365
Sum of electronic and thermal Enthalpies= -2240.331420
Sum of electronic and thermal Free Energies= -2240.437501

HOMO -0.15637 LUMO -0.12198

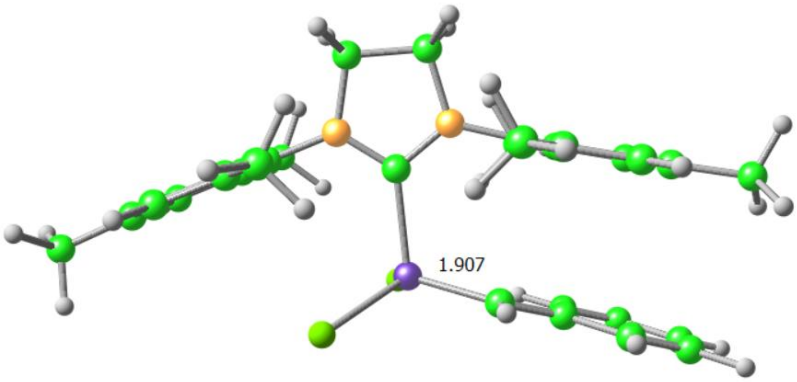
| | | | |
|---|---|---|---|
| Fe | 0.488411000 | -0.991805000 | -0.184944000 |
| Cl | 0.794215000 | -1.845311000 | 1.887587000 |
| Cl | 1.698068000 | -2.173876000 | -1.599652000 |
| N | 1.795482000 | 1.457960000 | 0.451894000 |
| N | -0.357346000 | 1.846289000 | 0.301252000 |
| C | 0.596139000 | 0.895644000 | 0.186198000 |
| C | 1.704481000 | 2.918156000 | 0.684824000 |
| H | 2.170493000 | 3.454348000 | -0.158053000 |
| H | 2.232809000 | 3.195286000 | 1.607286000 |
| C | 0.184618000 | 3.145633000 | 0.767796000 |
| H | -0.159035000 | 3.342378000 | 1.795894000 |
| H | -0.167818000 | 3.962830000 | 0.122600000 |
| C | 3.055337000 | 0.827405000 | 0.177432000 |
| C | 3.831784000 | 0.362200000 | 1.254403000 |
| C | 3.345624000 | 0.489986000 | 2.672237000 |
| H | 4.099392000 | 0.112347000 | 3.375981000 |
| H | 2.419572000 | -0.091767000 | 2.807871000 |
| H | 3.125991000 | 1.536091000 | 2.939660000 |
| C | 5.050909000 | -0.258631000 | 0.959070000 |
| H | 5.656899000 | -0.645910000 | 1.782746000 |
| C | 5.504537000 | -0.407555000 | -0.358211000 |
| C | 6.790412000 | -1.138210000 | -0.654031000 |
| H | 7.290257000 | -0.729081000 | -1.544112000 |
| H | 6.590423000 | -2.204602000 | -0.849988000 |
| H | 7.489824000 | -1.083360000 | 0.192536000 |
| C | 4.719643000 | 0.104174000 | -1.399502000 |
| H | 5.061503000 | -0.001077000 | -2.432634000 |
| C | 3.492060000 | 0.728404000 | -1.157012000 |
| C | 2.642136000 | 1.213281000 | -2.301868000 |
| H | 3.249739000 | 1.343478000 | -3.207600000 |
| H | 2.141685000 | 2.167863000 | -2.081369000 |
| H | 1.862114000 | 0.466218000 | -2.521997000 |
| C | -1.765949000 | 1.647400000 | 0.175857000 |
| C | -2.380153000 | 1.966251000 | -1.048819000 |
| C | -1.557346000 | 2.441999000 | -2.218249000 |
| H | -2.178316000 | 2.540647000 | -3.118585000 |
| H | -0.734881000 | 1.744028000 | -2.435981000 |
| H | -1.096886000 | 3.423720000 | -2.021154000 |
| C | -3.764871000 | 1.793248000 | -1.155745000 |
| H | -4.255426000 | 2.018098000 | -2.106851000 |
| C | -4.530602000 | 1.317550000 | -0.082776000 |
| C | -6.020361000 | 1.132310000 | -0.212696000 |
| H | -6.566499000 | 1.930226000 | 0.316650000 |
| H | -6.333348000 | 0.172010000 | 0.222864000 |
| H | -6.336729000 | 1.151521000 | -1.264936000 |
| C | -3.881391000 | 1.013196000 | 1.121688000 |
| H | -4.463052000 | 0.618629000 | 1.958761000 |
| C | -2.500921000 | 1.173270000 | 1.278156000 |
| C | -1.810936000 | 0.803781000 | 2.562636000 |
| H | -1.299058000 | 1.669349000 | 3.013432000 |
| H | -1.042842000 | 0.029668000 | 2.400209000 |
| H | -2.534556000 | 0.421610000 | 3.294372000 |
| C | -1.082141000 | -1.011906000 | -1.000154000 |
| C | -3.442842000 | -1.516076000 | -1.456753000 |
| C | -2.341848000 | -1.547922000 | -0.562284000 |
| C | -4.682510000 | -2.029816000 | -1.084111000 |
| C | -2.535272000 | -2.118641000 | 0.720831000 |
| C | -4.856029000 | -2.580554000 | 0.191099000 |
| H | -5.517112000 | -2.000390000 | -1.787482000 |
| C | -3.776992000 | -2.624628000 | 1.086994000 |
| H | -1.684614000 | -2.171645000 | 1.403673000 |
| H | -5.826376000 | -2.988352000 | 0.482517000 |




| South West | North West | North East | North West | **Total %V_Bur** |
|---|---|---|---|---|
| 49.3 | 58.4 | 45.4 | 65.6 | 54.7 |

| | | | |
|---|---|---|---|
| H | -3.908195000 | -3.067249000 | 2.076497000 |
| H | -3.302609000 | -1.082292000 | -2.448881000 |
| H | -1.042914000 | -0.690934000 | -2.054350000 |

# Fe-IIq



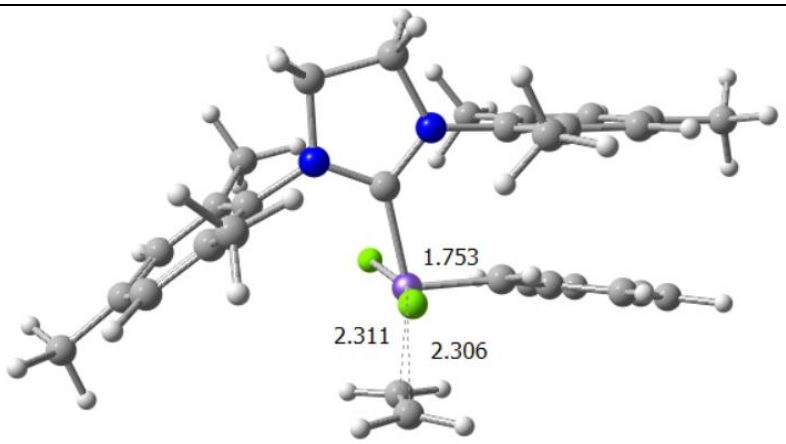

Zero-point correction= 0.513872 (Hartree/Particle)
Thermal correction to Energy= 0.549130
Thermal correction to Enthalpy= 0.550074
Thermal correction to Gibbs Free Energy= 0.445649
Sum of electronic and zero-point Energies= -2240.364328
Sum of electronic and thermal Energies= -2240.329070
Sum of electronic and thermal Enthalpies= -2240.328125
Sum of electronic and thermal Free Energies= -2240.432550

HOMO -0.21609 LUMO -0.10364

| | | | |
|---|---|---|---|
| Fe | 0.328268000 | -1.145471000 | -0.355222000 |
| Cl | 0.454056000 | -2.242083000 | 1.607235000 |
| Cl | 1.827550000 | -1.720769000 | -1.897313000 |
| N | 1.951685000 | 1.359717000 | 0.483556000 |
| N | -0.193048000 | 1.749757000 | 0.509432000 |
| C | 0.747113000 | 0.832542000 | 0.221086000 |
| C | 1.885721000 | 2.760369000 | 0.979694000 |
| H | 2.426480000 | 3.425491000 | 0.289908000 |
| H | 2.361837000 | 2.828338000 | 1.968383000 |
| C | 0.370817000 | 3.029034000 | 1.018675000 |
| H | -0.007100000 | 3.226798000 | 2.032742000 |
| H | 0.060873000 | 3.859809000 | 0.367536000 |
| C | 3.220078000 | 0.729520000 | 0.255303000 |
| C | 3.838663000 | 0.033219000 | 1.306928000 |
| C | 3.181880000 | -0.086338000 | 2.656720000 |
| H | 3.847614000 | -0.595816000 | 3.366115000 |
| H | 2.248291000 | -0.666093000 | 2.586501000 |
| H | 2.929348000 | 0.899231000 | 3.079889000 |
| C | 5.077190000 | -0.568418000 | 1.049683000 |
| H | 5.565892000 | -1.128669000 | 1.851559000 |
| C | 5.696126000 | -0.479025000 | -0.203639000 |
| C | 7.001845000 | -1.185324000 | -0.472160000 |
| H | 7.633299000 | -0.614228000 | -1.168487000 |
| H | 6.819713000 | -2.172663000 | -0.927662000 |
| H | 7.569656000 | -1.348742000 | 0.454956000 |
| C | 5.058506000 | 0.250995000 | -1.215785000 |
| H | 5.527971000 | 0.328832000 | -2.200221000 |
| C | 3.818393000 | 0.863252000 | -1.009994000 |
| C | 3.114626000 | 1.584465000 | -2.128943000 |
| H | 3.789016000 | 1.726588000 | -2.983916000 |
| H | 2.738819000 | 2.572251000 | -1.820544000 |
| H | 2.253198000 | 0.988954000 | -2.470137000 |
| C | -1.604172000 | 1.622304000 | 0.311372000 |
| C | -2.147789000 | 1.993670000 | -0.932868000 |
| C | -1.247154000 | 2.389931000 | -2.073644000 |
| H | -1.834751000 | 2.636321000 | -2.967903000 |
| H | -0.554929000 | 1.572117000 | -2.327269000 |
| H | -0.626335000 | 3.265157000 | -1.824457000 |
| C | -3.537224000 | 1.940664000 | -1.083482000 |
| H | -3.976408000 | 2.212890000 | -2.047380000 |
| C | -4.376322000 | 1.532608000 | -0.036879000 |
| C | -5.873159000 | 1.512160000 | -0.210589000 |
| H | -6.322329000 | 2.459776000 | 0.130733000 |
| H | -6.327833000 | 0.698660000 | 0.371759000 |
| H | -6.150664000 | 1.374245000 | -1.265163000 |
| C | -3.794062000 | 1.150348000 | 1.178497000 |
| H | -4.433360000 | 0.794098000 | 1.990083000 |
| C | -2.409077000 | 1.187802000 | 1.377705000 |
| C | -1.787702000 | 0.720679000 | 2.666242000 |
| H | -1.166982000 | 1.502703000 | 3.131846000 |

| | | | |
|---|---|---|---|
| H | -1.129849000 | -0.146624000 | 2.492602000 |
| H | -2.561708000 | 0.428420000 | 3.388059000 |
| C | -1.412127000 | -1.138379000 | -1.135241000 |
| C | -3.849149000 | -1.364937000 | -1.573356000 |
| C | -2.729185000 | -1.507342000 | -0.708101000 |
| C | -5.125213000 | -1.743067000 | -1.168817000 |
| C | -2.959550000 | -2.037117000 | 0.590206000 |
| C | -5.324986000 | -2.257893000 | 0.119885000 |
| H | -5.971332000 | -1.634551000 | -1.850614000 |
| C | -4.237973000 | -2.404484000 | 0.994479000 |
| H | -2.102398000 | -2.166958000 | 1.253566000 |
| H | -6.326597000 | -2.555518000 | 0.438243000 |
| H | -4.394771000 | -2.815527000 | 1.994018000 |
| H | -3.686269000 | -0.956813000 | -2.573574000 |
| H | -1.407798000 | -0.781475000 | -2.182852000 |

# Fe-III



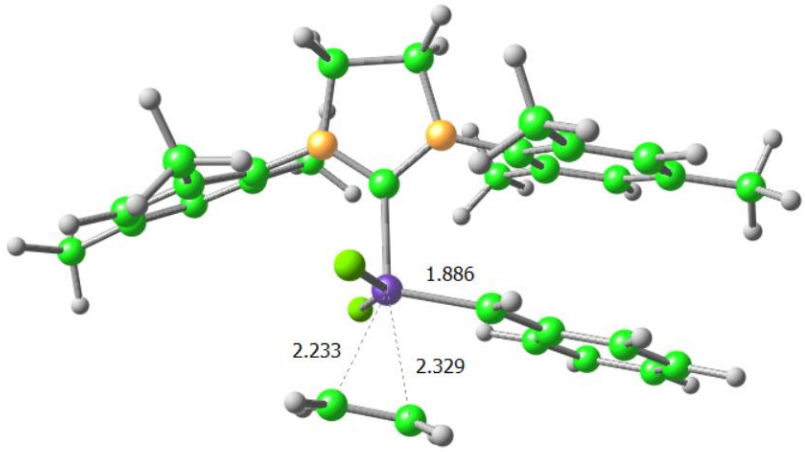

Zero-point correction= 0.570359 (Hartree/Particle)
Thermal correction to Energy= 0.608267
Thermal correction to Enthalpy= 0.609211
Thermal correction to Gibbs Free Energy= 0.501317
Sum of electronic and zero-point Energies= -2318.935248
Sum of electronic and thermal Energies= -2318.897341
Sum of electronic and thermal Enthalpies= -2318.896397
Sum of electronic and thermal Free Energies= -2319.004291

HOMO -0.15134 LUMO -0.10954

| | | | |
|---|---|---|---|
| Fe | 0.451482000 | 0.832803000 | 0.661847000 |
| Cl | 0.690191000 | 1.656361000 | -1.484532000 |
| Cl | 0.838214000 | -0.344668000 | 2.640593000 |
| N | 1.843403000 | -1.454070000 | -0.452202000 |
| N | -0.316734000 | -1.818890000 | -0.463986000 |
| C | 0.637619000 | -0.915433000 | -0.147485000 |
| C | 1.749844000 | -2.811255000 | -1.032436000 |
| H | 2.331706000 | -3.518905000 | -0.423671000 |
| H | 2.157734000 | -2.810763000 | -2.054671000 |
| C | 0.236690000 | -3.088771000 | -0.993218000 |
| H | -0.189807000 | -3.298429000 | -1.985239000 |
| H | -0.024658000 | -3.919485000 | -0.320607000 |
| C | 3.101454000 | -0.764557000 | -0.395346000 |
| C | 3.556833000 | -0.082173000 | -1.545785000 |
| C | 2.869157000 | -0.213268000 | -2.880396000 |
| H | 2.952601000 | 0.718611000 | -3.454798000 |
| H | 1.802440000 | -0.436313000 | -2.775547000 |
| H | 3.348783000 | -1.014613000 | -3.469919000 |
| C | 4.733345000 | 0.666819000 | -1.445947000 |
| H | 5.075512000 | 1.224410000 | -2.322490000 |
| C | 5.479929000 | 0.718944000 | -0.260641000 |
| C | 6.702442000 | 1.596590000 | -0.156986000 |
| H | 7.399407000 | 1.227547000 | 0.609120000 |
| H | 6.420506000 | 2.625674000 | 0.121473000 |
| H | 7.239589000 | 1.653699000 | -1.115171000 |
| C | 5.062671000 | -0.066325000 | 0.818909000 |
| H | 5.669170000 | -0.095174000 | 1.728857000 |
| C | 3.894323000 | -0.841275000 | 0.767274000 |
| C | 3.593125000 | -1.798263000 | 1.890653000 |
| H | 3.667993000 | -1.301527000 | 2.867269000 |
| H | 4.326385000 | -2.622786000 | 1.871166000 |
| H | 2.581745000 | -2.210222000 | 1.821717000 |
| C | -1.737499000 | -1.659856000 | -0.385930000 |
| C | -2.425201000 | -2.146322000 | 0.742764000 |
| C | -1.686422000 | -2.783086000 | 1.888497000 |
| H | -2.359419000 | -2.946499000 | 2.741053000 |
| H | -0.840598000 | -2.159333000 | 2.220641000 |
| H | -1.275514000 | -3.765193000 | 1.599542000 |
| C | -3.819309000 | -2.007202000 | 0.772625000 |
| H | -4.363392000 | -2.359217000 | 1.653609000 |
| C | -4.528839000 | -1.432337000 | -0.289011000 |
| C | -6.023698000 | -1.256419000 | -0.222674000 |
| H | -6.514135000 | -1.647572000 | -1.127205000 |
| H | -6.280118000 | -0.187038000 | -0.148679000 |
| H | -6.451652000 | -1.769559000 | 0.649808000 |
| C | -3.814026000 | -1.005280000 | -1.416877000 |
| H | -4.352747000 | -0.559462000 | -2.257260000 |
| C | -2.423508000 | -1.119802000 | -1.494749000 |
| C | -1.678656000 | -0.657653000 | -2.714597000 |
| H | -1.099493000 | -1.478424000 | -3.168948000 |
| H | -0.960212000 | 0.138145000 | -2.461022000 |
| H | -2.375469000 | -0.276206000 | -3.472637000 |
| C | -1.278451000 | 0.784227000 | 0.938778000 |
| C | -3.632263000 | 1.383785000 | 1.178639000 |
| C | -2.428247000 | 1.508905000 | 0.436977000 |
| C | -4.797336000 | 2.033987000 | 0.777497000 |
| C | -2.445756000 | 2.309070000 | -0.729417000 |
| C | -4.797832000 | 2.803101000 | -0.392145000 |
| H | -5.708276000 | 1.936942000 | 1.372100000 |
| C | -3.619440000 | 2.934165000 | -1.140939000 |
| H | -1.524883000 | 2.405680000 | -1.306176000 |
| H | -5.711994000 | 3.305231000 | -0.716637000 |
| H | -3.618367000 | 3.537524000 | -2.051387000 |
| C | 0.837115000 | 2.502604000 | 2.204838000 |
| C | 0.725612000 | 3.104206000 | 0.985272000 |

| | | | | |
|---|---|---|---|---|
| H | -0.011946000 | 2.397602000 | 2.879199000 |
| H | 1.809512000 | 2.233732000 | 2.618093000 |
| H | -0.223298000 | 3.501362000 | 0.623257000 |
| H | -3.630148000 | 0.761557000 | 2.075774000 |
| H | -1.541921000 | 0.143709000 | 1.795636000 |
| H | 1.604800000 | 3.341598000 | 0.387146000 |

# Fe-IIIt



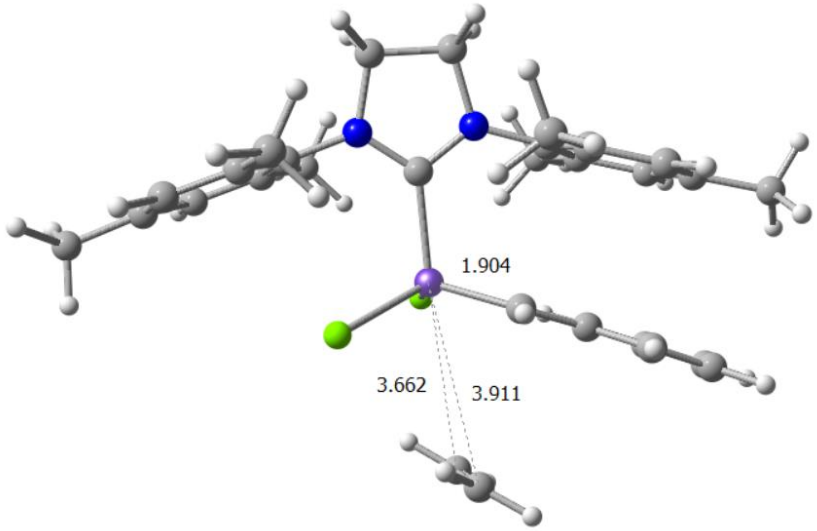

Zero-point correction= 0.569577 (Hartree/Particle)
Thermal correction to Energy= 0.607907
Thermal correction to Enthalpy= 0.608851
Thermal correction to Gibbs Free Energy= 0.498804
Sum of electronic and zero-point Energies= -2318.933990
Sum of electronic and thermal Energies= -2318.895661
Sum of electronic and thermal Enthalpies= -2318.894716
Sum of electronic and thermal Free Energies= -2319.004764

HOMO -0.16030 LUMO -0.11867

| | | | |
|---|---|---|---|
| Fe | 0.378125000 | 0.729492000 | 0.928504000 |
| Cl | 1.072722000 | 2.110634000 | -0.815547000 |
| Cl | 0.788660000 | -0.603014000 | 2.840894000 |
| N | 1.880568000 | -1.383342000 | -0.419142000 |
| N | -0.269561000 | -1.818296000 | -0.371072000 |
| C | 0.668626000 | -0.883126000 | -0.076744000 |
| C | 1.807716000 | -2.805488000 | -0.824919000 |
| H | 2.201049000 | -3.437683000 | -0.012475000 |
| H | 2.409436000 | -2.974716000 | -1.728046000 |
| C | 0.304147000 | -3.007159000 | -1.045495000 |
| H | 0.023885000 | -3.001043000 | -2.112595000 |
| H | -0.078802000 | -3.928999000 | -0.587897000 |
| C | 3.135589000 | -0.685715000 | -0.474436000 |
| C | 3.467913000 | -0.039383000 | -1.685261000 |
| C | 2.550841000 | -0.101343000 | -2.877255000 |
| H | 3.021613000 | 0.371072000 | -3.749874000 |
| H | 1.613044000 | 0.429239000 | -2.661875000 |
| H | 2.302295000 | -1.140687000 | -3.146931000 |
| C | 4.679715000 | 0.651719000 | -1.755725000 |
| H | 4.934638000 | 1.174173000 | -2.681954000 |
| C | 5.567762000 | 0.695740000 | -0.671000000 |
| C | 6.836073000 | 1.509087000 | -0.747799000 |
| H | 7.581087000 | 1.162870000 | -0.017289000 |
| H | 6.630842000 | 2.571268000 | -0.534643000 |
| H | 7.286292000 | 1.459194000 | -1.750486000 |
| C | 5.244061000 | -0.028798000 | 0.479686000 |
| H | 5.947314000 | -0.048412000 | 1.317395000 |
| C | 4.046086000 | -0.752317000 | 0.594061000 |
| C | 3.817385000 | -1.633137000 | 1.792905000 |
| H | 4.224546000 | -1.171274000 | 2.703222000 |
| H | 4.336116000 | -2.597478000 | 1.653085000 |
| H | 2.752702000 | -1.820416000 | 1.972325000 |
| C | -1.684165000 | -1.621295000 | -0.428645000 |
| C | -2.497105000 | -2.191667000 | 0.569554000 |
| C | -1.882425000 | -2.898611000 | 1.747242000 |
| H | -2.640424000 | -3.110597000 | 2.513635000 |
| H | -1.073370000 | -2.300443000 | 2.196513000 |
| H | -1.438804000 | -3.862271000 | 1.445227000 |
| C | -3.886442000 | -2.066696000 | 0.433621000 |
| H | -4.531262000 | -2.486458000 | 1.210932000 |
| C | -4.466227000 | -1.416058000 | -0.663227000 |
| C | -5.963132000 | -1.303274000 | -0.797650000 |
| H | -6.351231000 | -2.037270000 | -1.522936000 |
| H | -6.250936000 | -0.303340000 | -1.154903000 |
| H | -6.466952000 | -1.484935000 | 0.162157000 |
| C | -3.623839000 | -0.871972000 | -1.643960000 |
| H | -4.061348000 | -0.337197000 | -2.491014000 |
| C | -2.233611000 | -0.963520000 | -1.550171000 |
| C | -1.340389000 | -0.326267000 | -2.577807000 |
| H | -0.672426000 | -1.060647000 | -3.055385000 |
| H | -0.692902000 | 0.436853000 | -2.115713000 |
| H | -1.935211000 | 0.154357000 | -3.365293000 |
| C | -1.499095000 | 0.776959000 | 1.099005000 |
| C | -3.918887000 | 1.274069000 | 0.979164000 |
| C | -2.609400000 | 1.447153000 | 0.466585000 |
| C | -5.010059000 | 1.906895000 | 0.386338000 |
| C | -2.432227000 | 2.284351000 | -0.662641000 |
| C | -4.816446000 | 2.712368000 | -0.741737000 |
| H | -6.012267000 | 1.769879000 | 0.797347000 |
| C | -3.525806000 | 2.900592000 | -1.260985000 |
| H | -1.418024000 | 2.435003000 | -1.041028000 |
| H | -5.670308000 | 3.205142000 | -1.212279000 |
| H | -3.378688000 | 3.540596000 | -2.133503000 |
| C | -0.309770000 | 2.553446000 | 2.203230000 |
| C | 1.068788000 | 2.396579000 | 2.243935000 |

| | | | | |
|---|---|---|---|---|
| H | -0.759870000 | 3.257526000 | 1.503216000 |
| H | -0.924541000 | 2.222018000 | 3.042828000 |
| H | 1.699857000 | 2.972137000 | 1.567400000 |
| H | -4.058706000 | 0.631349000 | 1.850576000 |
| H | -1.814160000 | 0.164132000 | 1.959361000 |
| H | 1.539650000 | 1.883438000 | 3.081209000 |

