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**1\_S0**

Pt -0.000002000 -0.670014000 0.000206000

Cl 0.000035000 -3.103144000 -0.000060000

C -1.216915000 3.293769000 0.000144000

C -1.