# Fe-IIIq



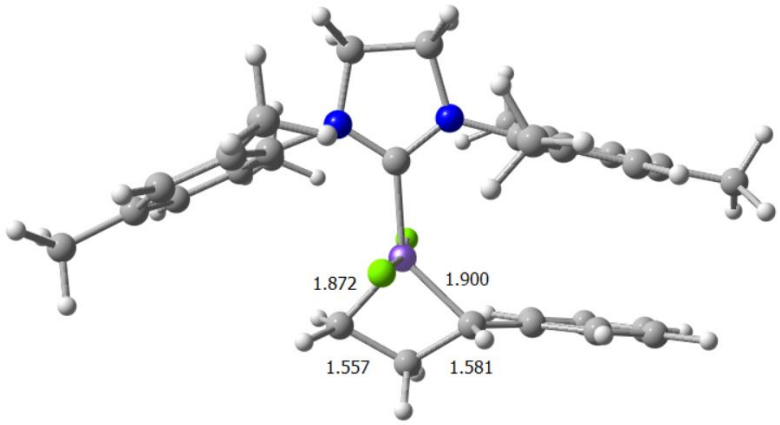

Zero-point correction= 0.564469 (Hartree/Particle)
Thermal correction to Energy= 0.605547
Thermal correction to Enthalpy= 0.606492
Thermal correction to Gibbs Free Energy= 0.484504
Sum of electronic and zero-point Energies= -2318.937594
Sum of electronic and thermal Energies= -2318.896515
Sum of electronic and thermal Enthalpies= -2318.895571
Sum of electronic and thermal Free Energies= -2319.017558

HOMO -0.16237 LUMO -0.12201

| | | | |
|---|---|---|---|
| Fe | 0.321347000 | 0.929022000 | 0.007174000 |
| Cl | 0.395268000 | 1.523640000 | -2.167504000 |
| Cl | 1.799505000 | 1.944613000 | 1.339265000 |
| N | 2.076519000 | -1.634303000 | -0.068375000 |
| N | -0.051415000 | -2.108431000 | -0.072553000 |
| C | 0.844981000 | -1.106203000 | -0.024520000 |
| C | 2.077939000 | -3.119176000 | -0.155801000 |
| H | 2.616712000 | -3.544211000 | 0.703902000 |
| H | 2.592227000 | -3.435433000 | -1.075107000 |
| C | 0.575587000 | -3.454691000 | -0.158205000 |
| H | 0.247404000 | -3.963563000 | -1.076753000 |
| H | 0.268234000 | -4.066404000 | 0.702978000 |
| C | 3.313244000 | -0.907814000 | -0.048916000 |
| C | 3.879770000 | -0.488903000 | -1.264348000 |
| C | 3.194743000 | -0.752934000 | -2.578856000 |
| H | 3.863801000 | -0.517927000 | -3.417499000 |
| H | 2.290833000 | -0.130741000 | -2.676524000 |
| H | 2.881401000 | -1.803997000 | -2.677799000 |
| C | 5.093059000 | 0.209126000 | -1.210975000 |
| H | 5.542802000 | 0.553444000 | -2.146374000 |
| C | 5.737253000 | 0.479546000 | 0.002988000 |
| C | 7.015875000 | 1.279607000 | 0.035571000 |
| H | 7.659558000 | 0.976432000 | 0.874141000 |
| H | 6.797138000 | 2.353095000 | 0.159725000 |
| H | 7.586033000 | 1.165012000 | -0.897514000 |
| C | 5.150142000 | 0.021465000 | 1.190212000 |
| H | 5.638918000 | 0.227772000 | 2.146341000 |
| C | 3.935980000 | -0.672213000 | 1.188984000 |
| C | 3.280362000 | -1.093430000 | 2.477259000 |
| H | 3.954171000 | -0.927627000 | 3.328355000 |
| H | 2.989578000 | -2.155552000 | 2.473546000 |
| H | 2.369690000 | -0.496753000 | 2.642333000 |
| C | -1.473936000 | -1.982176000 | 0.022506000 |
| C | -2.075888000 | -2.042292000 | 1.293838000 |
| C | -1.232888000 | -2.129263000 | 2.539662000 |
| H | -1.856710000 | -2.035822000 | 3.438514000 |
| H | -0.473646000 | -1.332942000 | 2.558898000 |
| H | -0.694234000 | -3.088621000 | 2.606214000 |
| C | -3.471643000 | -1.979486000 | 1.363082000 |
| H | -3.954739000 | -2.008783000 | 2.343630000 |
| C | -4.261789000 | -1.859791000 | 0.211740000 |
| C | -5.765468000 | -1.816444000 | 0.304763000 |
| H | -6.200693000 | -2.812640000 | 0.119784000 |
| H | -6.186862000 | -1.125029000 | -0.438595000 |
| H | -6.094528000 | -1.487532000 | 1.300262000 |
| C | -3.623258000 | -1.787645000 | -1.033288000 |
| H | -4.225076000 | -1.662796000 | -1.937055000 |
| C | -2.230297000 | -1.849474000 | -1.154550000 |
| C | -1.554500000 | -1.721028000 | -2.493095000 |
| H | -0.854586000 | -2.550020000 | -2.681541000 |
| H | -0.967085000 | -0.789577000 | -2.549365000 |
| H | -2.295232000 | -1.710271000 | -3.303613000 |
| C | -1.404988000 | 1.051822000 | 0.801340000 |
| C | -3.834786000 | 1.342079000 | 1.231622000 |
| C | -2.739973000 | 1.269329000 | 0.328815000 |
| C | -5.125305000 | 1.598294000 | 0.779778000 |
| C | -3.006802000 | 1.448615000 | -1.053402000 |
| C | -5.361383000 | 1.776106000 | -0.591037000 |
| H | -5.953518000 | 1.660396000 | 1.488893000 |
| C | -4.298394000 | 1.701275000 | -1.503064000 |
| H | -2.166825000 | 1.412623000 | -1.749395000 |
| H | -6.373140000 | 1.983017000 | -0.947059000 |
| H | -4.484072000 | 1.847821000 | -2.569226000 |
| C | -1.126516000 | 4.315378000 | 1.324330000 |
| C | -0.770981000 | 4.424023000 | 0.042211000 |

| | | | | |
|---|---|---|---|---|
| H | -2.120242000 | 4.607600000 | 1.674212000 |
| H | -0.432899000 | 3.911573000 | 2.065801000 |
| H | -1.457919000 | 4.805160000 | -0.717538000 |
| H | -3.640232000 | 1.203375000 | 2.297739000 |
| H | -1.365359000 | 0.991297000 | 1.905709000 |
| H | 0.216398000 | 4.109685000 | -0.301833000 |

# Fe-IV



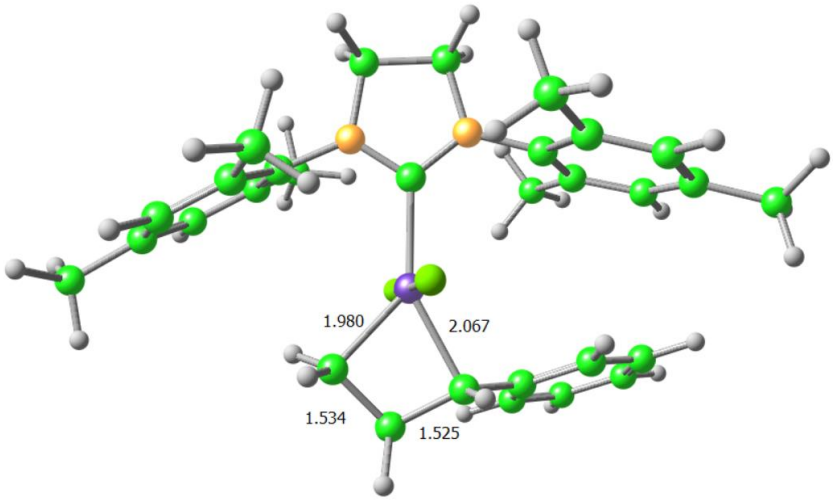

Zero-point correction= 0.571565 (Hartree/Particle)
Thermal correction to Energy= 0.608059
Thermal correction to Enthalpy= 0.609003
Thermal correction to Gibbs Free Energy= 0.504189
Sum of electronic and zero-point Energies= -2318.946020
Sum of electronic and thermal Energies= -2318.909526
Sum of electronic and thermal Enthalpies= -2318.908582
Sum of electronic and thermal Free Energies= -2319.013396

HOMO -0.15155 LUMO -0.10941

| | | | |
|---|---|---|---|
| Fe | -0.360452000 | 0.903924000 | -0.265548000 |
| Cl | 0.022310000 | 1.426265000 | 1.907807000 |
| Cl | -1.027846000 | 0.287878000 | -2.375122000 |
| N | -1.957182000 | -1.374880000 | 0.603414000 |
| N | 0.193198000 | -1.827336000 | 0.535776000 |
| C | -0.739337000 | -0.886866000 | 0.298519000 |
| C | -1.887159000 | -2.741952000 | 1.174650000 |
| H | -2.567254000 | -3.412335000 | 0.631615000 |
| H | -2.186712000 | -2.717701000 | 2.233870000 |
| C | -0.402873000 | -3.109481000 | 0.986397000 |
| H | 0.077965000 | -3.439584000 | 1.917170000 |
| H | -0.247929000 | -3.882656000 | 0.217116000 |
| C | -3.211250000 | -0.715590000 | 0.363760000 |
| C | -3.762844000 | 0.118583000 | 1.355625000 |
| C | -3.135099000 | 0.245057000 | 2.716998000 |
| H | -3.666007000 | 0.995254000 | 3.318556000 |
| H | -2.076869000 | 0.536970000 | 2.654260000 |
| H | -3.186808000 | -0.713187000 | 3.260646000 |
| C | -4.953766000 | 0.793335000 | 1.056160000 |
| H | -5.382499000 | 1.458273000 | 1.811239000 |
| C | -5.611510000 | 0.627726000 | -0.169263000 |
| C | -6.859436000 | 1.413083000 | -0.488901000 |
| H | -7.529136000 | 0.851129000 | -1.155900000 |
| H | -6.606112000 | 2.357899000 | -0.998068000 |
| H | -7.416566000 | 1.670960000 | 0.423394000 |
| C | -5.078330000 | -0.280862000 | -1.092561000 |
| H | -5.598932000 | -0.453765000 | -2.038548000 |
| C | -3.889757000 | -0.977215000 | -0.843107000 |
| C | -3.392080000 | -2.010189000 | -1.819197000 |
| H | -3.853642000 | -1.864210000 | -2.804710000 |
| H | -3.653967000 | -3.026660000 | -1.477148000 |
| H | -2.304798000 | -1.948426000 | -1.947789000 |
| C | 1.605702000 | -1.715516000 | 0.294362000 |
| C | 2.104176000 | -2.007327000 | -0.991713000 |
| C | 1.191368000 | -2.389925000 | -2.124259000 |
| H | 1.774866000 | -2.734671000 | -2.988690000 |
| H | 0.563065000 | -1.540365000 | -2.438083000 |
| H | 0.503411000 | -3.200390000 | -1.835809000 |
| C | 3.489516000 | -1.943917000 | -1.188172000 |
| H | 3.888182000 | -2.160956000 | -2.183360000 |
| C | 4.371342000 | -1.618688000 | -0.150928000 |
| C | 5.861303000 | -1.593189000 | -0.379507000 |
| H | 6.338439000 | -0.796077000 | 0.208076000 |
| H | 6.101567000 | -1.430979000 | -1.439733000 |
| H | 6.321207000 | -2.549078000 | -0.077973000 |
| C | 3.840393000 | -1.358620000 | 1.117473000 |
| H | 4.514168000 | -1.106456000 | 1.940666000 |
| C | 2.465928000 | -1.429246000 | 1.373209000 |
| C | 1.946129000 | -1.260742000 | 2.775396000 |
| H | 1.763856000 | -2.244397000 | 3.242463000 |
| H | 1.012096000 | -0.685141000 | 2.793338000 |
| H | 2.681855000 | -0.734054000 | 3.398125000 |
| C | 1.104855000 | 1.792915000 | -1.084660000 |
| C | 3.510759000 | 1.459168000 | -1.404038000 |
| C | 2.473826000 | 1.898843000 | -0.552206000 |
| C | 4.850466000 | 1.581518000 | -1.037750000 |
| C | 2.831772000 | 2.449192000 | 0.695769000 |
| C | 5.187889000 | 2.129342000 | 0.202784000 |
| H | 5.632078000 | 1.245571000 | -1.721766000 |
| C | 4.170575000 | 2.558245000 | 1.065998000 |
| H | 2.048055000 | 2.759994000 | 1.385347000 |
| H | 6.235492000 | 2.225283000 | 0.496360000 |
| H | 4.425300000 | 2.984628000 | 2.038771000 |
| C | -1.394653000 | 2.453366000 | -0.453688000 |
| C | 0.037184000 | 2.931994000 | -0.833931000 |

| | | | |
|---|---|---|---|
| H | -2.114731000 | 2.444634000 | -1.275436000 |
| H | -1.756391000 | 2.852933000 | 0.497799000 |
| H | -0.056280000 | 3.413356000 | -1.818044000 |
| H | 3.247917000 | 1.030397000 | -2.373623000 |
| H | 1.118232000 | 1.505598000 | -2.140879000 |
| H | 0.420102000 | 3.603012000 | -0.058292000 |

# Fe-IVt



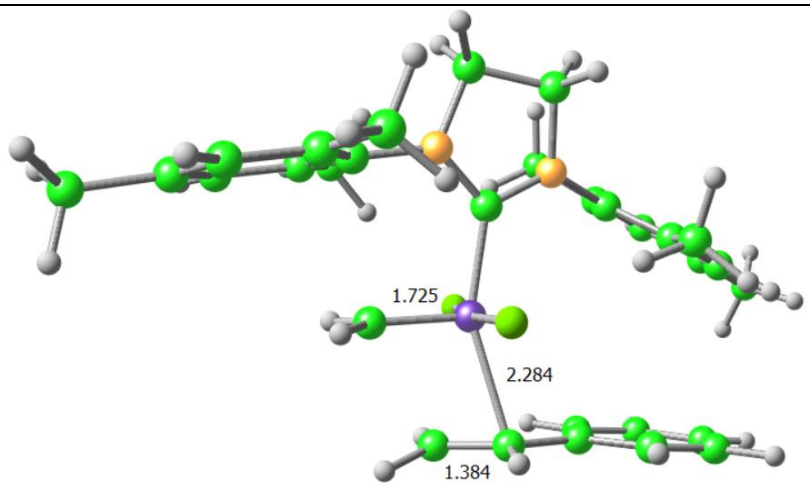

Zero-point correction= 0.570221 (Hartree/Particle)
Thermal correction to Energy= 0.609239
Thermal correction to Enthalpy= 0.610183
Thermal correction to Gibbs Free Energy= 0.495474
Sum of electronic and zero-point Energies= -2318.961013
Sum of electronic and thermal Energies= -2318.921995
Sum of electronic and thermal Enthalpies= -2318.921051
Sum of electronic and thermal Free Energies= -2319.035760

HOMO -0.15821 LUMO -0.12402

| | | | |
|---|---|---|---|
| Fe | -0.399802000 | 0.682211000 | -0.653369000 |
| Cl | -0.620904000 | 1.726217000 | 1.319167000 |
| Cl | -0.133228000 | -0.439975000 | -2.580224000 |
| N | -1.750586000 | -1.569097000 | 0.751275000 |
| N | 0.400955000 | -1.941323000 | 0.716780000 |
| C | -0.564077000 | -1.090841000 | 0.330245000 |
| C | -1.641736000 | -2.867177000 | 1.462258000 |
| H | -2.157943000 | -3.653518000 | 0.889586000 |
| H | -2.106263000 | -2.796727000 | 2.455859000 |
| C | -0.116665000 | -3.076658000 | 1.527040000 |
| H | 0.281082000 | -3.010646000 | 2.551552000 |
| H | 0.204762000 | -4.032450000 | 1.090218000 |
| C | -3.003822000 | -0.911862000 | 0.517339000 |
| C | -3.562981000 | -0.114557000 | 1.534811000 |
| C | -2.954136000 | -0.052799000 | 2.910807000 |
| H | -3.239529000 | 0.876652000 | 3.421095000 |
| H | -1.858851000 | -0.086737000 | 2.865939000 |
| H | -3.311154000 | -0.894682000 | 3.529292000 |
| C | -4.734761000 | 0.594723000 | 1.243909000 |
| H | -5.163815000 | 1.239336000 | 2.016100000 |
| C | -5.364999000 | 0.502448000 | -0.004020000 |
| C | -6.591678000 | 1.325062000 | -0.312247000 |
| H | -7.238252000 | 0.823067000 | -1.046367000 |
| H | -6.309155000 | 2.302687000 | -0.736996000 |
| H | -7.183585000 | 1.519840000 | 0.593718000 |
| C | -4.823761000 | -0.365489000 | -0.961583000 |
| H | -5.328505000 | -0.486307000 | -1.924116000 |
| C | -3.653104000 | -1.095295000 | -0.720022000 |
| C | -3.124724000 | -2.062383000 | -1.745020000 |
| H | -3.848450000 | -2.190964000 | -2.561235000 |
| H | -2.935069000 | -3.051468000 | -1.299608000 |
| H | -2.174531000 | -1.713020000 | -2.176996000 |
| C | 1.805073000 | -1.815309000 | 0.450535000 |
| C | 2.349489000 | -2.522749000 | -0.641179000 |
| C | 1.478831000 | -3.371021000 | -1.529486000 |
| H | 2.059302000 | -3.771186000 | -2.371462000 |
| H | 0.643899000 | -2.779683000 | -1.932481000 |
| H | 1.054580000 | -4.227910000 | -0.980133000 |
| C | 3.725023000 | -2.418198000 | -0.873631000 |
| H | 4.155545000 | -2.948324000 | -1.728033000 |
| C | 4.560328000 | -1.666446000 | -0.034671000 |
| C | 6.035820000 | -1.545703000 | -0.325683000 |
| H | 6.581945000 | -1.139230000 | 0.537254000 |
| H | 6.214034000 | -0.873181000 | -1.181494000 |
| H | 6.477876000 | -2.519800000 | -0.584030000 |
| C | 3.988897000 | -1.011907000 | 1.060789000 |
| H | 4.624360000 | -0.424250000 | 1.727644000 |
| C | 2.613182000 | -1.064922000 | 1.323573000 |
| C | 2.033520000 | -0.315888000 | 2.491225000 |
| H | 1.360407000 | -0.946072000 | 3.093112000 |
| H | 1.435071000 | 0.543049000 | 2.150067000 |
| H | 2.833002000 | 0.057455000 | 3.144654000 |
| C | 0.755391000 | 2.192853000 | -1.462181000 |
| C | 3.103527000 | 1.735922000 | -0.866004000 |
| C | 1.926276000 | 2.484201000 | -0.634704000 |
| C | 4.267232000 | 1.985646000 | -0.141881000 |
| C | 1.956145000 | 3.477291000 | 0.369187000 |
| C | 4.281082000 | 2.974850000 | 0.847640000 |
| H | 5.166029000 | 1.401010000 | -0.344593000 |
| C | 3.118124000 | 3.716309000 | 1.099075000 |
| H | 1.055389000 | 4.051649000 | 0.582971000 |
| H | 5.191256000 | 3.170130000 | 1.418698000 |
| H | 3.121050000 | 4.489441000 | 1.870602000 |
| C | -0.499572000 | 3.055499000 | -1.549250000 |
| C | -1.623726000 | 2.015219000 | -1.457734000 |

| | | | | |
|---|---|---|---|---|
| H | -0.565081000 | 3.748646000 | -0.701765000 |
| H | -0.527276000 | 3.631286000 | -2.491504000 |
| H | -2.415925000 | 2.210659000 | -0.728405000 |
| H | 3.084334000 | 0.945377000 | -1.620460000 |
| H | 1.028216000 | 1.747397000 | -2.422119000 |
| H | -1.975460000 | 1.612900000 | -2.412194000 |

# Fe-Vs

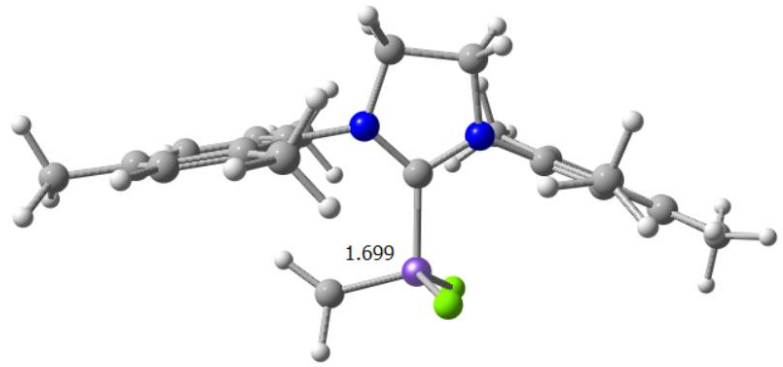



Zero-point correction= 0.570266 (Hartree/Particle)
Thermal correction to Energy= 0.608766
Thermal correction to Enthalpy= 0.609710
Thermal correction to Gibbs Free Energy= 0.500036
Sum of electronic and zero-point Energies= -2318.934912
Sum of electronic and thermal Energies= -2318.896413
Sum of electronic and thermal Enthalpies= -2318.895469
Sum of electronic and thermal Free Energies= -2319.005142

HOMO -0.16526 LUMO -0.11470

| | | | |
|---|---|---|---|
| Fe | -0.303849000 | -0.980705000 | -0.203274000 |
| Cl | 0.298065000 | -0.257578000 | -2.296282000 |
| Cl | -0.639000000 | -1.546900000 | 2.015337000 |
| N | -1.932977000 | 1.341683000 | 0.540283000 |
| N | 0.220623000 | 1.736010000 | 0.672861000 |
| C | -0.702967000 | 0.810237000 | 0.326746000 |
| C | -1.870291000 | 2.763594000 | 0.951289000 |
| H | -2.542463000 | 2.949191000 | 1.798960000 |
| H | -2.175104000 | 3.409287000 | 0.110245000 |
| C | -0.389291000 | 2.925315000 | 1.313400000 |
| H | 0.059016000 | 3.845281000 | 0.916344000 |
| H | -0.216443000 | 2.886480000 | 2.401300000 |
| C | -3.188956000 | 0.742665000 | 0.210054000 |
| C | -3.644960000 | 0.793064000 | -1.126000000 |
| C | -2.828171000 | 1.452862000 | -2.202457000 |
| H | -3.379005000 | 1.465599000 | -3.152420000 |
| H | -1.870642000 | 0.929055000 | -2.361571000 |
| H | -2.581871000 | 2.493646000 | -1.939465000 |
| C | -4.879694000 | 0.200299000 | -1.422601000 |
| H | -5.235104000 | 0.217222000 | -2.456715000 |
| C | -5.667589000 | -0.400512000 | -0.432969000 |
| C | -6.968432000 | -1.078252000 | -0.785263000 |
| H | -7.707811000 | -0.974334000 | 0.022165000 |
| H | -6.814088000 | -2.157550000 | -0.950695000 |
| H | -7.401483000 | -0.663109000 | -1.706574000 |
| C | -5.214067000 | -0.367634000 | 0.893651000 |
| H | -5.832826000 | -0.803681000 | 1.682957000 |
| C | -3.989296000 | 0.211841000 | 1.243820000 |
| C | -3.542556000 | 0.266353000 | 2.678626000 |
| H | -4.218577000 | -0.317724000 | 3.317458000 |
| H | -3.541278000 | 1.302749000 | 3.056464000 |
| H | -2.522928000 | -0.134097000 | 2.783630000 |
| C | 1.630604000 | 1.695755000 | 0.405174000 |
| C | 2.520261000 | 1.167008000 | 1.356941000 |
| C | 2.043603000 | 0.642327000 | 2.683769000 |
| H | 2.845700000 | 0.084253000 | 3.185582000 |
| H | 1.171192000 | -0.019014000 | 2.581405000 |
| H | 1.752953000 | 1.472466000 | 3.350036000 |
| C | 3.889754000 | 1.192541000 | 1.055991000 |
| H | 4.591421000 | 0.773349000 | 1.780637000 |
| C | 4.378740000 | 1.737273000 | -0.134077000 |
| C | 5.852401000 | 1.714407000 | -0.451852000 |
| H | 6.070219000 | 0.971457000 | -1.236550000 |
| H | 6.449044000 | 1.449863000 | 0.432413000 |
| H | 6.200351000 | 2.690630000 | -0.822644000 |
| C | 3.464666000 | 2.300716000 | -1.035112000 |
| H | 3.830151000 | 2.754446000 | -1.960760000 |
| C | 2.090924000 | 2.308152000 | -0.780109000 |
| C | 1.136908000 | 2.974489000 | -1.735256000 |
| H | 0.628058000 | 3.833362000 | -1.266410000 |
| H | 0.371426000 | 2.262341000 | -2.073355000 |
| H | 1.673714000 | 3.347444000 | -2.617754000 |
| C | 0.895327000 | -2.923014000 | -0.122961000 |
| C | 3.006182000 | -2.466016000 | 1.040873000 |
| C | 2.280218000 | -2.439895000 | -0.169811000 |
| C | 4.360869000 | -2.141233000 | 1.069474000 |
| C | 2.943557000 | -2.034691000 | -1.346733000 |
| C | 5.011084000 | -1.759510000 | -0.108387000 |
| H | 4.910550000 | -2.182027000 | 2.012161000 |
| C | 4.293180000 | -1.692219000 | -1.308862000 |
| H | 2.390887000 | -1.975057000 | -2.283790000 |
| H | 6.072332000 | -1.503596000 | -0.090129000 |
| H | 4.793553000 | -1.378339000 | -2.227198000 |
| C | -1.867174000 | -1.529919000 | -0.684634000 |
| C | -0.009267000 | -3.102557000 | -1.155276000 |
| H | -2.544277000 | -2.039942000 | 0.018052000 |
| H | -2.209108000 | -1.448666000 | -1.727576000 |
| H | -0.862171000 | -3.762172000 | -0.986033000 |
| H | 2.485203000 | -2.753073000 | 1.956938000 |
| H | 0.616339000 | -3.343914000 | 0.844093000 |
| H | 0.212144000 | -2.831900000 | -2.186733000 |

# Fe-VI

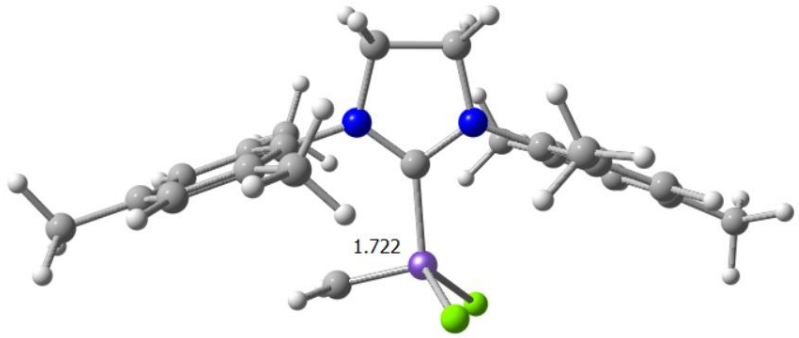



Zero-point correction= 0.435715 (Hartree/Particle)
Thermal correction to Energy= 0.467447
Thermal correction to Enthalpy= 0.468391
Thermal correction to Gibbs Free Energy= 0.371218
Sum of electronic and zero-point Energies= -2009.272579
Sum of electronic and thermal Energies= -2009.240846
Sum of electronic and thermal Enthalpies= -2009.239902
Sum of electronic and thermal Free Energies= -2009.337075

HOMO -0.17119 LUMO -0.11164

| | | | |
|---|---|---|---|
| Fe | -0.085573000 | 0.401707000 | -1.414517000 |
| Cl | -1.273014000 | -1.214067000 | -2.236084000 |
| Cl | -0.207670000 | 2.569661000 | -1.245269000 |
| N | 1.207715000 | 0.020196000 | 1.171026000 |
| N | -0.987483000 | 0.028623000 | 1.223040000 |
| C | 0.092314000 | 0.070993000 | 0.393291000 |
| C | 0.894763000 | -0.189866000 | 2.602145000 |
| H | 1.482465000 | 0.499238000 | 3.223729000 |
| H | 1.145572000 | -1.223830000 | 2.895292000 |
| C | -0.612367000 | 0.087668000 | 2.651309000 |
| H | -1.175494000 | -0.662403000 | 3.223510000 |
| H | -0.843751000 | 1.086526000 | 3.056398000 |
| C | 2.558831000 | -0.135548000 | 0.733947000 |
| C | 3.021427000 | -1.420067000 | 0.391931000 |
| C | 2.078565000 | -2.595105000 | 0.369540000 |
| H | 2.614254000 | -3.521897000 | 0.125728000 |
| H | 1.291496000 | -2.440778000 | -0.386494000 |
| H | 1.569328000 | -2.739663000 | 1.334613000 |
| C | 4.354304000 | -1.552019000 | -0.017425000 |
| H | 4.724529000 | -2.541147000 | -0.301030000 |
| C | 5.214768000 | -0.446597000 | -0.090733000 |
| C | 6.655671000 | -0.616529000 | -0.504609000 |
| H | 7.301079000 | -0.766891000 | 0.376812000 |
| H | 7.027643000 | 0.271658000 | -1.035336000 |
| H | 6.785620000 | -1.489549000 | -1.159941000 |
| C | 4.711404000 | 0.817635000 | 0.246504000 |
| H | 5.364719000 | 1.691642000 | 0.173469000 |
| C | 3.385981000 | 0.998435000 | 0.663311000 |
| C | 2.836985000 | 2.365574000 | 0.969760000 |
| H | 3.621460000 | 3.129391000 | 0.885362000 |
| H | 2.417744000 | 2.417088000 | 1.987074000 |
| H | 2.019911000 | 2.618635000 | 0.275608000 |
| C | -2.362723000 | -0.083422000 | 0.834725000 |
| C | -3.175608000 | 1.060566000 | 0.752483000 |
| C | -2.675552000 | 2.424338000 | 1.149846000 |
| H | -3.204996000 | 3.210853000 | 0.594959000 |
| H | -1.603940000 | 2.543036000 | 0.950926000 |
| H | -2.856312000 | 2.599038000 | 2.224673000 |
| C | -4.506783000 | 0.888161000 | 0.344659000 |
| H | -5.143631000 | 1.772022000 | 0.247790000 |
| C | -5.039153000 | -0.374841000 | 0.066222000 |
| C | -6.456663000 | -0.527710000 | -0.426436000 |
| H | -6.924564000 | -1.440581000 | -0.029206000 |
| H | -6.478511000 | -0.600393000 | -1.526391000 |
| H | -7.077953000 | 0.332631000 | -0.139515000 |
| C | -4.217711000 | -1.499092000 | 0.238280000 |
| H | -4.625529000 | -2.496589000 | 0.052840000 |
| C | -2.881580000 | -1.377917000 | 0.626256000 |
| C | -2.013863000 | -2.595057000 | 0.806940000 |
| H | -1.541320000 | -2.616043000 | 1.802184000 |
| H | -1.212069000 | -2.608933000 | 0.054860000 |
| H | -2.605794000 | -3.512856000 | 0.691874000 |
| C | 1.455963000 | 0.126664000 | -2.073245000 |
| H | 2.340854000 | -0.349636000 | -1.638982000 |
| H | 1.528269000 | 0.450650000 | -3.131020000 |

# Fe-VIt

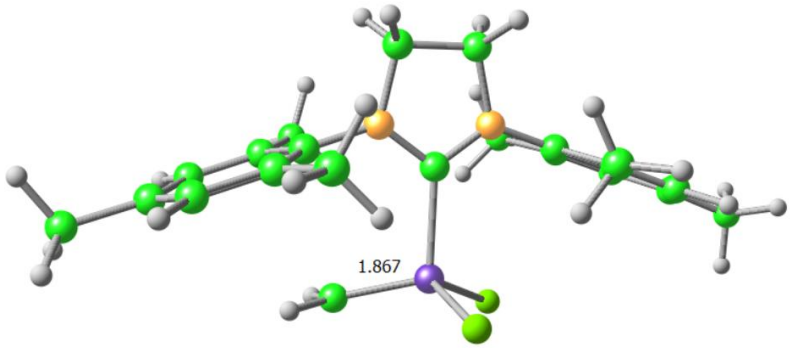



Zero-point correction= 0.434208 (Hartree/Particle)
Thermal correction to Energy= 0.465808
Thermal correction to Enthalpy= 0.466752
Thermal correction to Gibbs Free Energy= 0.367828
Sum of electronic and zero-point Energies= -2009.278595
Sum of electronic and thermal Energies= -2009.246995
Sum of electronic and thermal Enthalpies= -2009.246051
Sum of electronic and thermal Free Energies= -2009.344975

HOMO -0.16163 LUMO -0.12140

| | | | |
|---|---|---|---|
| Fe | -0.096627000 | 0.934412000 | -0.950782000 |
| Cl | -1.438355000 | 0.645517000 | -2.667873000 |
| Cl | -0.359394000 | 2.854825000 | 0.145227000 |
| N | 1.236585000 | -0.975725000 | 0.908900000 |
| N | -0.949730000 | -0.923970000 | 1.062003000 |
| C | 0.111856000 | -0.423037000 | 0.399305000 |
| C | 0.965018000 | -1.872699000 | 2.057485000 |
| H | 1.375477000 | -1.434889000 | 2.981074000 |
| H | 1.440385000 | -2.851181000 | 1.898437000 |
| C | -0.574781000 | -1.942372000 | 2.070113000 |
| H | -0.959747000 | -2.928103000 | 1.764324000 |
| H | -1.009435000 | -1.690044000 | 3.047725000 |
| C | 2.570321000 | -0.625853000 | 0.537462000 |
| C | 3.214724000 | -1.384616000 | -0.457252000 |
| C | 2.496009000 | -2.521667000 | -1.135308000 |
| H | 3.129535000 | -2.980609000 | -1.905650000 |
| H | 1.567500000 | -2.169689000 | -1.611041000 |
| H | 2.209838000 | -3.308048000 | -0.419140000 |
| C | 4.514295000 | -1.017228000 | -0.827526000 |
| H | 5.021921000 | -1.587031000 | -1.610696000 |
| C | 5.170713000 | 0.067172000 | -0.228888000 |
| C | 6.580729000 | 0.430492000 | -0.623687000 |
| H | 7.310955000 | -0.033396000 | 0.060006000 |
| H | 6.740197000 | 1.517735000 | -0.583792000 |
| H | 6.814932000 | 0.084681000 | -1.640357000 |
| C | 4.494526000 | 0.798656000 | 0.759306000 |
| H | 4.987943000 | 1.658142000 | 1.221536000 |
| C | 3.193753000 | 0.472940000 | 1.160522000 |
| C | 2.447058000 | 1.316922000 | 2.157609000 |
| H | 3.108700000 | 2.071169000 | 2.603460000 |
| H | 2.020232000 | 0.713383000 | 2.973314000 |
| H | 1.606236000 | 1.840671000 | 1.670977000 |
| C | -2.316696000 | -0.674677000 | 0.705179000 |
| C | -3.035839000 | 0.303672000 | 1.415147000 |
| C | -2.390702000 | 1.099635000 | 2.517284000 |
| H | -3.143628000 | 1.677246000 | 3.070128000 |
| H | -1.655017000 | 1.804418000 | 2.095378000 |
| H | -1.857511000 | 0.457213000 | 3.234902000 |
| C | -4.362729000 | 0.539945000 | 1.035072000 |
| H | -4.933336000 | 1.306869000 | 1.565874000 |
| C | -4.969367000 | -0.169604000 | -0.009082000 |
| C | -6.380259000 | 0.146741000 | -0.438335000 |
| H | -6.898729000 | -0.748732000 | -0.810676000 |
| H | -6.377381000 | 0.888508000 | -1.253985000 |
| H | -6.968014000 | 0.568616000 | 0.389497000 |
| C | -4.226438000 | -1.157271000 | -0.670974000 |
| H | -4.686875000 | -1.720503000 | -1.487154000 |
| C | -2.898186000 | -1.429563000 | -0.330449000 |
| C | -2.098028000 | -2.454423000 | -1.089985000 |
| H | -1.548866000 | -3.136389000 | -0.422700000 |
| H | -1.363876000 | -1.947247000 | -1.735857000 |
| H | -2.752718000 | -3.058358000 | -1.732021000 |
| C | 1.484085000 | 0.923651000 | -1.632554000 |
| H | 1.682042000 | 0.368060000 | -2.557869000 |
| H | 2.264934000 | 1.573942000 | -1.219359000 |

# Fe-VIq

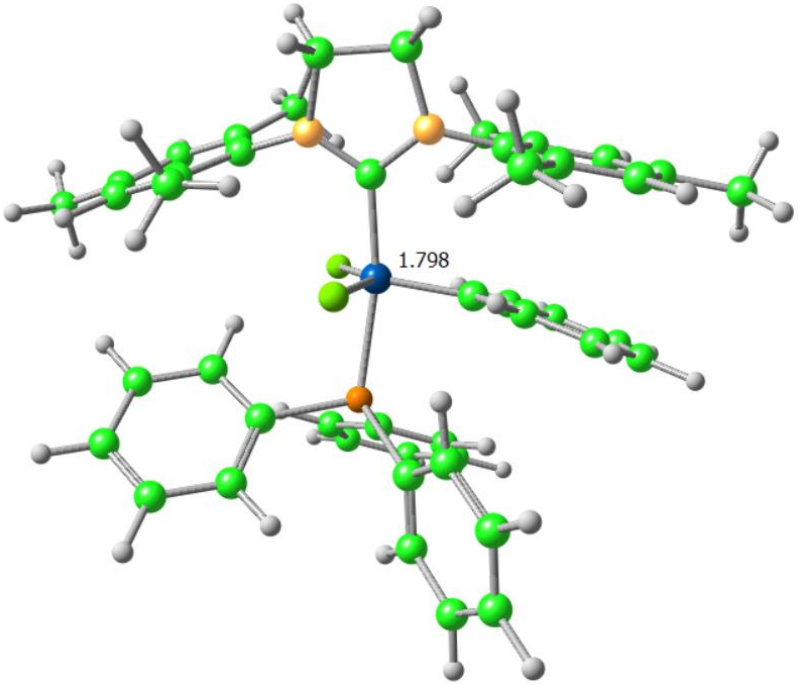



Zero-point correction= 0.433438 (Hartree/Particle)
Thermal correction to Energy= 0.466108
Thermal correction to Enthalpy= 0.467052
Thermal correction to Gibbs Free Energy= 0.365656
Sum of electronic and zero-point Energies= -2009.270881
Sum of electronic and thermal Energies= -2009.238212
Sum of electronic and thermal Enthalpies= -2009.237267
Sum of electronic and thermal Free Energies= -2009.338663

HOMO -0.24098 LUMO -0.11423

| | | | |
|---|---|---|---|
| Fe | 0.098491000 | 1.177964000 | -0.957995000 |
| Cl | -1.592018000 | 0.947255000 | -2.378625000 |
| Cl | -0.032026000 | 2.926892000 | 0.432782000 |
| N | 1.164390000 | -0.998183000 | 0.888840000 |
| N | -1.017885000 | -1.031634000 | 0.905203000 |
| C | 0.056426000 | -0.437190000 | 0.371042000 |
| C | 0.869839000 | -2.071146000 | 1.874833000 |
| H | 1.290877000 | -1.805109000 | 2.855861000 |
| H | 1.326749000 | -3.016968000 | 1.548849000 |
| C | -0.670286000 | -2.109740000 | 1.869637000 |
| H | -1.078345000 | -3.069117000 | 1.518688000 |
| H | -1.111534000 | -1.885334000 | 2.851449000 |
| C | 2.510180000 | -0.689888000 | 0.515199000 |
| C | 3.086773000 | -1.384977000 | -0.566075000 |
| C | 2.285307000 | -2.396431000 | -1.343715000 |
| H | 2.860799000 | -2.774843000 | -2.198569000 |
| H | 1.353678000 | -1.949820000 | -1.722908000 |
| H | 1.999640000 | -3.260139000 | -0.721774000 |
| C | 4.406239000 | -1.076394000 | -0.917912000 |
| H | 4.861792000 | -1.596285000 | -1.765114000 |
| C | 5.145684000 | -0.108597000 | -0.223746000 |
| C | 6.573773000 | 0.191655000 | -0.606221000 |
| H | 7.274149000 | -0.439370000 | -0.034187000 |
| H | 6.832173000 | 1.239926000 | -0.398759000 |
| H | 6.752474000 | -0.002501000 | -1.673355000 |
| C | 4.534390000 | 0.562181000 | 0.845148000 |
| H | 5.093547000 | 1.331029000 | 1.385413000 |
| C | 3.218267000 | 0.287314000 | 1.237550000 |
| C | 2.556723000 | 1.057898000 | 2.347757000 |
| H | 3.287641000 | 1.683447000 | 2.876981000 |
| H | 2.078860000 | 0.393214000 | 3.083773000 |
| H | 1.767862000 | 1.714809000 | 1.944679000 |
| C | -2.388448000 | -0.734641000 | 0.601551000 |
| C | -3.064237000 | 0.233882000 | 1.362058000 |
| C | -2.368221000 | 0.990434000 | 2.462009000 |
| H | -3.093735000 | 1.556035000 | 3.061880000 |
| H | -1.641044000 | 1.703298000 | 2.040756000 |
| H | -1.814264000 | 0.321607000 | 3.139016000 |
| C | -4.400733000 | 0.499712000 | 1.037754000 |
| H | -4.938662000 | 1.259904000 | 1.610915000 |
| C | -5.057412000 | -0.171782000 | -0.001154000 |
| C | -6.479747000 | 0.173685000 | -0.366088000 |
| H | -7.022812000 | -0.703888000 | -0.745988000 |
| H | -6.499383000 | 0.941060000 | -1.157477000 |
| H | -7.030738000 | 0.575035000 | 0.496462000 |
| C | -4.351801000 | -1.145778000 | -0.720715000 |
| H | -4.847552000 | -1.674617000 | -1.539354000 |
| C | -3.014478000 | -1.441231000 | -0.439945000 |
| C | -2.246115000 | -2.428910000 | -1.277497000 |
| H | -1.717863000 | -3.178604000 | -0.667949000 |
| H | -1.494298000 | -1.897949000 | -1.882422000 |
| H | -2.917987000 | -2.961099000 | -1.963707000 |
| C | 1.764527000 | 1.066663000 | -1.793055000 |
| H | 1.956250000 | 0.507221000 | -2.724142000 |
| H | 2.694298000 | 1.509899000 | -1.400604000 |

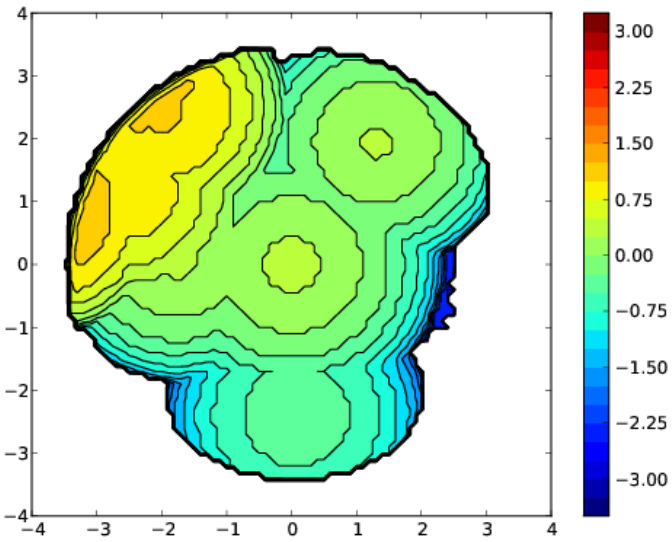
# Co-Id




Zero-point correction= 0.782905 (Hartree/Particle)
Thermal correction to Energy= 0.836801
Thermal correction to Enthalpy= 0.837745
Thermal correction to Gibbs Free Energy= 0.691350
Sum of electronic and zero-point Energies= -3298.698649
Sum of electronic and thermal Energies= -3298.644752
Sum of electronic and thermal Enthalpies= -3298.643808
Sum of electronic and thermal Free Energies= -3298.790204

HOMO -0.13657 LUMO -0.11705

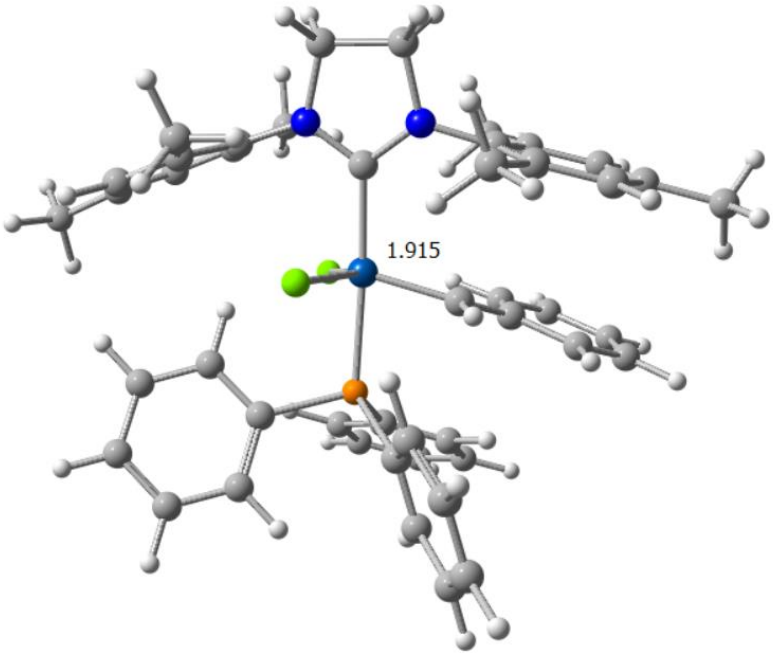
| | | | |
|---|---|---|---|
| Co | -0.150039000 | -0.315557000 | -0.188613000 |
| Cl | -1.030690000 | -0.252222000 | 1.991772000 |
| Cl | -0.699026000 | -0.190768000 | -2.537339000 |
| P | -0.251242000 | 1.942560000 | -0.206200000 |
| N | -1.601311000 | -2.844262000 | -0.443379000 |
| N | 0.556940000 | -3.085458000 | -0.737031000 |
| C | -0.411993000 | -2.198937000 | -0.397567000 |
| C | -1.478926000 | -4.215542000 | -0.991047000 |
| H | -1.879831000 | -4.234744000 | -2.017162000 |
| H | -2.050416000 | -4.923236000 | -0.375031000 |
| C | 0.036117000 | -4.455291000 | -0.951144000 |
| H | 0.346211000 | -5.108093000 | -0.117090000 |
| H | 0.428665000 | -4.874790000 | -1.887426000 |
| C | -2.876771000 | -2.384145000 | 0.031316000 |
| C | -3.191516000 | -2.629057000 | 1.386992000 |
| C | -2.233360000 | -3.358356000 | 2.289896000 |
| H | -2.714124000 | -3.598628000 | 3.247895000 |
| H | -1.356003000 | -2.727022000 | 2.491022000 |
| H | -1.880356000 | -4.299437000 | 1.839105000 |
| C | -4.418913000 | -2.176853000 | 1.875206000 |
| H | -4.656182000 | -2.335912000 | 2.930804000 |
| C | -5.344680000 | -1.522082000 | 1.048698000 |
| C | -6.632986000 | -0.978115000 | 1.615381000 |
| H | -7.369799000 | -0.783379000 | 0.822934000 |
| H | -6.457070000 | -0.028684000 | 2.148663000 |
| H | -7.082060000 | -1.675267000 | 2.338745000 |
| C | -5.038250000 | -1.383665000 | -0.306801000 |
| H | -5.766323000 | -0.922248000 | -0.979927000 |
| C | -3.820162000 | -1.827015000 | -0.847786000 |
| C | -3.606402000 | -1.760249000 | -2.335167000 |
| H | -3.981682000 | -0.810139000 | -2.740924000 |
| H | -4.162215000 | -2.576057000 | -2.829163000 |
| H | -2.546503000 | -1.822682000 | -2.604772000 |
| C | 1.962464000 | -2.892310000 | -0.576270000 |
| C | 2.762785000 | -2.694253000 | -1.717776000 |
| C | 2.130495000 | -2.570117000 | -3.077144000 |
| H | 2.860876000 | -2.213480000 | -3.816254000 |
| H | 1.273035000 | -1.876397000 | -3.052769000 |
| H | 1.746943000 | -3.541588000 | -3.431396000 |
| C | 4.146632000 | -2.570985000 | -1.533361000 |
| H | 4.780678000 | -2.391564000 | -2.406289000 |
| C | 4.734119000 | -2.657214000 | -0.264388000 |
| C | 6.223389000 | -2.509075000 | -0.085048000 |
| H | 6.679211000 | -3.452515000 | 0.256203000 |
| H | 6.450551000 | -1.742701000 | 0.672168000 |
| H | 6.713465000 | -2.218661000 | -1.024806000 |
| C | 3.905703000 | -2.872164000 | 0.848108000 |
| H | 4.346764000 | -2.912320000 | 1.847567000 |
| C | 2.521755000 | -2.996364000 | 0.716547000 |
| C | 1.628527000 | -3.149561000 | 1.914591000 |
| H | 1.018733000 | -4.065242000 | 1.858137000 |
| H | 0.923030000 | -2.304108000 | 1.978275000 |
| H | 2.216448000 | -3.184327000 | 2.840766000 |
| C | 1.635151000 | -0.191708000 | -0.363581000 |
| C | 3.957317000 | 0.500643000 | 0.111561000 |
| C | 2.665808000 | 0.156599000 | 0.583317000 |
| C | 4.977774000 | 0.827452000 | 1.001606000 |
| C | 2.432454000 | 0.152989000 | 1.980238000 |
| C | 4.735231000 | 0.786965000 | 2.381575000 |
| H | 5.964703000 | 1.106668000 | 0.626609000 |
| C | 3.463301000 | 0.448345000 | 2.865730000 |
| H | 1.422698000 | -0.067398000 | 2.335257000 |
| H | 5.537680000 | 1.031649000 | 3.081497000 |
| H | 3.272678000 | 0.441552000 | 3.940654000 |
| C | -1.990125000 | 2.390118000 | -0.641077000 |
| C | -2.266570000 | 3.347194000 | -1.628280000 |
| C | -3.047127000 | 1.709175000 | -0.012771000 |
| C | -3.590873000 | 3.639958000 | -1.965653000 |
| H | -1.450318000 | 3.853977000 | -2.143555000 |
| C | -4.367305000 | 2.016757000 | -0.348480000 |
| H | -2.832481000 | 0.933956000 | 0.726975000 |
| C | -4.644014000 | 2.980751000 | -1.323145000 |
| H | -3.798163000 | 4.382347000 | -2.739436000 |
| H | -5.179542000 | 1.480981000 | 0.145245000 |
| H | -5.677901000 | 3.211050000 | -1.589984000 |
| C | 0.792929000 | 2.945281000 | -1.360055000 |
| C | 0.972173000 | 4.319317000 | -1.116091000 |
| C | 1.402431000 | 2.361717000 | -2.479678000 |
| C | 1.762223000 | 5.090668000 | -1.971420000 |
| H | 0.498526000 | 4.784085000 | -0.250299000 |




| South West | North West | North East | North West | **Total %V_Bur** |
|---|---|---|---|---|
| 43.0 | 62.5 | 46.0 | 33.0 | 46.1 |

| | | | |
|---|---|---|---|
| C | 2.198468000 | 3.136588000 | -3.328978000 |
| H | 1.202335000 | 1.313622000 | -2.706092000 |
| C | 2.384713000 | 4.498951000 | -3.076555000 |
| H | 1.893638000 | 6.156137000 | -1.771062000 |
| H | 2.667027000 | 2.670708000 | -4.198642000 |
| H | 3.005794000 | 5.101755000 | -3.742815000 |
| C | 0.097542000 | 2.784031000 | 1.397909000 |
| C | -0.924033000 | 3.060291000 | 2.317565000 |
| C | 1.429634000 | 3.073560000 | 1.737104000 |
| C | -0.617143000 | 3.632316000 | 3.554458000 |
| H | -1.958732000 | 2.829262000 | 2.065904000 |
| C | 1.732689000 | 3.641357000 | 2.976449000 |
| H | 2.231974000 | 2.867066000 | 1.028133000 |
| C | 0.710462000 | 3.921378000 | 3.888684000 |
| H | -1.420178000 | 3.846740000 | 4.262589000 |
| H | 2.772778000 | 3.858523000 | 3.227923000 |
| H | 0.947085000 | 4.365794000 | 4.857891000 |
| H | 4.134251000 | 0.511443000 | -0.965663000 |
| H | 2.012746000 | -0.212231000 | -1.399379000 |

# Co-Iq




Zero-point correction= 0.781835 (Hartree/Particle)
Thermal correction to Energy= 0.835116
Thermal correction to Enthalpy= 0.836060
Thermal correction to Gibbs Free Energy= 0.691955
Sum of electronic and zero-point Energies= -3298.681529
Sum of electronic and thermal Energies= -3298.628248

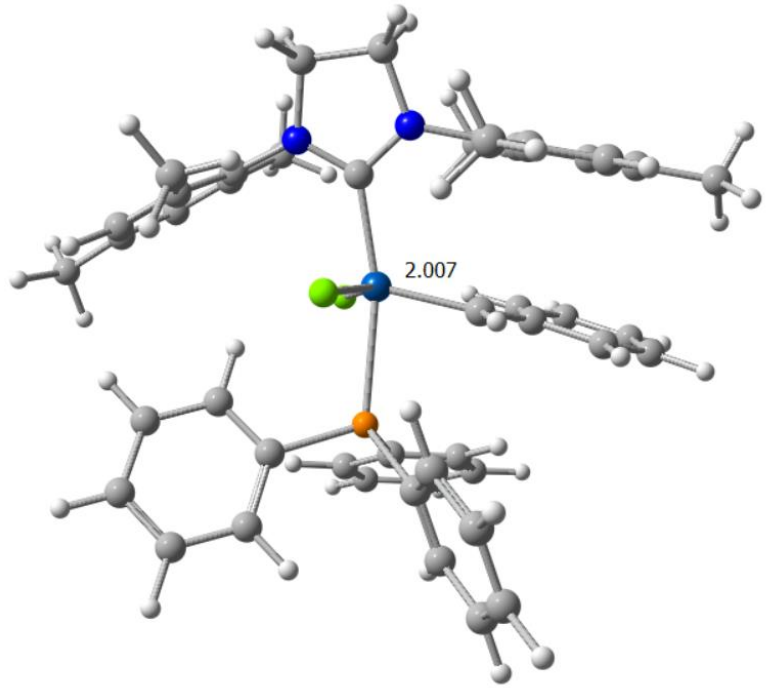
| | | | |
|---|---|---|---|
| Co | -0.268983000 | -0.349971000 | -0.181929000 |
| Cl | -1.106306000 | -0.110270000 | 1.932025000 |
| Cl | -1.264307000 | -0.184588000 | -2.256008000 |
| P | -0.138278000 | 1.933344000 | -0.227267000 |
| N | -1.667915000 | -3.024917000 | -0.246023000 |
| N | 0.484395000 | -3.241889000 | -0.524705000 |
| C | -0.494937000 | -2.356930000 | -0.265098000 |
| C | -1.520171000 | -4.481415000 | -0.493683000 |
| H | -2.102638000 | -4.769602000 | -1.381141000 |
| H | -1.899312000 | -5.046359000 | 0.371138000 |
| C | -0.003216000 | -4.635040000 | -0.696072000 |
| H | 0.470110000 | -5.290408000 | 0.050356000 |
| H | 0.262952000 | -5.003393000 | -1.697843000 |
| C | -2.946779000 | -2.479692000 | 0.106761000 |
| C | -3.292051000 | -2.395949000 | 1.472091000 |
| C | -2.419103000 | -2.997291000 | 2.543113000 |
| H | -2.602152000 | -2.511604000 | 3.510161000 |
| H | -1.353787000 | -2.884987000 | 2.312475000 |
| H | -2.641403000 | -4.072773000 | 2.659078000 |
| C | -4.502816000 | -1.784391000 | 1.809035000 |
| H | -4.761275000 | -1.678276000 | 2.866271000 |
| C | -5.378464000 | -1.291681000 | 0.830798000 |
| C | -6.645000000 | -0.573175000 | 1.227312000 |
| H | -7.299341000 | -0.406429000 | 0.360022000 |
| H | -6.416719000 | 0.409350000 | 1.672402000 |
| H | -7.212400000 | -1.142903000 | 1.979288000 |
| C | -5.047546000 | -1.483040000 | -0.514589000 |
| H | -5.738488000 | -1.145490000 | -1.292268000 |
| C | -3.847887000 | -2.098942000 | -0.902896000 |
| C | -3.595667000 | -2.400659000 | -2.356756000 |
| H | -3.959067000 | -1.584609000 | -2.995440000 |
| H | -4.133955000 | -3.320326000 | -2.646082000 |
| H | -2.528168000 | -2.527134000 | -2.566329000 |
| C | 1.893602000 | -2.992022000 | -0.500630000 |
| C | 2.564996000 | -2.722995000 | -1.704600000 |
| C | 1.796003000 | -2.576552000 | -2.991108000 |
| H | 2.459409000 | -2.261176000 | -3.807799000 |
| H | 0.985435000 | -1.837324000 | -2.887850000 |
| H | 1.322794000 | -3.525364000 | -3.292969000 |
| C | 3.954719000 | -2.551792000 | -1.653658000 |
| H | 4.493024000 | -2.325426000 | -2.578397000 |
| C | 4.665967000 | -2.648210000 | -0.450698000 |
| C | 6.157758000 | -2.438314000 | -0.408787000 |
| H | 6.674560000 | -3.318502000 | 0.005064000 |
| H | 6.405316000 | -1.578649000 | 0.233586000 |

Sum of electronic and thermal Enthalpies= -3298.627304
Sum of electronic and thermal Free Energies= -3298.771409

HOMO -0.13132 LUMO -0.13177

| | | | |
|---|---|---|---|
| H | 6.564997000 | -2.244668000 | -1.411054000 |
| C | 3.956732000 | -2.909632000 | 0.730212000 |
| H | 4.492649000 | -2.941590000 | 1.682359000 |
| C | 2.570813000 | -3.085668000 | 0.728873000 |
| C | 1.804769000 | -3.301703000 | 2.006630000 |
| H | 1.268852000 | -4.265115000 | 2.009727000 |
| H | 1.052013000 | -2.510320000 | 2.145156000 |
| H | 2.480542000 | -3.284961000 | 2.871533000 |
| C | 1.609846000 | -0.053596000 | -0.404800000 |
| C | 3.947977000 | 0.545873000 | 0.057731000 |
| C | 2.648863000 | 0.175089000 | 0.526571000 |
| C | 5.002533000 | 0.740163000 | 0.940144000 |
| C | 2.477799000 | 0.029891000 | 1.935203000 |
| C | 4.815395000 | 0.561631000 | 2.321968000 |
| H | 5.981344000 | 1.038158000 | 0.556092000 |
| C | 3.544810000 | 0.209453000 | 2.805096000 |
| H | 1.481485000 | -0.201640000 | 2.315254000 |
| H | 5.646446000 | 0.712925000 | 3.013692000 |
| H | 3.385522000 | 0.094851000 | 3.879778000 |
| C | -1.864695000 | 2.586190000 | -0.458633000 |
| C | -2.052616000 | 3.905597000 | -0.896286000 |
| C | -2.979189000 | 1.780327000 | -0.182900000 |
| C | -3.344361000 | 4.419881000 | -1.040102000 |
| H | -1.191873000 | 4.532328000 | -1.133856000 |
| C | -4.267517000 | 2.298515000 | -0.331934000 |
| H | -2.846795000 | 0.752644000 | 0.150975000 |
| C | -4.454908000 | 3.616769000 | -0.759724000 |
| H | -3.480925000 | 5.448017000 | -1.382284000 |
| H | -5.124977000 | 1.656246000 | -0.123402000 |
| H | -5.464037000 | 4.017510000 | -0.878701000 |
| C | 0.829188000 | 2.802595000 | -1.547938000 |
| C | 1.347379000 | 4.090976000 | -1.327721000 |
| C | 1.022240000 | 2.195460000 | -2.799861000 |
| C | 2.056337000 | 4.751210000 | -2.336098000 |
| H | 1.205103000 | 4.579581000 | -0.363685000 |
| C | 1.732299000 | 2.858688000 | -3.802612000 |
| H | 0.586713000 | 1.213957000 | -2.991039000 |
| C | 2.256185000 | 4.135921000 | -3.574950000 |
| H | 2.454026000 | 5.750643000 | -2.146972000 |
| H | 1.873195000 | 2.372402000 | -4.770338000 |
| H | 2.812502000 | 4.651210000 | -4.360840000 |
| C | 0.412902000 | 2.766131000 | 1.319287000 |
| C | -0.538209000 | 3.112575000 | 2.292611000 |
| C | 1.774605000 | 3.003226000 | 1.568978000 |
| C | -0.130945000 | 3.694308000 | 3.494569000 |
| H | -1.595179000 | 2.922759000 | 2.108198000 |
| C | 2.176444000 | 3.588524000 | 2.772035000 |
| H | 2.525517000 | 2.735775000 | 0.827105000 |
| C | 1.226657000 | 3.931365000 | 3.738404000 |
| H | -0.878367000 | 3.959204000 | 4.245181000 |
| H | 3.239004000 | 3.760206000 | 2.953415000 |
| H | 1.542654000 | 4.383993000 | 4.680890000 |
| H | 4.092219000 | 0.681961000 | -1.016296000 |
| H | 1.869803000 | 0.084557000 | -1.462440000 |

# Co-Is



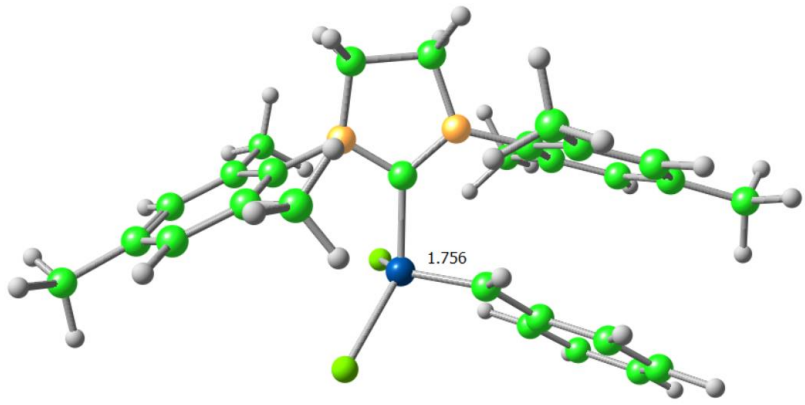

Zero-point correction= 0.779003 (Hartree/Particle)
Thermal correction to Energy= 0.833745
Thermal correction to Enthalpy= 0.834690
Thermal correction to Gibbs Free Energy= 0.681624
Sum of electronic and zero-point Energies= -3298.633770
Sum of electronic and thermal Energies= -3298.579028
Sum of electronic and thermal Enthalpies= -3298.578083
Sum of electronic and thermal Free Energies= -3298.731150

HOMO -0.12791 LUMO -0.16796

| | | | |
|---|---|---|---|
| Co | -0.061645000 | -0.427746000 | -0.219832000 |
| Cl | -0.850342000 | -0.328016000 | 1.879913000 |
| Cl | -0.853238000 | -0.395597000 | -2.358126000 |
| P | -0.568159000 | 2.108613000 | -0.223900000 |
| N | -1.226703000 | -3.344184000 | -0.283372000 |
| N | 0.927673000 | -3.302403000 | -0.618420000 |
| C | -0.138970000 | -2.553872000 | -0.299241000 |
| C | -0.930486000 | -4.757039000 | -0.643376000 |
| H | -1.451799000 | -5.017982000 | -1.576870000 |
| H | -1.280346000 | -5.431207000 | 0.151606000 |
| C | 0.601676000 | -4.743475000 | -0.797478000 |
| H | 1.118651000 | -5.337105000 | -0.027688000 |
| H | 0.938465000 | -5.088554000 | -1.785144000 |
| C | -2.543704000 | -2.934881000 | 0.109190000 |
| C | -2.864349000 | -2.956955000 | 1.483669000 |
| C | -1.879403000 | -3.474317000 | 2.498889000 |
| H | -2.272027000 | -3.350486000 | 3.516672000 |
| H | -0.926027000 | -2.933427000 | 2.434674000 |
| H | -1.671161000 | -4.546219000 | 2.344809000 |
| C | -4.123496000 | -2.497372000 | 1.875273000 |
| H | -4.371680000 | -2.483067000 | 2.940135000 |
| C | -5.068784000 | -2.048760000 | 0.939330000 |
| C | -6.399977000 | -1.504808000 | 1.396459000 |
| H | -7.101654000 | -1.402500000 | 0.556538000 |
| H | -6.279893000 | -0.510760000 | 1.858095000 |
| H | -6.863412000 | -2.157885000 | 2.151471000 |
| C | -4.741219000 | -2.110525000 | -0.417939000 |
| H | -5.477644000 | -1.797623000 | -1.163681000 |
| C | -3.488394000 | -2.564956000 | -0.861548000 |
| C | -3.219563000 | -2.695186000 | -2.337442000 |
| H | -3.577378000 | -1.809081000 | -2.879163000 |
| H | -3.749988000 | -3.574226000 | -2.741637000 |
| H | -2.149944000 | -2.795943000 | -2.551298000 |
| C | 2.293622000 | -2.866643000 | -0.574760000 |
| C | 2.942665000 | -2.516061000 | -1.770251000 |
| C | 2.201050000 | -2.518708000 | -3.080383000 |
| H | 2.856842000 | -2.188782000 | -3.897406000 |
| H | 1.327094000 | -1.849392000 | -3.039626000 |
| H | 1.824720000 | -3.522415000 | -3.336834000 |
| C | 4.283439000 | -2.117157000 | -1.693532000 |
| H | 4.798276000 | -1.821138000 | -2.611964000 |
| C | 4.971626000 | -2.066831000 | -0.475104000 |
| C | 6.412615000 | -1.629519000 | -0.411154000 |
| H | 7.078644000 | -2.484156000 | -0.207817000 |
| H | 6.557525000 | -0.893229000 | 0.392835000 |
| H | 6.733294000 | -1.170855000 | -1.357066000 |
| C | 4.288603000 | -2.425350000 | 0.694926000 |
| H | 4.797805000 | -2.349153000 | 1.658872000 |
| C | 2.949765000 | -2.825617000 | 0.669231000 |
| C | 2.206920000 | -3.136341000 | 1.941632000 |
| H | 1.771152000 | -4.148462000 | 1.932365000 |
| H | 1.377419000 | -2.427514000 | 2.088623000 |
| H | 2.875550000 | -3.059822000 | 2.808674000 |
| C | 1.809393000 | 0.251045000 | -0.475328000 |
| C | 4.049507000 | 1.141541000 | 0.034361000 |
| C | 2.813641000 | 0.555302000 | 0.465641000 |
| C | 5.054662000 | 1.458261000 | 0.937960000 |
| C | 2.669242000 | 0.321811000 | 1.869322000 |
| C | 4.893151000 | 1.194697000 | 2.310121000 |
| H | 5.981124000 | 1.912181000 | 0.576478000 |
| C | 3.687998000 | 0.628010000 | 2.759806000 |
| H | 1.724991000 | -0.082760000 | 2.233909000 |
| H | 5.687726000 | 1.441107000 | 3.017008000 |
| H | 3.541810000 | 0.439396000 | 3.826297000 |
| C | -2.367861000 | 2.405871000 | -0.526558000 |
| C | -2.845763000 | 3.611188000 | -1.063614000 |
| C | -3.271340000 | 1.371838000 | -0.229417000 |
| C | -4.215228000 | 3.788904000 | -1.279456000 |
| H | -2.144630000 | 4.407988000 | -1.318382000 |
| C | -4.639744000 | 1.556649000 | -0.442172000 |
| H | -2.906144000 | 0.423263000 | 0.168142000 |
| C | -5.114803000 | 2.762983000 | -0.967258000 |
| H | -4.579866000 | 4.729756000 | -1.697804000 |
| H | -5.330690000 | 0.744746000 | -0.209793000 |
| H | -6.184369000 | 2.902566000 | -1.139333000 |
| C | 0.273265000 | 3.236182000 | -1.423119000 |
| C | 0.552471000 | 4.575833000 | -1.102535000 |
| C | 0.627171000 | 2.744768000 | -2.690176000 |
| C | 1.175714000 | 5.409208000 | -2.036135000 |
| H | 0.288482000 | 4.964429000 | -0.117908000 |
| C | 1.247574000 | 3.582329000 | -3.620591000 |
| H | 0.405290000 | 1.706737000 | -2.944182000 |
| C | 1.526483000 | 4.914719000 | -3.296409000 |
| H | 1.388471000 | 6.448259000 | -1.774964000 |
| H | 1.518095000 | 3.189084000 | -4.603003000 |
| H | 2.016089000 | 5.565852000 | -4.023794000 |
| C | -0.242466000 | 2.914903000 | 1.392902000 |
| C | -1.276792000 | 3.164955000 | 2.308030000 |
| C | 1.089648000 | 3.164342000 | 1.767565000 |
| C | -0.982021000 | 3.668090000 | 3.578019000 |
| H | -2.310746000 | 2.962612000 | 2.024774000 |
| C | 1.378081000 | 3.665835000 | 3.037424000 |
| H | 1.901875000 | 2.956857000 | 1.070546000 |
| C | 0.344206000 | 3.918965000 | 3.946443000 |
| H | -1.793175000 | 3.862226000 | 4.283188000 |

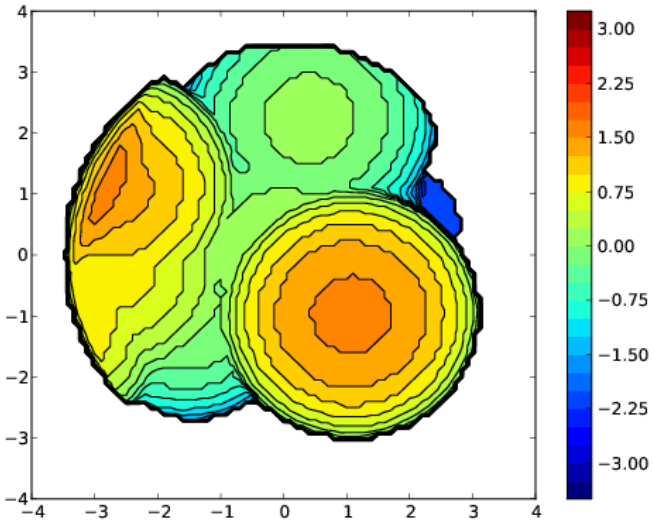
| | | | | |
|---|---|---|---|---|
| H | 2.417728000 | 3.845179000 | 3.318177000 |
| H | 0.572169000 | 4.307476000 | 4.941350000 |
| H | 4.183323000 | 1.340352000 | -1.031490000 |
| H | 2.041881000 | 0.448023000 | -1.529591000 |

# Co-IId




Zero-point correction= 0.514716 (Hartree/Particle)
Thermal correction to Energy= 0.551529
Thermal correction to Enthalpy= 0.552473
Thermal correction to Gibbs Free Energy= 0.441666
Sum of electronic and zero-point Energies= -2262.294425
Sum of electronic and thermal Energies= -2262.257613
Sum of electronic and thermal Enthalpies= -2262.256668
Sum of electronic and thermal Free Energies= -2262.367475

HOMO -0.16584 LUMO -0.12642

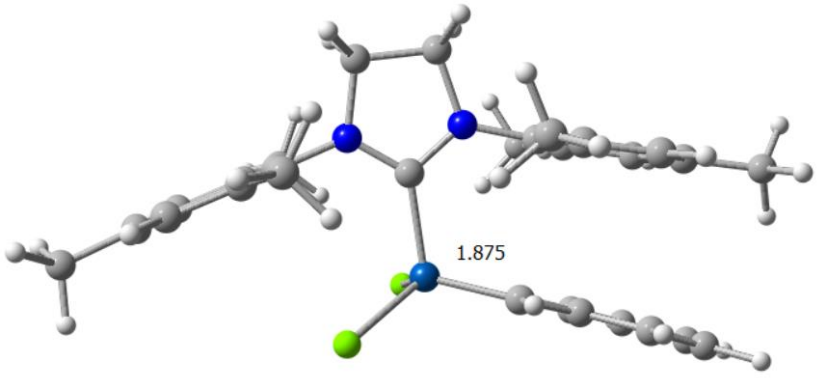



| South West | North West | North East | North West | **Total %V_Bur** |
|---|---|---|---|---|
| 52.2 | 61.3 | 45.1 | 66.5 | 56.3 |

| | | | |
|---|---|---|---|
| Co | -0.488163000 | 0.912779000 | -0.058488000 |
| Cl | -0.778449000 | 1.380037000 | 2.156931000 |
| Cl | -1.447245000 | 2.514675000 | -1.191661000 |
| N | -1.809919000 | -1.516312000 | 0.301109000 |
| N | 0.350848000 | -1.903370000 | 0.228889000 |
| C | -0.597166000 | -0.938357000 | 0.156567000 |
| C | -1.730818000 | -2.992884000 | 0.365070000 |
| H | -2.111925000 | -3.424099000 | -0.576217000 |
| H | -2.336614000 | -3.377840000 | 1.196036000 |
| C | -0.222455000 | -3.229542000 | 0.559927000 |
| H | 0.030765000 | -3.494334000 | 1.599344000 |
| H | 0.182981000 | -4.003820000 | -0.105744000 |
| C | -3.044939000 | -0.833662000 | 0.037413000 |
| C | -3.889033000 | -0.515983000 | 1.118474000 |
| C | -3.504180000 | -0.863773000 | 2.530392000 |
| H | -4.273359000 | -0.522712000 | 3.236093000 |
| H | -2.549773000 | -0.378500000 | 2.790431000 |
| H | -3.379371000 | -1.950306000 | 2.668124000 |
| C | -5.075127000 | 0.171309000 | 0.840258000 |
| H | -5.731623000 | 0.443765000 | 1.671206000 |
| C | -5.432764000 | 0.532484000 | -0.466040000 |
| C | -6.684440000 | 1.331380000 | -0.729971000 |
| H | -7.101312000 | 1.109758000 | -1.723099000 |
| H | -6.465022000 | 2.411389000 | -0.698092000 |
| H | -7.458688000 | 1.129496000 | 0.024268000 |
| C | -4.583382000 | 0.167634000 | -1.517382000 |
| H | -4.850305000 | 0.436958000 | -2.542849000 |
| C | -3.384781000 | -0.517869000 | -1.291695000 |
| C | -2.472223000 | -0.845777000 | -2.445233000 |
| H | -3.042774000 | -0.918575000 | -3.381364000 |
| H | -1.931018000 | -1.791586000 | -2.296531000 |
| H | -1.724043000 | -0.045403000 | -2.568634000 |
| C | 1.762053000 | -1.705449000 | 0.116963000 |
| C | 2.380933000 | -1.974114000 | -1.119893000 |
| C | 1.573085000 | -2.447735000 | -2.300578000 |
| H | 2.159980000 | -2.385937000 | -3.226683000 |
| H | 0.657208000 | -1.851376000 | -2.426256000 |
| H | 1.256389000 | -3.496932000 | -2.179729000 |
| C | 3.760374000 | -1.760715000 | -1.229932000 |
| H | 4.250352000 | -1.944915000 | -2.189986000 |
| C | 4.519970000 | -1.297178000 | -0.148165000 |
| C | 5.993668000 | -1.020480000 | -0.291898000 |
| H | 6.576294000 | -1.536505000 | 0.486561000 |
| H | 6.190551000 | 0.058725000 | -0.187798000 |
| H | 6.371191000 | -1.341082000 | -1.272781000 |
| C | 3.874434000 | -1.073040000 | 1.076689000 |
| H | 4.455024000 | -0.713211000 | 1.930174000 |
| C | 2.502371000 | -1.282467000 | 1.240320000 |
| C | 1.827703000 | -1.025888000 | 2.556368000 |
| H | 1.288457000 | -1.917721000 | 2.913559000 |
| H | 1.079128000 | -0.219351000 | 2.475337000 |
| H | 2.562784000 | -0.744293000 | 3.321754000 |
| C | 1.064638000 | 0.842099000 | -0.874627000 |
| C | 3.354343000 | 1.567259000 | -1.378121000 |
| C | 2.254190000 | 1.543789000 | -0.482221000 |
| C | 4.540461000 | 2.210518000 | -1.034777000 |
| C | 2.391179000 | 2.182070000 | 0.777115000 |
| C | 4.661822000 | 2.823901000 | 0.218223000 |
| H | 5.373666000 | 2.232088000 | -1.740153000 |
| C | 3.584877000 | 2.806098000 | 1.118685000 |
| H | 1.543923000 | 2.167208000 | 1.467574000 |
| H | 5.593273000 | 3.324483000 | 0.491735000 |
| H | 3.681071000 | 3.292031000 | 2.091607000 |
| H | 3.253803000 | 1.074820000 | -2.347195000 |
| H | 1.130923000 | 0.338645000 | -1.852664000 |

| | |
|---|---|
| | |

# Co-IIq

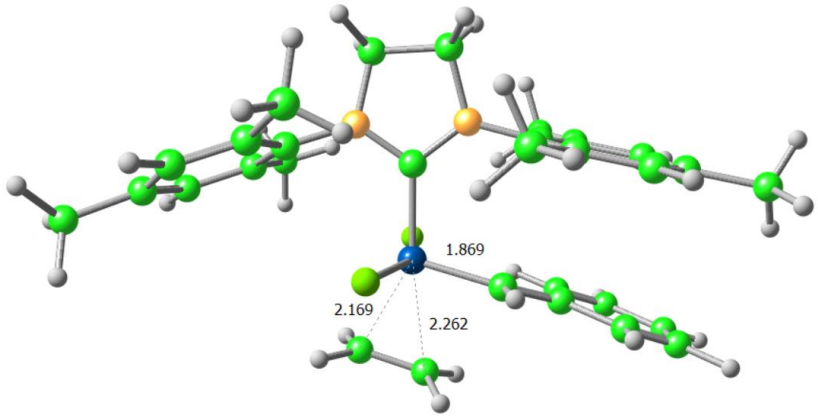



Zero-point correction= 0.513868 (Hartree/Particle)
Thermal correction to Energy= 0.548295
Thermal correction to Enthalpy= 0.549239
Thermal correction to Gibbs Free Energy= 0.446818
Sum of electronic and zero-point Energies= -2262.281826
Sum of electronic and thermal Energies= -2262.247400
Sum of electronic and thermal Enthalpies= -2262.246455
Sum of electronic and thermal Free Energies= -2262.348876

HOMO -0.16320 LUMO -0.14031

| | | | |
|---|---|---|---|
| Co | -0.303089000 | 1.043517000 | -0.375869000 |
| Cl | -0.506867000 | 2.180071000 | 1.549198000 |
| Cl | -1.752711000 | 1.713945000 | -1.912983000 |
| N | -1.937070000 | -1.316710000 | 0.510849000 |
| N | 0.203025000 | -1.745599000 | 0.482755000 |
| C | -0.730245000 | -0.807647000 | 0.217387000 |
| C | -1.879461000 | -2.720068000 | 0.996986000 |
| H | -2.434549000 | -3.373460000 | 0.307017000 |
| H | -2.345138000 | -2.792754000 | 1.990275000 |
| C | -0.367600000 | -3.008833000 | 1.016691000 |
| H | 0.020633000 | -3.197155000 | 2.029157000 |
| H | -0.080448000 | -3.854865000 | 0.374772000 |
| C | -3.207221000 | -0.695180000 | 0.266977000 |
| C | -3.853964000 | -0.023175000 | 1.317776000 |
| C | -3.217864000 | 0.098440000 | 2.676791000 |
| H | -3.913597000 | 0.562730000 | 3.388695000 |
| H | -2.310162000 | 0.720657000 | 2.622774000 |
| H | -2.922910000 | -0.882194000 | 3.083527000 |
| C | -5.099788000 | 0.557999000 | 1.049672000 |
| H | -5.610163000 | 1.099398000 | 1.851092000 |
| C | -5.699271000 | 0.471900000 | -0.213395000 |
| C | -7.013903000 | 1.157597000 | -0.492326000 |
| H | -7.610215000 | 0.600785000 | -1.229938000 |
| H | -6.843382000 | 2.167093000 | -0.901639000 |
| H | -7.612671000 | 1.269684000 | 0.423051000 |
| C | -5.034830000 | -0.235423000 | -1.223915000 |
| H | -5.489979000 | -0.312444000 | -2.215131000 |
| C | -3.787140000 | -0.828702000 | -1.007015000 |
| C | -3.061256000 | -1.533553000 | -2.121971000 |
| H | -3.730204000 | -1.699334000 | -2.977089000 |
| H | -2.656057000 | -2.508294000 | -1.808844000 |
| H | -2.219588000 | -0.909628000 | -2.462543000 |
| C | 1.614610000 | -1.615873000 | 0.303662000 |
| C | 2.183005000 | -2.022263000 | -0.918400000 |
| C | 1.307645000 | -2.484568000 | -2.054335000 |
| H | 1.900090000 | -2.638554000 | -2.966079000 |
| H | 0.516813000 | -1.751060000 | -2.271079000 |
| H | 0.803672000 | -3.436129000 | -1.819100000 |
| C | 3.576559000 | -1.967629000 | -1.045543000 |
| H | 4.034904000 | -2.273443000 | -1.990074000 |
| C | 4.394054000 | -1.528419000 | 0.003809000 |
| C | 5.893523000 | -1.487330000 | -0.141276000 |
| H | 6.381710000 | -2.144768000 | 0.595318000 |
| H | 6.271926000 | -0.467246000 | 0.026336000 |
| H | 6.209093000 | -1.807508000 | -1.143963000 |
| C | 3.788012000 | -1.118707000 | 1.201324000 |
| H | 4.413019000 | -0.748217000 | 2.017938000 |
| C | 2.401843000 | -1.154919000 | 1.376212000 |
| C | 1.754803000 | -0.668746000 | 2.643935000 |
| H | 1.135529000 | -1.449513000 | 3.113495000 |
| H | 1.087269000 | 0.185969000 | 2.442133000 |
| H | 2.513364000 | -0.353848000 | 3.372596000 |
| C | 1.412736000 | 1.042212000 | -1.130975000 |
| C | 3.843602000 | 1.332858000 | -1.535983000 |
| C | 2.705651000 | 1.464121000 | -0.692136000 |
| C | 5.090445000 | 1.801633000 | -1.135460000 |
| C | 2.883733000 | 2.064673000 | 0.583838000 |
| C | 5.239923000 | 2.385355000 | 0.130866000 |
| H | 5.951386000 | 1.709988000 | -1.800758000 |
| C | 4.135458000 | 2.513770000 | 0.987006000 |
| H | 2.005288000 | 2.183892000 | 1.222259000 |
| H | 6.219207000 | 2.751412000 | 0.447672000 |
| H | 4.257650000 | 2.979595000 | 1.966943000 |
| H | 3.715321000 | 0.871129000 | -2.517386000 |
| H | 1.438401000 | 0.623887000 | -2.155056000 |

# Co-IIId

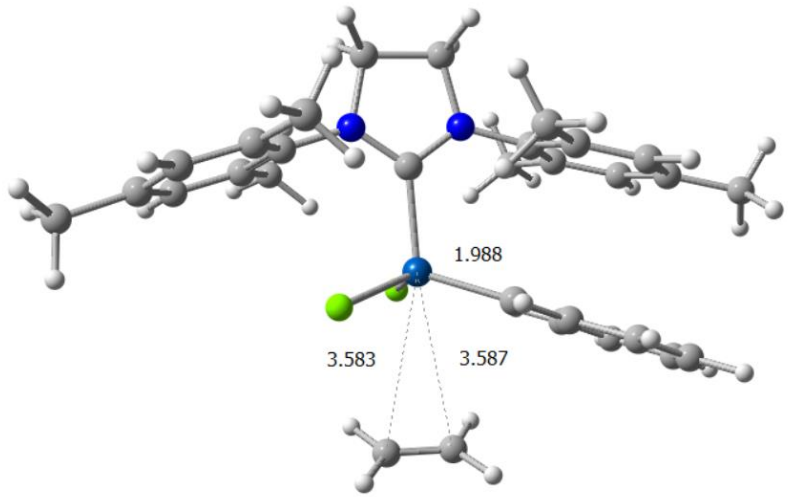



Zero-point correction= 0.569221 (Hartree/Particle)
Thermal correction to Energy= 0.608513
Thermal correction to Enthalpy= 0.609457
Thermal correction to Gibbs Free Energy= 0.495733
Sum of electronic and zero-point Energies= -2340.859842
Sum of electronic and thermal Energies= -2340.820551
Sum of electronic and thermal Enthalpies= -2340.819606
Sum of electronic and thermal Free Energies= -2340.933330

HOMO -0.14138 LUMO -0.12422

| | | | |
|---|---|---|---|
| Co | -0.410892000 | 1.000564000 | -0.343824000 |
| Cl | -0.237549000 | 1.835855000 | 1.833199000 |
| Cl | -1.378744000 | 0.267076000 | -2.340143000 |
| N | -1.890806000 | -1.154091000 | 0.854912000 |
| N | 0.260103000 | -1.587605000 | 0.819393000 |
| C | -0.684787000 | -0.696347000 | 0.446514000 |
| C | -1.775388000 | -2.376057000 | 1.684341000 |
| H | -2.503348000 | -3.129658000 | 1.356765000 |
| H | -1.979433000 | -2.121664000 | 2.737149000 |
| C | -0.318418000 | -2.797427000 | 1.452300000 |
| H | 0.214947000 | -3.032593000 | 2.382952000 |
| H | -0.224006000 | -3.655766000 | 0.766936000 |
| C | -3.184021000 | -0.651023000 | 0.478805000 |
| C | -3.833626000 | 0.320810000 | 1.256840000 |
| C | -3.284857000 | 0.809746000 | 2.570772000 |
| H | -3.172514000 | 1.903099000 | 2.574601000 |
| H | -2.292841000 | 0.398531000 | 2.782005000 |
| H | -3.974778000 | 0.538393000 | 3.386627000 |
| C | -5.077514000 | 0.796422000 | 0.807771000 |
| H | -5.582271000 | 1.571251000 | 1.392386000 |
| C | -5.689949000 | 0.298941000 | -0.344507000 |
| C | -7.002244000 | 0.859351000 | -0.834526000 |
| H | -7.682724000 | 0.060059000 | -1.165092000 |
| H | -6.843399000 | 1.528643000 | -1.696081000 |
| H | -7.508739000 | 1.440364000 | -0.050813000 |
| C | -5.051377000 | -0.737800000 | -1.042633000 |
| H | -5.530389000 | -1.164433000 | -1.928255000 |
| C | -3.808935000 | -1.235040000 | -0.646789000 |
| C | -3.172259000 | -2.380689000 | -1.387461000 |
| H | -3.719825000 | -2.590547000 | -2.315829000 |
| H | -3.179012000 | -3.303621000 | -0.782160000 |
| H | -2.135021000 | -2.142621000 | -1.654619000 |
| C | 1.639447000 | -1.590622000 | 0.444723000 |
| C | 2.000335000 | -2.067434000 | -0.832398000 |
| C | 0.955971000 | -2.496460000 | -1.827283000 |
| H | 1.426003000 | -2.831278000 | -2.761646000 |
| H | 0.254853000 | -1.678503000 | -2.064624000 |
| H | 0.351927000 | -3.332947000 | -1.439671000 |
| C | 3.365013000 | -2.129383000 | -1.145027000 |
| H | 3.661700000 | -2.481638000 | -2.136850000 |
| C | 4.351608000 | -1.754620000 | -0.225122000 |
| C | 5.815093000 | -1.828288000 | -0.575888000 |
| H | 6.312584000 | -0.868404000 | -0.368442000 |
| H | 5.962938000 | -2.069021000 | -1.637841000 |
| H | 6.327907000 | -2.599868000 | 0.020630000 |
| C | 3.951260000 | -1.310878000 | 1.044458000 |
| H | 4.709774000 | -0.999986000 | 1.767849000 |
| C | 2.604304000 | -1.228885000 | 1.405080000 |
| C | 2.187626000 | -0.736088000 | 2.763350000 |
| H | 1.762937000 | -1.551126000 | 3.373429000 |
| H | 1.415533000 | 0.045228000 | 2.680317000 |
| H | 3.049853000 | -0.328588000 | 3.308040000 |
| C | 1.342541000 | 0.912514000 | -0.983998000 |
| C | 3.749739000 | 1.145825000 | -1.481535000 |
| C | 2.669012000 | 1.323334000 | -0.580968000 |
| C | 5.033921000 | 1.582208000 | -1.159926000 |
| C | 2.932443000 | 1.934039000 | 0.669967000 |
| C | 5.271386000 | 2.178763000 | 0.083824000 |
| H | 5.851425000 | 1.452841000 | -1.872092000 |
| C | 4.218548000 | 2.351269000 | 0.995745000 |
| H | 2.096525000 | 2.069273000 | 1.360041000 |
| H | 6.277487000 | 2.517439000 | 0.341996000 |
| H | 4.408250000 | 2.820939000 | 1.963204000 |
| C | -1.157433000 | 2.959146000 | -0.901420000 |
| C | 0.175826000 | 2.957261000 | -1.315484000 |
| H | -1.952710000 | 2.729452000 | -1.609264000 |
| H | -1.423638000 | 3.413217000 | 0.052757000 |
| H | 0.415438000 | 2.781773000 | -2.366525000 |
| H | 3.553625000 | 0.669179000 | -2.444325000 |
| H | 1.362768000 | 0.453208000 | -1.988912000 |
| H | 0.934583000 | 3.440661000 | -0.700617000 |

# Co-IIIs

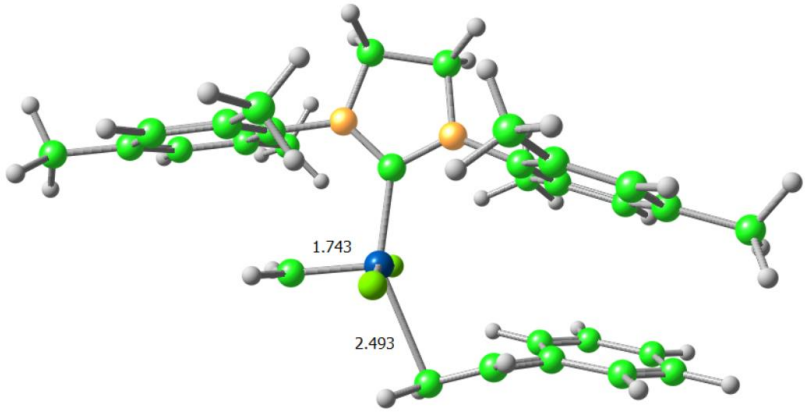



Zero-point correction= 0.563553 (Hartree/Particle)
Thermal correction to Energy= 0.604703
Thermal correction to Enthalpy= 0.605648
Thermal correction to Gibbs Free Energy= 0.484412
Sum of electronic and zero-point Energies= -2340.813668
Sum of electronic and thermal Energies= -2340.772517
Sum of electronic and thermal Enthalpies= -2340.771573
Sum of electronic and thermal Free Energies= -2340.892808

HOMO -0.13634 LUMO -0.18176

| | | | |
|---|---|---|---|
| Co | -0.301865000 | 0.932596000 | -0.092379000 |
| Cl | -0.242784000 | 1.568407000 | 2.029533000 |
| Cl | -1.860201000 | 1.693784000 | -1.407807000 |
| N | -2.038019000 | -1.574723000 | 0.337665000 |
| N | 0.102556000 | -2.008735000 | 0.374793000 |
| C | -0.813663000 | -1.050539000 | 0.172897000 |
| C | -2.007125000 | -3.022435000 | 0.681756000 |
| H | -2.565867000 | -3.597013000 | -0.071555000 |
| H | -2.483663000 | -3.180277000 | 1.660137000 |
| C | -0.499923000 | -3.332633000 | 0.688995000 |
| H | -0.137474000 | -3.687772000 | 1.664074000 |
| H | -0.203137000 | -4.062824000 | -0.078644000 |
| C | -3.294093000 | -0.910722000 | 0.146761000 |
| C | -3.931029000 | -0.310281000 | 1.245477000 |
| C | -3.305683000 | -0.331638000 | 2.614716000 |
| H | -3.955673000 | 0.168448000 | 3.344849000 |
| H | -2.331443000 | 0.180658000 | 2.614216000 |
| H | -3.133337000 | -1.361289000 | 2.967848000 |
| C | -5.162545000 | 0.318766000 | 1.021218000 |
| H | -5.666635000 | 0.801981000 | 1.862750000 |
| C | -5.759154000 | 0.346974000 | -0.245818000 |
| C | -7.061777000 | 1.073978000 | -0.470294000 |
| H | -7.657513000 | 0.596643000 | -1.261818000 |
| H | -6.875784000 | 2.115428000 | -0.780791000 |
| H | -7.668040000 | 1.107162000 | 0.446287000 |
| C | -5.103200000 | -0.288320000 | -1.309242000 |
| H | -5.555860000 | -0.276097000 | -2.304498000 |
| C | -3.869320000 | -0.923169000 | -1.136729000 |
| C | -3.148683000 | -1.548547000 | -2.302021000 |
| H | -3.778254000 | -1.533057000 | -3.201458000 |
| H | -2.863121000 | -2.594006000 | -2.105610000 |
| H | -2.225559000 | -0.990931000 | -2.522622000 |
| C | 1.514167000 | -1.904309000 | 0.138715000 |
| C | 1.989515000 | -2.049707000 | -1.177923000 |
| C | 1.033217000 | -2.195999000 | -2.332667000 |
| H | 1.580332000 | -2.330744000 | -3.275076000 |
| H | 0.397717000 | -1.302298000 | -2.430245000 |
| H | 0.358483000 | -3.057929000 | -2.207264000 |
| C | 3.371622000 | -2.013131000 | -1.383343000 |
| H | 3.757276000 | -2.100320000 | -2.402652000 |
| C | 4.270501000 | -1.844254000 | -0.320736000 |
| C | 5.757634000 | -1.819151000 | -0.561929000 |
| H | 6.249421000 | -1.096481000 | 0.104025000 |
| H | 5.986938000 | -1.535023000 | -1.598200000 |
| H | 6.204781000 | -2.810192000 | -0.376693000 |
| C | 3.756136000 | -1.700158000 | 0.972940000 |
| H | 4.443544000 | -1.531324000 | 1.805439000 |
| C | 2.380118000 | -1.728192000 | 1.229757000 |
| C | 1.840260000 | -1.528210000 | 2.620885000 |
| H | 1.320510000 | -2.426952000 | 2.992291000 |
| H | 1.118031000 | -0.697685000 | 2.647481000 |
| H | 2.654330000 | -1.300663000 | 3.321553000 |
| C | 1.473623000 | 1.083195000 | -0.972874000 |
| C | 3.874564000 | 1.353350000 | -1.463930000 |
| C | 2.788423000 | 1.313688000 | -0.527387000 |
| C | 5.178454000 | 1.587424000 | -1.051592000 |
| C | 3.120062000 | 1.515965000 | 0.848886000 |
| C | 5.473459000 | 1.781598000 | 0.309142000 |
| H | 5.982009000 | 1.617612000 | -1.791749000 |
| C | 4.429500000 | 1.746013000 | 1.248596000 |
| H | 2.315202000 | 1.492647000 | 1.584349000 |
| H | 6.499673000 | 1.971738000 | 0.629310000 |
| H | 4.647647000 | 1.901890000 | 2.308034000 |
| C | -0.261757000 | 4.510592000 | -0.269447000 |
| C | 1.048695000 | 4.252412000 | -0.245551000 |
| H | -0.755158000 | 4.910454000 | -1.158231000 |
| H | -0.898391000 | 4.301710000 | 0.592814000 |
| H | 1.690911000 | 4.433118000 | -1.110577000 |
| H | 3.652090000 | 1.199588000 | -2.522643000 |
| H | 1.319562000 | 0.993205000 | -2.059901000 |
| H | 1.533820000 | 3.832109000 | 0.636908000 |

# Co-Vd

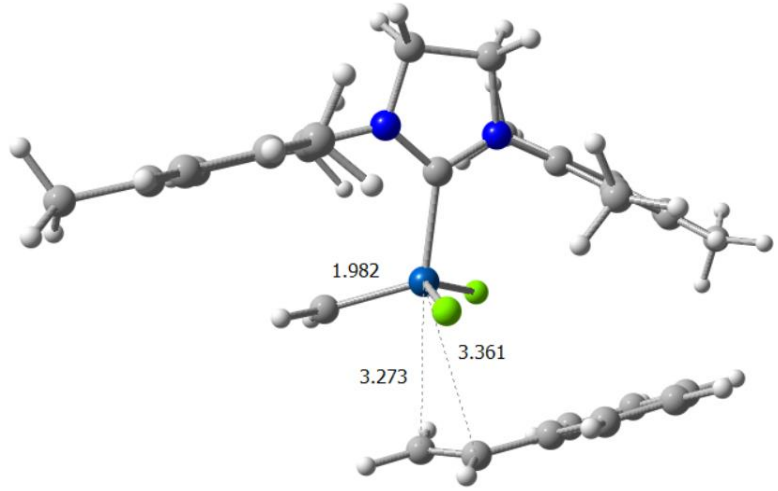



Zero-point correction= 0.567518 (Hartree/Particle)
Thermal correction to Energy= 0.607084
Thermal correction to Enthalpy= 0.608029
Thermal correction to Gibbs Free Energy= 0.493527
Sum of electronic and zero-point Energies= -2340.853619
Sum of electronic and thermal Energies= -2340.814053
Sum of electronic and thermal Enthalpies= -2340.813108
Sum of electronic and thermal Free Energies= -2340.927610

HOMO -0.15765 LUMO -0.12131

| | | | |
|---|---|---|---|
| Co | -0.534244000 | -0.873334000 | 0.725984000 |
| Cl | -0.222453000 | -2.208075000 | -1.053049000 |
| Cl | -0.554017000 | 0.246719000 | 2.670485000 |
| N | -2.113327000 | 0.951796000 | -0.941756000 |
| N | 0.025888000 | 1.421186000 | -0.976393000 |
| C | -0.907222000 | 0.618198000 | -0.431827000 |
| C | -2.046323000 | 2.105167000 | -1.871814000 |
| H | -2.591249000 | 2.961450000 | -1.443659000 |
| H | -2.512203000 | 1.844091000 | -2.832201000 |
| C | -0.534249000 | 2.353708000 | -1.987046000 |
| H | -0.136340000 | 2.102120000 | -2.981618000 |
| H | -0.242906000 | 3.385542000 | -1.744893000 |
| C | -3.391325000 | 0.445335000 | -0.545434000 |
| C | -4.016338000 | -0.536382000 | -1.340778000 |
| C | -3.325626000 | -1.102672000 | -2.551044000 |
| H | -3.938078000 | -1.886738000 | -3.015765000 |
| H | -2.346356000 | -1.530015000 | -2.280823000 |
| H | -3.141076000 | -0.326368000 | -3.311491000 |
| C | -5.277654000 | -0.994885000 | -0.944103000 |
| H | -5.763854000 | -1.775209000 | -1.536387000 |
| C | -5.927060000 | -0.484701000 | 0.189268000 |
| C | -7.296984000 | -0.981841000 | 0.579731000 |
| H | -8.083229000 | -0.439662000 | 0.028394000 |
| H | -7.485437000 | -0.835175000 | 1.652625000 |
| H | -7.415634000 | -2.051002000 | 0.351679000 |
| C | -5.291297000 | 0.520346000 | 0.930689000 |
| H | -5.788881000 | 0.933125000 | 1.812573000 |
| C | -4.029296000 | 1.013100000 | 0.576918000 |
| C | -3.352322000 | 2.074983000 | 1.397765000 |
| H | -4.044442000 | 2.493339000 | 2.140621000 |
| H | -2.980296000 | 2.901759000 | 0.773185000 |
| H | -2.481016000 | 1.656832000 | 1.929394000 |
| C | 1.417962000 | 1.514451000 | -0.635916000 |
| C | 1.787358000 | 2.373519000 | 0.421048000 |
| C | 0.753687000 | 3.116040000 | 1.224070000 |
| H | 1.237515000 | 3.801348000 | 1.932806000 |
| H | 0.119918000 | 2.417895000 | 1.791857000 |
| H | 0.091759000 | 3.712945000 | 0.575554000 |
| C | 3.151538000 | 2.550556000 | 0.674894000 |
| H | 3.451189000 | 3.208209000 | 1.495993000 |
| C | 4.135944000 | 1.943873000 | -0.117954000 |
| C | 5.597081000 | 2.203958000 | 0.148955000 |
| H | 6.234656000 | 1.564272000 | -0.475240000 |
| H | 5.851876000 | 2.013840000 | 1.203086000 |
| H | 5.854948000 | 3.254367000 | -0.063220000 |
| C | 3.730253000 | 1.126563000 | -1.176947000 |
| H | 4.484761000 | 0.635586000 | -1.795266000 |
| C | 2.377499000 | 0.900679000 | -1.462824000 |
| C | 1.979749000 | 0.062612000 | -2.647515000 |
| H | 1.617083000 | 0.693824000 | -3.477044000 |
| H | 1.181343000 | -0.647646000 | -2.389382000 |
| H | 2.842919000 | -0.505552000 | -3.018268000 |
| C | 2.145000000 | -1.498420000 | 1.749893000 |
| C | 4.527699000 | -1.027551000 | 1.284330000 |
| C | 3.311852000 | -1.611637000 | 0.875910000 |
| C | 5.689763000 | -1.192512000 | 0.530427000 |
| C | 3.281906000 | -2.324816000 | -0.340156000 |
| C | 5.648136000 | -1.902530000 | -0.674509000 |
| H | 6.628765000 | -0.756464000 | 0.876917000 |
| C | 4.436701000 | -2.456836000 | -1.109532000 |
| H | 2.335429000 | -2.741150000 | -0.689766000 |
| H | 6.554012000 | -2.023443000 | -1.272466000 |
| H | 4.394861000 | -3.000709000 | -2.056002000 |
| C | 1.118520000 | -2.386000000 | 1.819233000 |
| C | -2.122018000 | -1.530067000 | 1.017917000 |
| H | 1.094208000 | -3.282695000 | 1.199853000 |
| H | 0.380952000 | -2.305616000 | 2.618133000 |
| H | -2.573613000 | -2.231642000 | 0.308723000 |
| H | 4.554271000 | -0.456290000 | 2.215360000 |
| H | 2.144282000 | -0.657357000 | 2.450349000 |
| H | -2.731114000 | -1.169035000 | 1.853535000 |

# Co-Vs

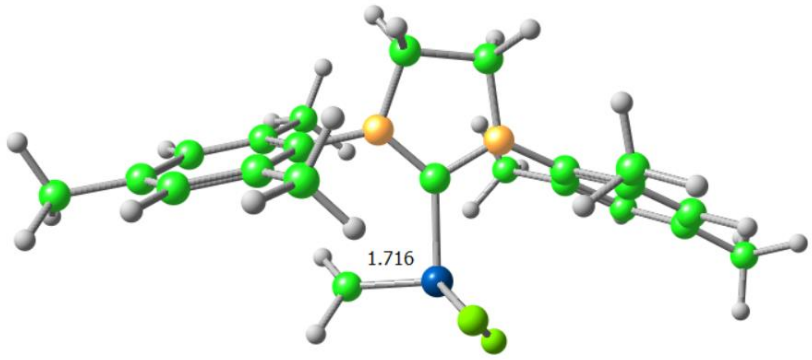



Zero-point correction= 0.562652 (Hartree/Particle)
Thermal correction to Energy= 0.604446
Thermal correction to Enthalpy= 0.605390
Thermal correction to Gibbs Free Energy= 0.482775
Sum of electronic and zero-point Energies= -2340.794391
Sum of electronic and thermal Energies= -2340.752597
Sum of electronic and thermal Enthalpies= -2340.751653
Sum of electronic and thermal Free Energies= -2340.874268

HOMO -0.14310 LUMO -0.17590

| | | | |
|---|---|---|---|
| Co | -0.418861000 | -0.854447000 | -0.348203000 |
| Cl | 1.103627000 | -0.380760000 | -1.847190000 |
| Cl | -0.442612000 | -1.685716000 | 1.708727000 |
| N | -2.132906000 | 1.469048000 | 0.582723000 |
| N | -0.039793000 | 2.091446000 | 0.531135000 |
| C | -0.886972000 | 1.086072000 | 0.264285000 |
| C | -2.205075000 | 2.885464000 | 1.031839000 |
| H | -2.740840000 | 2.956756000 | 1.988062000 |
| H | -2.749675000 | 3.480385000 | 0.281470000 |
| C | -0.719089000 | 3.267954000 | 1.140078000 |
| H | -0.462296000 | 4.182469000 | 0.588130000 |
| H | -0.381440000 | 3.384527000 | 2.181606000 |
| C | -3.323001000 | 0.735237000 | 0.265326000 |
| C | -3.778728000 | 0.725635000 | -1.065930000 |
| C | -3.006336000 | 1.424056000 | -2.153816000 |
| H | -3.566458000 | 1.411551000 | -3.098139000 |
| H | -2.042500000 | 0.917411000 | -2.320146000 |
| H | -2.787300000 | 2.472877000 | -1.899472000 |
| C | -4.946749000 | 0.010945000 | -1.354127000 |
| H | -5.303887000 | -0.020109000 | -2.387123000 |
| C | -5.649299000 | -0.684832000 | -0.361064000 |
| C | -6.913266000 | -1.438317000 | -0.694728000 |
| H | -7.796546000 | -0.783340000 | -0.611110000 |
| H | -7.065912000 | -2.285297000 | -0.010609000 |
| H | -6.888002000 | -1.826776000 | -1.722997000 |
| C | -5.161683000 | -0.650487000 | 0.952406000 |
| H | -5.692368000 | -1.197403000 | 1.736784000 |
| C | -4.003408000 | 0.060198000 | 1.292217000 |
| C | -3.479431000 | 0.067659000 | 2.703681000 |
| H | -4.121672000 | -0.535374000 | 3.359278000 |
| H | -3.438992000 | 1.087359000 | 3.119801000 |
| H | -2.459886000 | -0.346129000 | 2.739281000 |
| C | 1.374235000 | 2.109509000 | 0.289255000 |
| C | 2.257964000 | 1.599467000 | 1.254064000 |
| C | 1.762713000 | 1.004502000 | 2.543677000 |
| H | 2.579357000 | 0.931917000 | 3.274422000 |
| H | 1.359930000 | -0.006820000 | 2.377172000 |
| H | 0.950348000 | 1.597240000 | 2.989903000 |
| C | 3.628142000 | 1.627074000 | 0.961930000 |
| H | 4.327692000 | 1.220454000 | 1.695522000 |
| C | 4.118704000 | 2.142646000 | -0.242026000 |
| C | 5.591857000 | 2.093028000 | -0.559132000 |
| H | 5.915599000 | 2.979059000 | -1.124810000 |
| H | 5.821115000 | 1.207117000 | -1.174132000 |
| H | 6.198000000 | 2.026083000 | 0.355465000 |
| C | 3.206164000 | 2.671528000 | -1.165876000 |
| H | 3.572604000 | 3.079631000 | -2.111965000 |
| C | 1.830490000 | 2.666274000 | -0.921141000 |
| C | 0.856218000 | 3.172138000 | -1.952629000 |
| H | 0.212102000 | 3.976420000 | -1.562269000 |
| H | 0.199289000 | 2.355243000 | -2.287534000 |
| H | 1.388524000 | 3.564348000 | -2.829237000 |
| C | 1.371593000 | -3.693909000 | -0.182089000 |
| C | 3.038287000 | -2.635916000 | 1.313672000 |
| C | 2.633381000 | -2.972292000 | 0.006142000 |
| C | 4.210619000 | -1.914407000 | 1.540189000 |
| C | 3.453134000 | -2.571597000 | -1.068243000 |
| C | 5.010262000 | -1.519305000 | 0.462306000 |
| H | 4.501800000 | -1.659476000 | 2.561722000 |
| C | 4.625271000 | -1.852138000 | -0.841685000 |
| H | 3.168893000 | -2.835762000 | -2.087835000 |
| H | 5.932956000 | -0.962055000 | 0.636560000 |
| H | 5.247448000 | -1.553155000 | -1.688120000 |
| C | 0.656670000 | -3.789080000 | -1.320298000 |
| C | -1.893862000 | -1.750496000 | -1.322955000 |
| H | 0.971328000 | -3.312242000 | -2.249557000 |
| H | -0.282453000 | -4.341214000 | -1.345629000 |
| H | -1.900209000 | -1.830711000 | -2.415702000 |
| H | 2.404143000 | -2.930020000 | 2.152798000 |
| H | 0.960544000 | -4.146948000 | 0.724904000 |
| H | -2.703189000 | -2.240949000 | -0.770099000 |

# Co-VId

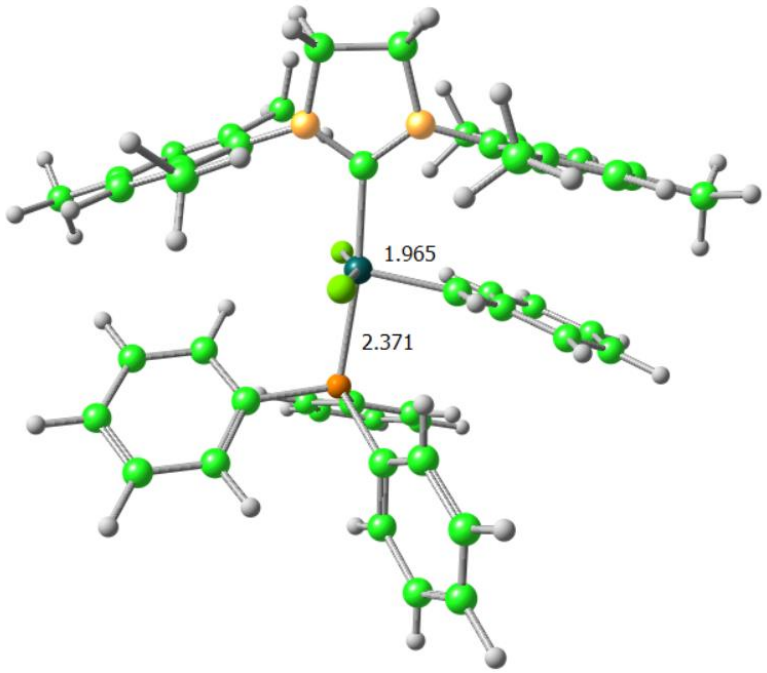



Zero-point correction= 0.434565 (Hartree/Particle)
Thermal correction to Energy= 0.466072
Thermal correction to Enthalpy= 0.467017
Thermal correction to Gibbs Free Energy= 0.368987
Sum of electronic and zero-point Energies= -2031.199330
Sum of electronic and thermal Energies= -2031.167823
Sum of electronic and thermal Enthalpies= -2031.166879
Sum of electronic and thermal Free Energies= -2031.264908

HOMO -0.17794 LUMO -0.12255

| | | | |
|---|---|---|---|
| Co | 0.169634000 | 0.906211000 | 0.998584000 |
| Cl | 1.657146000 | 0.823446000 | 2.574283000 |
| Cl | 0.378665000 | 2.813159000 | -0.196373000 |
| N | -1.273957000 | -0.699214000 | -1.008327000 |
| N | 0.917674000 | -0.707755000 | -1.151432000 |
| C | -0.131801000 | -0.258040000 | -0.432061000 |
| C | -1.020598000 | -1.417724000 | -2.280212000 |
| H | -1.358529000 | -0.799037000 | -3.126791000 |
| H | -1.570297000 | -2.368691000 | -2.301845000 |
| C | 0.507015000 | -1.601442000 | -2.258499000 |
| H | 0.810190000 | -2.636197000 | -2.028065000 |
| H | 0.989990000 | -1.297134000 | -3.196505000 |
| C | -2.607824000 | -0.479521000 | -0.543797000 |
| C | -3.218205000 | -1.491154000 | 0.227442000 |
| C | -2.453755000 | -2.733611000 | 0.605410000 |
| H | -3.039392000 | -3.358579000 | 1.292327000 |
| H | -1.497404000 | -2.485538000 | 1.091794000 |
| H | -2.208094000 | -3.346474000 | -0.276987000 |
| C | -4.528136000 | -1.286339000 | 0.671338000 |
| H | -5.004325000 | -2.053464000 | 1.288264000 |
| C | -5.237468000 | -0.118154000 | 0.352863000 |
| C | -6.658267000 | 0.071539000 | 0.822740000 |
| H | -7.368790000 | -0.392520000 | 0.118622000 |
| H | -6.916749000 | 1.137174000 | 0.896991000 |
| H | -6.822008000 | -0.392505000 | 1.806105000 |
| C | -4.607297000 | 0.853266000 | -0.435590000 |
| H | -5.149228000 | 1.766654000 | -0.695457000 |
| C | -3.297846000 | 0.693918000 | -0.909140000 |
| C | -2.644601000 | 1.743075000 | -1.763114000 |
| H | -3.339911000 | 2.568807000 | -1.963337000 |
| H | -2.324042000 | 1.328063000 | -2.732252000 |
| H | -1.742306000 | 2.153939000 | -1.279468000 |
| C | 2.288190000 | -0.623476000 | -0.731739000 |
| C | 3.139999000 | 0.296398000 | -1.369560000 |
| C | 2.629058000 | 1.205444000 | -2.453759000 |
| H | 3.429946000 | 1.863962000 | -2.815238000 |
| H | 1.807295000 | 1.831991000 | -2.070731000 |
| H | 2.244858000 | 0.638722000 | -3.317776000 |
| C | 4.469899000 | 0.359357000 | -0.937959000 |
| H | 5.140755000 | 1.082846000 | -1.409379000 |
| C | 4.955659000 | -0.465385000 | 0.085504000 |
| C | 6.376256000 | -0.331262000 | 0.574074000 |
| H | 6.756120000 | -1.282319000 | 0.974461000 |
| H | 6.435400000 | 0.414533000 | 1.383929000 |
| H | 7.049928000 | 0.000583000 | -0.229098000 |
| C | 4.082813000 | -1.390902000 | 0.671538000 |
| H | 4.447725000 | -2.042595000 | 1.469897000 |
| C | 2.744076000 | -1.489361000 | 0.279439000 |
| C | 1.811288000 | -2.447629000 | 0.971808000 |
| H | 1.119109000 | -2.939368000 | 0.271953000 |
| H | 1.206391000 | -1.903767000 | 1.715501000 |
| H | 2.376449000 | -3.226542000 | 1.500998000 |
| C | -1.351672000 | 0.600611000 | 1.730180000 |
| H | -1.792665000 | -0.358135000 | 2.023521000 |
| H | -1.856039000 | 1.516732000 | 2.079226000 |

# Rh-Id



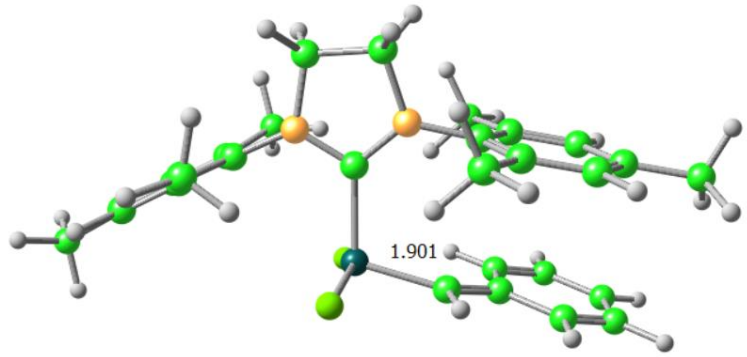

Zero-point correction= 0.782322 (Hartree/Particle)
Thermal correction to Energy= 0.835639
Thermal correction to Enthalpy= 0.836584
Thermal correction to Gibbs Free Energy= 0.691796
Sum of electronic and zero-point Energies= -3263.445673
Sum of electronic and thermal Energies= -3263.392356
Sum of electronic and thermal Enthalpies= -3263.391412
Sum of electronic and thermal Free Energies= -3263.536199

HOMO -0.11828 LUMO -0.09759

| | | | |
|---|---|---|---|
| Rh | -0.199254000 | -0.329538000 | -0.229431000 |
| Cl | -0.575166000 | -0.382903000 | 2.104153000 |
| Cl | -0.460242000 | -0.353339000 | -2.600474000 |
| P | -0.631821000 | 2.000997000 | -0.186502000 |
| N | -1.154727000 | -3.159117000 | -0.357992000 |
| N | 1.024703000 | -3.119458000 | -0.577556000 |
| C | -0.062878000 | -2.362339000 | -0.342047000 |
| C | -0.836854000 | -4.562841000 | -0.709997000 |
| H | -1.256038000 | -4.796512000 | -1.701550000 |
| H | -1.276235000 | -5.251190000 | 0.025048000 |
| C | 0.700520000 | -4.563318000 | -0.698334000 |
| H | 1.124186000 | -5.108262000 | 0.160391000 |
| H | 1.137226000 | -4.972661000 | -1.619323000 |
| C | -2.479304000 | -2.782277000 | 0.046919000 |
| C | -2.819376000 | -2.945785000 | 1.410825000 |
| C | -1.831881000 | -3.512757000 | 2.395002000 |
| H | -2.242203000 | -3.483040000 | 3.412990000 |
| H | -0.898526000 | -2.934766000 | 2.388002000 |
| H | -1.590224000 | -4.563294000 | 2.162078000 |
| C | -4.104411000 | -2.585766000 | 1.818530000 |
| H | -4.369610000 | -2.687669000 | 2.874581000 |
| C | -5.062015000 | -2.109061000 | 0.908097000 |
| C | -6.437394000 | -1.710807000 | 1.384694000 |
| H | -7.096325000 | -1.458166000 | 0.542094000 |
| H | -6.387780000 | -0.835011000 | 2.052567000 |
| H | -6.913422000 | -2.522492000 | 1.956546000 |
| C | -4.708655000 | -2.015725000 | -0.438797000 |
| H | -5.447327000 | -1.667095000 | -1.165844000 |
| C | -3.425615000 | -2.357184000 | -0.900064000 |
| C | -3.130125000 | -2.281911000 | -2.373131000 |
| H | -3.207649000 | -1.244704000 | -2.729600000 |
| H | -3.853501000 | -2.892193000 | -2.936689000 |
| H | -2.112881000 | -2.611596000 | -2.608755000 |
| C | 2.397658000 | -2.721935000 | -0.461438000 |
| C | 3.141159000 | -2.486993000 | -1.631210000 |
| C | 2.487033000 | -2.551734000 | -2.985231000 |
| H | 3.186212000 | -2.230627000 | -3.769388000 |
| H | 1.591569000 | -1.910521000 | -3.025018000 |
| H | 2.160369000 | -3.576166000 | -3.230796000 |
| C | 4.492836000 | -2.149796000 | -1.489441000 |
| H | 5.080761000 | -1.940927000 | -2.387701000 |
| C | 5.105392000 | -2.064320000 | -0.232131000 |
| C | 6.546981000 | -1.647690000 | -0.097934000 |
| H | 7.073583000 | -2.255463000 | 0.653115000 |
| H | 6.605957000 | -0.596791000 | 0.229146000 |
| H | 7.083473000 | -1.736594000 | -1.053327000 |
| C | 4.335016000 | -2.330643000 | 0.907208000 |
| H | 4.792813000 | -2.248061000 | 1.896168000 |
| C | 2.981130000 | -2.667320000 | 0.818667000 |
| C | 2.160608000 | -2.907608000 | 2.056332000 |
| H | 1.666963000 | -3.892913000 | 2.039742000 |
| H | 1.367347000 | -2.149915000 | 2.157464000 |
| H | 2.791961000 | -2.859914000 | 2.953287000 |
| C | 1.704068000 | 0.094213000 | -0.476366000 |
| C | 3.885288000 | 1.109248000 | -0.189526000 |
| C | 2.690000000 | 0.584262000 | 0.406189000 |
| C | 4.943491000 | 1.558193000 | 0.587101000 |
| C | 2.637317000 | 0.557538000 | 1.831586000 |
| C | 4.875115000 | 1.499313000 | 1.990975000 |
| H | 5.832213000 | 1.967530000 | 0.099919000 |
| C | 3.711190000 | 0.997448000 | 2.594849000 |
| H | 1.728872000 | 0.199874000 | 2.313782000 |
| H | 5.709004000 | 1.852863000 | 2.600358000 |
| H | 3.637689000 | 0.961156000 | 3.684623000 |
| C | -2.423100000 | 2.156516000 | -0.577909000 |
| C | -2.899034000 | 3.053503000 | -1.544381000 |
| C | -3.319382000 | 1.293125000 | 0.078392000 |

| | | | |
|---|---|---|---|
| C | -4.264906000 | 3.105106000 | -1.836691000 |
| H | -2.200033000 | 3.704657000 | -2.071020000 |
| C | -4.684713000 | 1.363260000 | -0.207696000 |
| H | -2.947856000 | 0.571863000 | 0.812054000 |
| C | -5.160262000 | 2.266919000 | -1.163871000 |
| H | -4.629803000 | 3.802806000 | -2.593497000 |
| H | -5.375109000 | 0.697965000 | 0.311118000 |
| H | -6.227708000 | 2.312297000 | -1.390345000 |
| C | 0.217615000 | 3.185662000 | -1.318276000 |
| C | 0.172114000 | 4.562917000 | -1.036327000 |
| C | 0.901694000 | 2.734393000 | -2.455197000 |
| C | 0.807558000 | 5.474580000 | -1.882572000 |
| H | -0.350774000 | 4.918507000 | -0.147095000 |
| C | 1.541993000 | 3.651261000 | -3.294671000 |
| H | 0.905188000 | 1.670765000 | -2.692833000 |
| C | 1.499859000 | 5.019431000 | -3.010513000 |
| H | 0.767989000 | 6.541864000 | -1.654866000 |
| H | 2.075840000 | 3.290207000 | -4.176266000 |
| H | 2.003836000 | 5.732134000 | -3.666960000 |
| C | -0.408352000 | 2.831885000 | 1.441959000 |
| C | -1.472397000 | 3.044809000 | 2.327415000 |
| C | 0.895458000 | 3.192639000 | 1.818975000 |
| C | -1.234204000 | 3.616608000 | 3.580615000 |
| H | -2.487010000 | 2.767051000 | 2.040347000 |
| C | 1.128403000 | 3.758523000 | 3.073102000 |
| H | 1.728734000 | 3.026850000 | 1.136010000 |
| C | 0.065087000 | 3.971352000 | 3.957330000 |
| H | -2.068588000 | 3.780882000 | 4.265728000 |
| H | 2.147811000 | 4.024402000 | 3.359276000 |
| H | 0.249195000 | 4.412639000 | 4.939208000 |
| H | 3.945080000 | 1.155500000 | -1.278931000 |
| H | 1.942237000 | 0.125779000 | -1.543666000 |

# Rh-IId



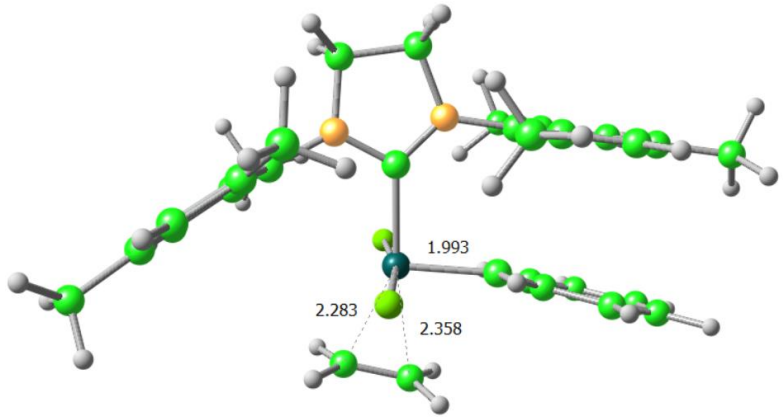

Zero-point correction= 0.515070 (Hartree/Particle)
Thermal correction to Energy= 0.550845
Thermal correction to Enthalpy= 0.551789
Thermal correction to Gibbs Free Energy= 0.445941
Sum of electronic and zero-point Energies= -2227.022622
Sum of electronic and thermal Energies= -2226.986848
Sum of electronic and thermal Enthalpies= -2226.985903
Sum of electronic and thermal Free Energies= -2227.091751

HOMO -0.14887 LUMO -0.12789

| | | | |
|---|---|---|---|
| Rh | -0.532959000 | 0.589253000 | -0.935545000 |
| Cl | -0.831539000 | 2.523015000 | 0.326695000 |
| Cl | -0.852151000 | -0.856668000 | -2.772783000 |
| N | -1.859770000 | -1.250122000 | 0.864500000 |
| N | 0.309483000 | -1.610157000 | 0.929356000 |
| C | -0.658621000 | -0.840135000 | 0.394399000 |
| C | -1.730859000 | -2.293792000 | 1.904768000 |
| H | -2.409874000 | -3.131049000 | 1.693457000 |
| H | -1.987093000 | -1.871579000 | 2.889853000 |
| C | -0.244778000 | -2.680820000 | 1.793668000 |
| H | 0.274503000 | -2.688447000 | 2.761765000 |
| H | -0.099717000 | -3.659455000 | 1.309733000 |
| C | -3.091054000 | -0.554762000 | 0.615464000 |
| C | -3.442338000 | 0.539228000 | 1.431282000 |
| C | -2.618101000 | 0.934410000 | 2.628522000 |
| H | -2.712474000 | 2.009613000 | 2.825380000 |
| H | -1.552222000 | 0.722930000 | 2.484318000 |
| H | -2.963716000 | 0.394231000 | 3.527119000 |
| C | -4.621997000 | 1.228678000 | 1.128159000 |
| H | -4.892115000 | 2.098289000 | 1.733402000 |
| C | -5.454470000 | 0.839613000 | 0.071124000 |
| C | -6.684452000 | 1.640339000 | -0.275612000 |
| H | -7.461595000 | 1.008642000 | -0.729334000 |
| H | -6.437188000 | 2.431936000 | -1.002171000 |
| H | -7.109646000 | 2.130597000 | 0.611934000 |
| C | -5.109656000 | -0.300064000 | -0.668589000 |
| H | -5.769202000 | -0.640200000 | -1.471551000 |
| C | -3.939890000 | -1.023468000 | -0.408763000 |
| C | -3.610367000 | -2.269474000 | -1.183788000 |
| H | -4.426541000 | -2.521257000 | -1.874035000 |
| H | -3.454764000 | -3.129477000 | -0.512795000 |
| H | -2.688525000 | -2.134057000 | -1.770264000 |
| C | 1.723565000 | -1.463632000 | 0.777537000 |
| C | 2.397206000 | -2.203816000 | -0.209780000 |
| C | 1.639626000 | -3.084048000 | -1.166544000 |
| H | 2.317198000 | -3.521099000 | -1.912189000 |
| H | 0.856643000 | -2.518229000 | -1.697093000 |
| H | 1.140254000 | -3.915483000 | -0.642921000 |
| C | 3.788554000 | -2.063505000 | -0.289533000 |
| H | 4.329299000 | -2.614097000 | -1.064352000 |
| C | 4.499671000 | -1.229344000 | 0.583942000 |
| C | 5.997920000 | -1.100164000 | 0.484419000 |
| H | 6.500515000 | -1.739428000 | 1.229032000 |
| H | 6.314094000 | -0.063365000 | 0.668288000 |
| H | 6.360424000 | -1.398704000 | -0.509342000 |
| C | 3.789264000 | -0.512962000 | 1.556516000 |
| H | 4.325693000 | 0.169368000 | 2.220361000 |
| C | 2.399828000 | -0.613832000 | 1.670699000 |
| C | 1.631744000 | 0.201961000 | 2.675980000 |
| H | 1.090519000 | -0.435115000 | 3.394745000 |
| H | 0.883619000 | 0.834896000 | 2.173374000 |
| H | 2.307325000 | 0.854824000 | 3.243267000 |
| C | 1.317081000 | 0.658069000 | -1.368494000 |

| | | | | |
|---|---|---|---|---|
| | C | 3.676561000 | 1.159310000 | -1.547168000 |
| | C | 2.437676000 | 1.396259000 | -0.878247000 |
| | C | 4.841800000 | 1.811330000 | -1.162453000 |
| | C | 2.441649000 | 2.323933000 | 0.196505000 |
| | C | 4.822733000 | 2.711703000 | -0.088136000 |
| | H | 5.773754000 | 1.612728000 | -1.695996000 |
| | C | 3.615035000 | 2.962308000 | 0.580504000 |
| | H | 1.502772000 | 2.539694000 | 0.703256000 |
| | H | 5.738081000 | 3.222760000 | 0.217448000 |
| | H | 3.590831000 | 3.672633000 | 1.410003000 |
| | H | 3.695100000 | 0.447779000 | -2.375146000 |
| | H | 1.541954000 | -0.032167000 | -2.191829000 |

# Rh-IIId



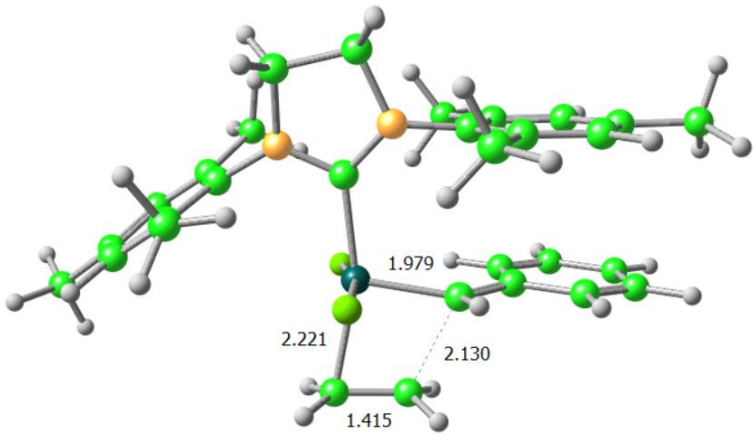

Zero-point correction= 0.568224 (Hartree/Particle)
Thermal correction to Energy= 0.607815
Thermal correction to Enthalpy= 0.608759
Thermal correction to Gibbs Free Energy= 0.493571
Sum of electronic and zero-point Energies= -2305.611524
Sum of electronic and thermal Energies= -2305.571933
Sum of electronic and thermal Enthalpies= -2305.570989
Sum of electronic and thermal Free Energies= -2305.686177

HOMO -0.13024 LUMO -0.10932

| | | | |
|---|---|---|---|
| Rh | 0.571429000 | -0.923278000 | -0.227312000 |
| Cl | 0.308731000 | -1.517291000 | 2.052165000 |
| Cl | 1.229788000 | -0.455129000 | -2.460651000 |
| N | 1.769384000 | 1.548377000 | 0.703150000 |
| N | -0.405754000 | 1.838504000 | 0.696752000 |
| C | 0.584218000 | 0.987742000 | 0.375670000 |
| C | 1.618408000 | 2.846434000 | 1.394234000 |
| H | 2.253860000 | 3.608955000 | 0.922691000 |
| H | 1.916844000 | 2.742419000 | 2.449339000 |
| C | 0.112627000 | 3.124919000 | 1.228938000 |
| H | -0.386569000 | 3.365749000 | 2.176954000 |
| H | -0.096937000 | 3.931098000 | 0.507983000 |
| C | 3.040082000 | 0.944058000 | 0.417801000 |
| C | 3.663522000 | 0.109220000 | 1.364451000 |
| C | 3.163191000 | -0.019052000 | 2.778413000 |
| H | 3.317273000 | -1.037234000 | 3.160370000 |
| H | 2.093193000 | 0.198509000 | 2.864388000 |
| H | 3.723776000 | 0.671376000 | 3.431910000 |
| C | 4.843661000 | -0.546621000 | 0.978566000 |
| H | 5.322159000 | -1.223963000 | 1.691549000 |
| C | 5.428177000 | -0.343121000 | -0.274978000 |
| C | 6.666538000 | -1.098155000 | -0.688788000 |
| H | 7.403011000 | -0.432524000 | -1.163741000 |
| H | 6.417285000 | -1.882335000 | -1.422289000 |
| H | 7.146473000 | -1.585662000 | 0.171229000 |
| C | 4.835498000 | 0.584562000 | -1.146650000 |
| H | 5.302038000 | 0.788292000 | -2.114224000 |
| C | 3.651351000 | 1.246964000 | -0.819649000 |
| C | 3.047555000 | 2.262494000 | -1.752201000 |
| H | 3.664062000 | 2.369958000 | -2.654272000 |
| H | 2.972390000 | 3.252549000 | -1.273226000 |
| H | 2.041598000 | 1.951542000 | -2.065697000 |
| C | -1.790396000 | 1.734867000 | 0.342480000 |
| C | -2.178165000 | 2.093927000 | -0.962663000 |
| C | -1.152005000 | 2.481444000 | -1.994219000 |
| H | -1.638231000 | 2.792954000 | -2.928216000 |
| H | -0.476747000 | 1.639541000 | -2.222196000 |
| H | -0.517041000 | 3.314140000 | -1.651438000 |
| C | -3.538171000 | 2.022559000 | -1.282431000 |
| H | -3.854949000 | 2.272765000 | -2.298695000 |
| C | -4.496382000 | 1.618043000 | -0.342561000 |
| C | -5.955329000 | 1.530791000 | -0.711364000 |
| H | -6.407114000 | 0.615600000 | -0.301416000 |
| H | -6.091714000 | 1.521099000 | -1.801894000 |
| H | -6.519347000 | 2.389134000 | -0.310392000 |
| C | -4.070468000 | 1.289878000 | 0.950407000 |
| H | -4.802796000 | 0.946197000 | 1.685574000 |
| C | -2.723077000 | 1.352902000 | 1.322600000 |
| C | -2.280785000 | 0.983420000 | 2.712218000 |
| H | -1.937176000 | 1.868617000 | 3.274300000 |
| H | -1.448190000 | 0.264541000 | 2.687364000 |
| H | -3.111551000 | 0.535432000 | 3.273302000 |
| C | -1.304204000 | -0.818571000 | -0.891462000 |
| C | -3.602671000 | -1.397426000 | -1.382367000 |
| C | -2.501458000 | -1.441681000 | -0.465983000 |
| C | -4.861622000 | -1.858140000 | -1.022902000 |
| C | -2.746655000 | -2.017048000 | 0.813413000 |
| C | -5.083507000 | -2.393417000 | 0.256342000 |
| H | -5.680002000 | -1.807998000 | -1.745044000 |
| C | -4.012645000 | -2.474051000 | 1.160047000 |
| H | -1.921707000 | -2.080364000 | 1.522336000 |
| H | -6.072327000 | -2.762193000 | 0.536104000 |
| H | -4.171633000 | -2.903710000 | 2.152127000 |
| C | 1.575025000 | -2.952359000 | -0.526974000 |
| C | 0.258670000 | -3.178043000 | -0.842179000 |
| H | 2.304958000 | -2.722053000 | -1.305578000 |
| H | 1.952493000 | -3.175585000 | 0.473285000 |
| H | -0.086015000 | -3.117654000 | -1.875029000 |

| | | | |
|---|---|---|---|
| H | -3.436629000 | -0.975642000 | -2.375840000 |
| H | -1.292993000 | -0.456885000 | -1.924787000 |
| H | -0.442204000 | -3.565397000 | -0.102104000 |

# Rh-III-IVd

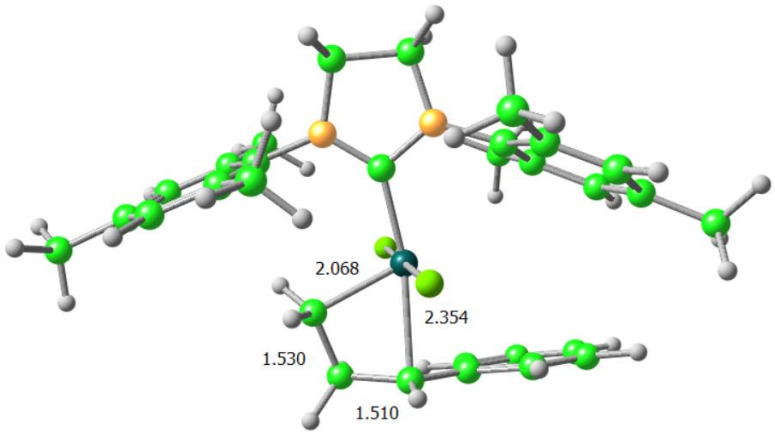



Zero-point correction= 0.568171 (Hartree/Particle)
Thermal correction to Energy= 0.606856
Thermal correction to Enthalpy= 0.607800
Thermal correction to Gibbs Free Energy= 0.496179
Sum of electronic and zero-point Energies= -2305.602712
Sum of electronic and thermal Energies= -2305.564027
Sum of electronic and thermal Enthalpies= -2305.563082
Sum of electronic and thermal Free Energies= -2305.674703

| | | | |
|---|---|---|---|
| Rh | 0.569912000 | -0.771282000 | -0.733338000 |
| Cl | 0.934348000 | -2.000167000 | 1.264378000 |
| Cl | 0.663734000 | 0.365962000 | -2.833923000 |
| N | 1.791606000 | 1.604084000 | 0.487290000 |
| N | -0.362326000 | 1.966621000 | 0.297117000 |
| C | 0.608717000 | 1.043856000 | 0.152594000 |
| C | 1.678360000 | 3.050613000 | 0.773386000 |
| H | 2.132475000 | 3.625694000 | -0.049067000 |
| H | 2.199062000 | 3.300460000 | 1.708189000 |
| C | 0.154811000 | 3.244019000 | 0.853673000 |
| H | -0.206545000 | 3.368107000 | 1.887480000 |
| H | -0.203718000 | 4.091466000 | 0.254218000 |
| C | 3.043989000 | 0.903033000 | 0.521997000 |
| C | 3.424031000 | 0.297404000 | 1.739047000 |
| C | 2.575983000 | 0.440409000 | 2.974007000 |
| H | 3.085328000 | 0.003399000 | 3.843240000 |
| H | 1.617375000 | -0.081254000 | 2.842152000 |
| H | 2.361080000 | 1.496884000 | 3.200199000 |
| C | 4.611705000 | -0.437303000 | 1.765985000 |
| H | 4.906023000 | -0.928636000 | 2.697349000 |
| C | 5.423960000 | -0.568934000 | 0.629541000 |
| C | 6.661936000 | -1.430010000 | 0.665948000 |
| H | 7.168853000 | -1.364606000 | 1.639985000 |
| H | 7.377270000 | -1.140129000 | -0.116726000 |
| H | 6.402604000 | -2.489188000 | 0.502890000 |
| C | 5.053866000 | 0.110047000 | -0.535733000 |
| H | 5.699600000 | 0.056852000 | -1.416829000 |
| C | 3.880013000 | 0.875705000 | -0.609914000 |
| C | 3.597396000 | 1.702753000 | -1.835393000 |
| H | 2.524537000 | 1.861170000 | -1.993290000 |
| H | 3.988137000 | 1.211648000 | -2.736905000 |
| H | 4.096703000 | 2.683315000 | -1.748903000 |
| C | -1.773422000 | 1.720301000 | 0.324896000 |
| C | -2.564225000 | 2.162128000 | -0.749746000 |
| C | -1.932674000 | 2.784725000 | -1.965515000 |
| H | -2.679655000 | 2.939398000 | -2.755958000 |
| H | -1.122329000 | 2.150835000 | -2.358957000 |
| H | -1.490737000 | 3.767464000 | -1.730101000 |
| C | -3.951191000 | 1.987895000 | -0.654969000 |
| H | -4.580669000 | 2.309012000 | -1.489720000 |
| C | -4.547967000 | 1.412515000 | 0.474320000 |
| C | -6.044159000 | 1.256235000 | 0.567594000 |
| H | -6.513926000 | 1.287377000 | -0.425782000 |
| H | -6.489019000 | 2.064431000 | 1.171568000 |
| H | -6.309335000 | 0.301644000 | 1.044609000 |
| C | -3.724802000 | 0.987597000 | 1.525053000 |
| H | -4.173328000 | 0.506703000 | 2.397779000 |
| C | -2.334897000 | 1.129363000 | 1.473420000 |
| C | -1.461537000 | 0.638161000 | 2.595859000 |
| H | -0.864860000 | 1.453082000 | 3.037182000 |
| H | -0.752312000 | -0.127436000 | 2.243292000 |
| H | -2.071227000 | 0.195296000 | 3.394018000 |
| C | -1.347410000 | -1.081155000 | -1.113399000 |
| C | -3.747284000 | -1.419221000 | -0.938871000 |
| C | -2.463019000 | -1.533679000 | -0.332786000 |
| C | -4.884705000 | -1.923728000 | -0.317610000 |
| C | -2.386303000 | -2.169570000 | 0.932724000 |
| C | -4.789016000 | -2.531932000 | 0.941191000 |
| H | -5.855765000 | -1.826931000 | -0.807996000 |
| C | -3.533464000 | -2.649434000 | 1.556298000 |
| H | -1.410380000 | -2.268025000 | 1.408493000 |
| H | -5.683343000 | -2.916552000 | 1.435798000 |
| H | -3.450428000 | -3.127288000 | 2.535185000 |
| C | -0.238521000 | -2.736205000 | -1.866252000 |
| C | 1.170178000 | -2.606350000 | -1.831074000 |
| H | -0.719892000 | -3.424272000 | -1.170283000 |
| H | -0.747132000 | -2.568299000 | -2.818229000 |
| H | 1.737159000 | -3.162882000 | -1.083733000 |

| | | | |
|---|---|---|---|
| H | -3.827587000 | -0.924123000 | -1.908736000 |
| H | -1.623931000 | -0.534389000 | -2.022634000 |
| H | 1.699443000 | -2.251420000 | -2.715778000 |

# Rh-IVd



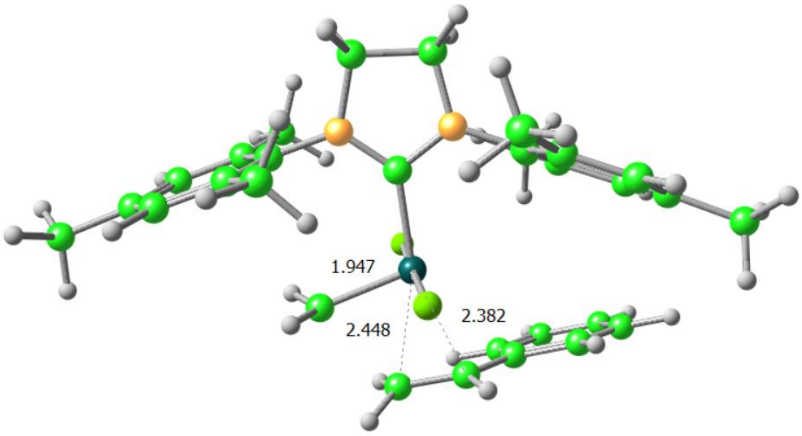

Zero-point correction= 0.570470 (Hartree/Particle)
Thermal correction to Energy= 0.609237
Thermal correction to Enthalpy= 0.610181
Thermal correction to Gibbs Free Energy= 0.497429
Sum of electronic and zero-point Energies= -2305.630676
Sum of electronic and thermal Energies= -2305.591909
Sum of electronic and thermal Enthalpies= -2305.590965
Sum of electronic and thermal Free Energies= -2305.703717

HOMO -0.15961 LUMO -0.13772

| | | | |
|---|---|---|---|
| Rh | 0.099002000 | -0.580432000 | 0.299235000 |
| Cl | -0.217613000 | -1.538399000 | -1.847633000 |
| Cl | 0.453207000 | 0.373092000 | 2.445136000 |
| N | -1.908796000 | 1.514215000 | -0.653069000 |
| N | 0.206180000 | 2.097971000 | -0.715018000 |
| C | -0.654631000 | 1.109322000 | -0.374755000 |
| C | -1.950202000 | 2.918241000 | -1.133368000 |
| H | -2.400498000 | 3.560756000 | -0.359362000 |
| H | -2.559247000 | 2.990702000 | -2.044321000 |
| C | -0.462533000 | 3.236406000 | -1.376969000 |
| H | -0.202316000 | 3.248602000 | -2.448081000 |
| H | -0.148464000 | 4.187940000 | -0.927216000 |
| C | -3.118039000 | 0.815434000 | -0.337000000 |
| C | -3.788108000 | 0.123918000 | -1.362768000 |
| C | -3.238903000 | 0.093872000 | -2.763165000 |
| H | -3.887662000 | -0.498987000 | -3.421822000 |
| H | -2.230173000 | -0.349840000 | -2.767672000 |
| H | -3.159997000 | 1.106424000 | -3.191310000 |
| C | -4.964264000 | -0.560856000 | -1.031442000 |
| H | -5.488862000 | -1.114138000 | -1.815425000 |
| C | -5.479573000 | -0.556235000 | 0.272149000 |
| C | -6.722633000 | -1.340958000 | 0.613028000 |
| H | -7.407794000 | -1.401080000 | -0.244927000 |
| H | -7.263799000 | -0.888920000 | 1.456673000 |
| H | -6.465974000 | -2.373742000 | 0.901840000 |
| C | -4.802318000 | 0.176277000 | 1.255862000 |
| H | -5.201410000 | 0.205691000 | 2.273674000 |
| C | -3.622217000 | 0.877068000 | 0.975082000 |
| C | -2.903270000 | 1.642875000 | 2.052519000 |
| H | -1.927874000 | 1.186316000 | 2.290148000 |
| H | -3.503172000 | 1.672787000 | 2.972010000 |
| H | -2.699668000 | 2.681619000 | 1.747934000 |
| C | 1.623627000 | 2.002725000 | -0.510075000 |
| C | 2.173810000 | 2.634852000 | 0.629375000 |
| C | 1.321070000 | 3.488025000 | 1.529600000 |
| H | 1.869826000 | 3.752722000 | 2.442945000 |
| H | 0.409636000 | 2.951730000 | 1.825879000 |
| H | 1.030133000 | 4.427704000 | 1.030104000 |
| C | 3.529173000 | 2.444550000 | 0.896791000 |
| H | 3.957324000 | 2.902114000 | 1.793024000 |
| C | 4.346392000 | 1.666700000 | 0.059525000 |
| C | 5.798930000 | 1.445247000 | 0.400893000 |
| H | 5.906565000 | 1.002930000 | 1.404048000 |
| H | 6.358585000 | 2.394267000 | 0.405374000 |
| H | 6.280744000 | 0.772490000 | -0.322214000 |
| C | 3.785711000 | 1.119398000 | -1.094665000 |
| H | 4.413022000 | 0.535848000 | -1.773916000 |
| C | 2.429481000 | 1.292871000 | -1.419749000 |
| C | 1.920295000 | 0.776886000 | -2.738781000 |
| H | 0.846777000 | 0.949716000 | -2.869686000 |
| H | 2.071726000 | -0.307870000 | -2.823911000 |
| H | 2.464462000 | 1.268058000 | -3.561749000 |
| C | 0.589611000 | -2.561340000 | 1.472475000 |
| C | 2.957815000 | -1.949572000 | 1.207013000 |
| C | 1.801558000 | -2.650259000 | 0.725366000 |
| C | 4.157365000 | -1.992897000 | 0.514840000 |
| C | 1.939994000 | -3.405892000 | -0.481071000 |
| C | 4.265296000 | -2.737702000 | -0.671709000 |
| H | 5.018651000 | -1.437911000 | 0.890572000 |
| C | 3.150762000 | -3.445301000 | -1.155017000 |
| H | 1.080011000 | -3.943864000 | -0.876132000 |
| H | 5.211168000 | -2.768676000 | -1.216182000 |
| H | 3.235193000 | -4.028845000 | -2.074084000 |
| C | -0.791867000 | -3.022056000 | 1.072813000 |
| C | -1.536261000 | -1.696789000 | 0.894808000 |
| H | -0.780024000 | -3.571672000 | 0.122877000 |
| H | -1.247986000 | -3.661448000 | 1.852593000 |
| H | -2.303005000 | -1.690913000 | 0.115107000 |
| H | 2.853997000 | -1.345661000 | 2.110461000 |
| H | 0.682657000 | -2.178458000 | 2.490961000 |

| | | | | |
|---|---|---|---|---|
| | H | -1.890857000 | -1.260872000 | 1.835640000 |

# Rh-IV-Vd

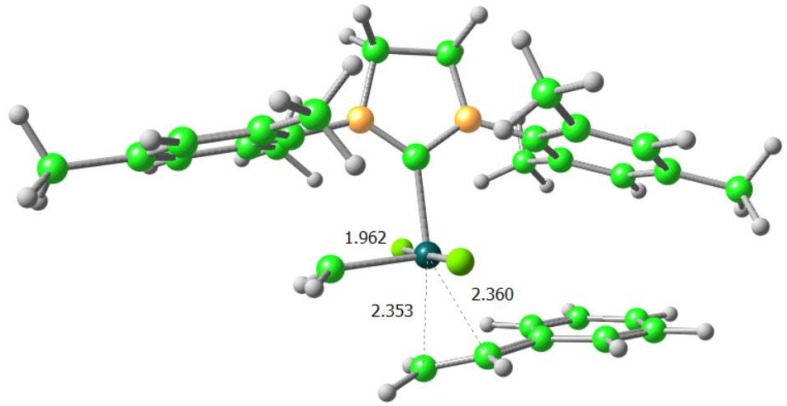



Zero-point correction= 0.566542 (Hartree/Particle)
Thermal correction to Energy= 0.604797
Thermal correction to Enthalpy= 0.605742
Thermal correction to Gibbs Free Energy= 0.494688
Sum of electronic and zero-point Energies= -2305.591639
Sum of electronic and thermal Energies= -2305.553383
Sum of electronic and thermal Enthalpies= -2305.552439
Sum of electronic and thermal Free Energies= -2305.663492

| | | | |
|---|---|---|---|
| Rh | 0.092279000 | -0.568229000 | -0.596821000 |
| Cl | 0.185322000 | -1.878540000 | 1.372418000 |
| Cl | -0.055046000 | 0.699632000 | -2.590712000 |
| N | 1.972120000 | 1.251575000 | 0.935596000 |
| N | -0.132048000 | 1.877078000 | 0.953815000 |
| C | 0.738901000 | 0.964531000 | 0.472681000 |
| C | 1.992716000 | 2.512398000 | 1.717997000 |
| H | 2.504934000 | 3.297675000 | 1.138458000 |
| H | 2.533082000 | 2.365965000 | 2.662430000 |
| C | 0.495891000 | 2.805403000 | 1.918576000 |
| H | 0.148668000 | 2.567829000 | 2.937484000 |
| H | 0.223663000 | 3.844453000 | 1.688974000 |
| C | 3.196662000 | 0.607769000 | 0.563066000 |
| C | 3.793880000 | -0.290386000 | 1.467411000 |
| C | 3.160130000 | -0.592356000 | 2.798049000 |
| H | 3.745591000 | -1.344248000 | 3.344003000 |
| H | 2.136788000 | -0.974687000 | 2.658729000 |
| H | 3.097826000 | 0.307427000 | 3.432065000 |
| C | 4.986288000 | -0.913114000 | 1.079202000 |
| H | 5.452811000 | -1.626769000 | 1.764064000 |
| C | 5.593548000 | -0.645889000 | -0.155833000 |
| C | 6.853711000 | -1.366343000 | -0.567302000 |
| H | 7.483175000 | -1.603918000 | 0.302511000 |
| H | 7.448561000 | -0.765922000 | -1.270553000 |
| H | 6.613553000 | -2.318650000 | -1.068655000 |
| C | 4.994606000 | 0.293669000 | -1.004830000 |
| H | 5.468344000 | 0.534058000 | -1.960758000 |
| C | 3.800396000 | 0.941917000 | -0.664469000 |
| C | 3.174390000 | 1.944393000 | -1.595547000 |
| H | 3.846047000 | 2.161011000 | -2.436868000 |
| H | 2.955574000 | 2.895194000 | -1.084511000 |
| H | 2.219258000 | 1.573487000 | -2.003379000 |
| C | -1.534547000 | 1.914262000 | 0.647665000 |
| C | -1.958544000 | 2.788034000 | -0.380598000 |
| C | -0.973574000 | 3.660365000 | -1.111068000 |
| H | -1.488967000 | 4.287390000 | -1.850788000 |
| H | -0.232907000 | 3.042499000 | -1.639706000 |
| H | -0.433303000 | 4.328736000 | -0.421154000 |
| C | -3.317128000 | 2.818728000 | -0.698977000 |
| H | -3.654058000 | 3.473614000 | -1.507193000 |
| C | -4.256042000 | 2.038017000 | -0.005240000 |
| C | -5.709821000 | 2.046815000 | -0.406690000 |
| H | -5.877535000 | 1.390452000 | -1.277136000 |
| H | -6.044455000 | 3.055003000 | -0.692721000 |
| H | -6.353788000 | 1.687820000 | 0.408481000 |
| C | -3.807919000 | 1.238149000 | 1.047221000 |
| H | -4.526725000 | 0.641722000 | 1.613878000 |
| C | -2.451959000 | 1.160984000 | 1.402355000 |
| C | -2.050578000 | 0.303322000 | 2.571778000 |
| H | -2.603342000 | 0.611709000 | 3.473210000 |
| H | -0.975750000 | 0.347122000 | 2.777477000 |
| H | -2.285989000 | -0.752610000 | 2.374233000 |
| C | -1.358288000 | -2.061284000 | -1.754331000 |
| C | -3.596658000 | -1.565571000 | -0.855156000 |
| C | -2.427336000 | -2.356649000 | -0.804653000 |
| C | -4.670251000 | -1.814259000 | -0.001064000 |
| C | -2.371832000 | -3.405909000 | 0.140469000 |
| C | -4.596990000 | -2.851286000 | 0.935425000 |
| H | -5.565942000 | -1.192698000 | -0.061420000 |
| C | -3.441004000 | -3.643629000 | 0.999096000 |
| H | -1.479320000 | -4.027194000 | 0.206554000 |
| H | -5.435197000 | -3.047869000 | 1.607043000 |
| H | -3.377007000 | -4.455791000 | 1.726369000 |
| C | -0.094062000 | -2.662257000 | -1.851724000 |
| C | 1.728008000 | -1.431756000 | -1.203907000 |
| H | 0.187676000 | -3.474527000 | -1.181494000 |
| H | 0.409748000 | -2.619420000 | -2.815983000 |
| H | 2.323958000 | -1.978790000 | -0.467843000 |
| H | -3.639540000 | -0.738226000 | -1.567722000 |
| H | -1.641842000 | -1.394717000 | -2.572550000 |

| | | | | |
|---|---|---|---|---|
| | H | 2.213095000 | -1.014370000 | -2.091080000 |

# Rh-Vd



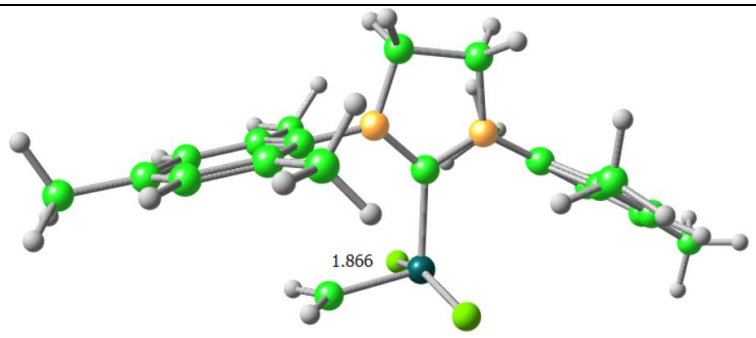

Zero-point correction= 0.566958 (Hartree/Particle)
Thermal correction to Energy= 0.605908
Thermal correction to Enthalpy= 0.606852
Thermal correction to Gibbs Free Energy= 0.494489
Sum of electronic and zero-point Energies= -2305.597211
Sum of electronic and thermal Energies= -2305.558262
Sum of electronic and thermal Enthalpies= -2305.557317
Sum of electronic and thermal Free Energies= -2305.669681

HOMO -0.13417 LUMO -0.10176

| | | | |
|---|---|---|---|
| Rh | 0.113130000 | -0.876232000 | -0.466961000 |
| Cl | 0.225055000 | -1.923606000 | 1.679781000 |
| Cl | -0.008051000 | 0.176302000 | -2.593259000 |
| N | 2.038612000 | 1.098657000 | 0.832893000 |
| N | -0.079996000 | 1.670372000 | 0.938831000 |
| C | 0.791633000 | 0.763210000 | 0.449219000 |
| C | 2.062161000 | 2.376426000 | 1.589183000 |
| H | 2.566752000 | 3.149049000 | 0.987041000 |
| H | 2.620090000 | 2.247318000 | 2.526085000 |
| C | 0.569781000 | 2.671391000 | 1.813105000 |
| H | 0.257520000 | 2.509666000 | 2.856677000 |
| H | 0.278093000 | 3.687251000 | 1.512155000 |
| C | 3.294429000 | 0.544337000 | 0.409479000 |
| C | 4.025603000 | -0.251172000 | 1.314703000 |
| C | 3.438781000 | -0.652677000 | 2.639801000 |
| H | 4.105518000 | -1.350583000 | 3.163952000 |
| H | 2.455757000 | -1.129855000 | 2.505077000 |
| H | 3.286983000 | 0.219325000 | 3.297946000 |
| C | 5.295215000 | -0.690582000 | 0.921904000 |
| H | 5.859809000 | -1.337019000 | 1.600097000 |
| C | 5.858862000 | -0.326071000 | -0.308269000 |
| C | 7.242472000 | -0.790837000 | -0.691310000 |
| H | 8.006977000 | -0.063989000 | -0.368824000 |
| H | 7.339996000 | -0.906802000 | -1.780517000 |
| H | 7.485926000 | -1.753910000 | -0.219831000 |
| C | 5.124364000 | 0.516492000 | -1.155310000 |
| H | 5.553330000 | 0.820873000 | -2.114311000 |
| C | 3.850353000 | 0.980540000 | -0.812743000 |
| C | 3.069631000 | 1.859008000 | -1.749876000 |
| H | 3.706489000 | 2.215897000 | -2.570462000 |
| H | 2.649078000 | 2.738687000 | -1.238001000 |
| H | 2.216616000 | 1.310586000 | -2.183135000 |
| C | -1.474524000 | 1.753151000 | 0.605874000 |
| C | -1.837699000 | 2.528279000 | -0.517332000 |
| C | -0.799078000 | 3.241897000 | -1.339259000 |
| H | -1.276602000 | 3.855786000 | -2.114551000 |
| H | -0.135563000 | 2.517841000 | -1.834399000 |
| H | -0.176599000 | 3.905919000 | -0.718084000 |
| C | -3.195398000 | 2.632324000 | -0.832094000 |
| H | -3.488387000 | 3.215557000 | -1.709705000 |
| C | -4.183851000 | 2.027942000 | -0.042198000 |
| C | -5.642002000 | 2.174577000 | -0.398841000 |
| H | -5.969614000 | 3.222641000 | -0.306149000 |
| H | -6.276309000 | 1.563539000 | 0.257652000 |
| H | -5.829468000 | 1.867949000 | -1.439592000 |
| C | -3.788308000 | 1.318031000 | 1.095040000 |
| H | -4.547619000 | 0.856762000 | 1.730121000 |
| C | -2.440405000 | 1.175871000 | 1.452160000 |
| C | -2.063347000 | 0.481773000 | 2.731844000 |
| H | -1.775531000 | 1.216734000 | 3.503024000 |
| H | -1.220652000 | -0.209721000 | 2.592789000 |
| H | -2.915701000 | -0.090515000 | 3.121589000 |
| C | -1.502699000 | -2.261733000 | -1.487321000 |
| C | -3.796924000 | -1.380774000 | -1.356101000 |
| C | -2.735645000 | -2.053339000 | -0.715789000 |
| C | -5.039020000 | -1.253244000 | -0.736192000 |
| C | -2.936311000 | -2.545916000 | 0.590380000 |
| C | -5.231555000 | -1.761343000 | 0.551981000 |
| H | -5.857028000 | -0.751749000 | -1.255721000 |
| C | -4.171154000 | -2.391915000 | 1.216946000 |
| H | -2.112450000 | -3.027956000 | 1.116901000 |
| H | -6.202777000 | -1.661224000 | 1.041565000 |
| H | -4.313083000 | -2.776576000 | 2.229084000 |
| C | -0.422304000 | -3.055939000 | -1.174738000 |
| C | 1.945432000 | -1.453351000 | -0.867962000 |
| H | -0.367713000 | -3.641297000 | -0.257561000 |
| H | 0.316510000 | -3.275228000 | -1.945604000 |
| H | 2.328735000 | -2.278970000 | -0.259374000 |

| | | | | |
|---|---|---|---|---|
| H | -3.634460000 | -0.973192000 | -2.356446000 |
| H | -1.532663000 | -1.837005000 | -2.493495000 |
| H | 2.256839000 | -1.362526000 | -1.913430000 |

# Rh-VId




Zero-point correction= 0.435605 (Hartree/Particle)
Thermal correction to Energy= 0.466686
Thermal correction to Enthalpy= 0.467630
Thermal correction to Gibbs Free Energy= 0.371760
Sum of electronic and zero-point Energies= -1995.935268
Sum of electronic and thermal Energies= -1995.904187
Sum of electronic and thermal Enthalpies= -1995.903243
Sum of electronic and thermal Free Energies= -1995.999112

HOMO -0.15804 LUMO -0.12692

| | | | |
|---|---|---|---|
| Rh | -0.155044000 | -0.012833000 | -1.342835000 |
| Cl | -0.412826000 | -2.322454000 | -1.607830000 |
| Cl | -0.247754000 | 2.299851000 | -1.698944000 |
| N | 1.129172000 | 0.209234000 | 1.343725000 |
| N | -1.070746000 | 0.211758000 | 1.403590000 |
| C | 0.008154000 | 0.116209000 | 0.600094000 |
| C | 0.827079000 | 0.306407000 | 2.792428000 |
| H | 1.356267000 | 1.163415000 | 3.230896000 |
| H | 1.162720000 | -0.609543000 | 3.304156000 |
| C | -0.705748000 | 0.472569000 | 2.813497000 |
| H | -1.207781000 | -0.246413000 | 3.476013000 |
| H | -1.015204000 | 1.489894000 | 3.098574000 |
| C | 2.477306000 | 0.063220000 | 0.887334000 |
| C | 3.022259000 | -1.230076000 | 0.776058000 |
| C | 2.182407000 | -2.450018000 | 1.041107000 |
| H | 2.799181000 | -3.358249000 | 1.022165000 |
| H | 1.392391000 | -2.554048000 | 0.278028000 |
| H | 1.679831000 | -2.400718000 | 2.019565000 |
| C | 4.350801000 | -1.342439000 | 0.348338000 |
| H | 4.786512000 | -2.339595000 | 0.240539000 |
| C | 5.128015000 | -0.215151000 | 0.047883000 |
| C | 6.565626000 | -0.364382000 | -0.385045000 |
| H | 7.242577000 | -0.331633000 | 0.484860000 |
| H | 6.865708000 | 0.445868000 | -1.064940000 |
| H | 6.733049000 | -1.323189000 | -0.896047000 |
| C | 4.549656000 | 1.055255000 | 0.182283000 |
| H | 5.141168000 | 1.942908000 | -0.058508000 |
| C | 3.225902000 | 1.221308000 | 0.606589000 |
| C | 2.595865000 | 2.584516000 | 0.698080000 |
| H | 3.327135000 | 3.367992000 | 0.458978000 |
| H | 2.201126000 | 2.786602000 | 1.706666000 |
| H | 1.748242000 | 2.671654000 | -0.002065000 |
| C | -2.426085000 | 0.089139000 | 0.946078000 |
| C | -3.164256000 | 1.247190000 | 0.628320000 |
| C | -2.594022000 | 2.625284000 | 0.829590000 |
| H | -3.240374000 | 3.380982000 | 0.364132000 |
| H | -1.594468000 | 2.718323000 | 0.381808000 |
| H | -2.520965000 | 2.867299000 | 1.903383000 |
| C | -4.470340000 | 1.075199000 | 0.152209000 |
| H | -5.049597000 | 1.961714000 | -0.119706000 |
| C | -5.051038000 | -0.193225000 | 0.021716000 |
| C | -6.438682000 | -0.351501000 | -0.547640000 |
| H | -6.956036000 | -1.218402000 | -0.111832000 |
| H | -6.393082000 | -0.510039000 | -1.637798000 |
| H | -7.051258000 | 0.543950000 | -0.370296000 |
| C | -4.309050000 | -1.313754000 | 0.419236000 |
| H | -4.761010000 | -2.307400000 | 0.358820000 |
| C | -2.998672000 | -1.198949000 | 0.896679000 |
| C | -2.231515000 | -2.412374000 | 1.346674000 |
| H | -1.748365000 | -2.250887000 | 2.322656000 |
| H | -1.443463000 | -2.660939000 | 0.618486000 |
| H | -2.900316000 | -3.278845000 | 1.435400000 |
| C | 1.616925000 | -0.075915000 | -1.924400000 |
| H | 2.114530000 | -1.045162000 | -2.022012000 |
| H | 2.165821000 | 0.858196000 | -2.073038000 |

**Table S2**. Computed stationary points (energies in kcal/mol) for the olefin metathesis reaction pathway for M(SIMes)$Cl_2$(=CHPh)$PPh_3$ (M = Fe and Co) with ethylene as a substrate (m = multiplicity; 1 = singlet, 2 = doublet, 3 = triplet, 4 = quadruplet, 5 = quintuplet, 6 = sextuplet; g = gas and s = solvent).

| | | Fe | | | | | | | | | Co | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | BP86-D3BJ(TZVP) | | BP86-D3BJ /TZVP | | M06L/TZVP | | M06/TZVP | | | BP86-D3BJ(TZVP) | | BP86-D3BJ /TZVP | | M06L/TZVP | | M06/TZVP | |
| | m | $E_g$ | $G_g$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ | m | $E_g$ | $G_g$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ |
| I | 1 | 0.00 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| | 3 | 5.1 | 3.1 | 4.1 | 2.0 | -4.2 | -6.2 | -18.7 | -20.8 | 4 | 11.4 | 11.7 | 13.8 | 14.2 | 7.8 | 8.1 | 2.3 | 2.7 |
| | 5 | 18.0 | 12.0 | 17.3 | 11.3 | -7.7 | -13.7 | -33.8 | -39.9 | 6 | 43.1 | 37.0 | 45.8 | 39.7 | 27.5 | 21.4 | 14.5 | 8.4 |
| II | 1 | 43.3 | 20.6 | 36.8 | 14.1 | 26.6 | 3.9 | 27.2 | 4.5 | 2 | 35.7 | 15.2 | 27.1 | 6.6 | 17.5 | -3.0 | 16.6 | -3.9 |
| | 3 | 38.4 | 17.5 | 29.3 | 8.4 | 10.8 | -10.1 | -3.3 | -24.2 | 4 | 44.1 | 26.9 | 36.1 | 18.9 | 15.8 | -1.5 | 7.6 | -9.7 |
| | 5 | 41.3 | 20.6 | 33.2 | 12.6 | 0.2 | -20.4 | -25.6 | -46.3 | | | | | | | | | |
| III | 1 | 34.0 | 31.2 | 30.0 | 27.2 | 21.9 | 19.0 | 22.7 | 19.8 | 2 | 32.9 | 29.2 | 29.6 | 25.9 | 22.8 | 19.1 | 22.1 | 18.4 |
| | 3 | 35.3 | 30.9 | 30.1 | 25.7 | 15.6 | 11.2 | -0.1 | -4.6 | | | | | | | | | |
| | 5 | 36.3 | 32.8 | 30.0 | 26.5 | -2.5 | -5.9 | -28.3 | -31.8 | 6 | 65.5 | 54.6 | 63.2 | 52.4 | 38.2 | 27.4 | 26.2 | 15.3 |
| IV | 1 | 26.5 | 25.4 | 23.2 | 22.1 | 10.5 | 9.4 | 8.7 | 7.7 | 2 | not stable in any multiplicity | | | | | | | |
| | 3 | 18.0 | 11.4 | 14.8 | 8.2 | -0.5 | -7.0 | -17.4 | -24.0 | 4 | | | | | | | | |
| | 5 | 3.5 | -6.3 | -2.6 | -12.4 | -39.6 | -49.4 | -69.4 | -79.2 | 6 | | | | | | | | |
| | 7 | 36.5 | 27.5 | 29.5 | 20.6 | -6.3 | -15.3 | -33.9 | -42.9 | 8 | | | | | | | | |
| V | 1 | 26.3 | 23.8 | 22.6 | 20.1 | 9.0 | 6.5 | 7.4 | 4.9 | 2 | 37.9 | 32.8 | 35.9 | 30.8 | 30.0 | 24.9 | 31.1 | 26.0 |
| | 3 | 25.5 | 22.0 | 21.5 | 18.0 | 5.9 | 2.4 | -4.6 | -7.1 | | | | | | | | | |
| | 5 | 29.9 | 30.7 | 25.6 | 26.4 | -0.2 | +0.7 | -21.7 | -20.9 | 6 | 78.1 | 66.2 | 76.0 | 64.1 | 48.3 | 36.4 | 35.9 | 24.0 |
| VI | 1 | 55.5 | 32.0 | 48.2 | 24.6 | 34.5 | 10.9 | 34.2 | 10.7 | 2 | 53.9 | 31.7 | 45.0 | 22.8 | 33.3 | 11.1 | 31.2 | 8.9 |
| | 3 | 52.7 | 27.0 | 42.9 | 17.3 | 22.3 | -3.3 | 6.6 | -19.1 | 4 | 54.0 | 30.6 | 49.5 | 26.1 | 19.2 | -4.1 | 8.4 | -15.0 |
| | 5 | 58.0 | 31.0 | 48.8 | 21.8 | 12.7 | -14.3 | -13.5 | -40.5 | | | | | | | | | |

**Table S3**. Computed stationary points (energies in kcal/mol) for the olefin metathesis reaction pathway for M(SIMes)$Cl_2$(=CHPh)$PPh_3$ (M = Ru and Rh) with ethylene as a substrate (m = multiplicity; 1 = singlet, 2 = doublet; g = gas and s = solvent).

| | | Ru | | Rh |
|---|---|---|---|---|

| | | BP86-D3BJ(TZVP) | | BP86-D3BJ /TZVP | | M06L/TZVP | | M06/TZVP | | | BP86-D3BJ(TZVP) | | BP86-D3BJ /TZVP | | M06L/TZVP | | M06/TZVP | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | m | $E_g$ | $G_g$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ | m | $E_g$ | $G_g$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ | $E_s$ | $G_s$ |
| **I** | 1 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **II** | 1 | 47.6 | 26.5 | 44.2 | 23.1 | 26.8 | 5.6 | 29.2 | 8.1 | 2 | 43.9 | 25.8 | 38.6 | 20.5 | 23.8 | 5.7 | 27.8 | 9.7 |
| **III** | 1 | 31.8 | 26.0 | 31.2 | 25.4 | 15.1 | 9.4 | 15.1 | 9.3 | 2 | 27.4 | 22.0 | 26.9 | 21.6 | 16.4 | 11.0 | 17.0 | 11.6 |
| **III-IV** | 1 | 34.0 | 30.7 | 34.0 | 30.7 | 18.7 | 15.4 | 16.8 | 13.5 | 2 | 32.9 | 29.2 | 31.9 | 28.2 | 23.6 | 19.9 | 24.7 | 21.0 |
| **IV** | 1 | 30.3 | 27.4 | 30.3 | 27.5 | 13.6 | 10.8 | 12.2 | 9.3 | 2 | 14.0 | 11.0 | 13.0 | 10.1 | -1.0 | -3.9 | -1.8 | -4.6 |
| **IV-V** | 1 | 39.4 | 34.2 | 38.5 | 33.3 | 22.9 | 17.6 | 20.6 | 15.3 | 2 | 40.9 | 36.3 | 39.4 | 34.7 | 28.7 | 24.0 | 28.8 | 24.2 |
| **V** | 1 | 36.9 | 32.2 | 36.5 | 31.8 | 20.7 | 16.1 | 18.8 | 14.1 | 2 | 37.2 | 32.4 | 36.2 | 31.5 | 24.7 | 20.0 | 23.4 | 18.6 |
| **VI** | 1 | 58.0 | 34.5 | 53.9 | 30.4 | 32.4 | 8.9 | 34.9 | 11.4 | 2 | 56.1 | 35.3 | 49.3 | 28.6 | 31.1 | 10.3 | 33.4 | 12.5 |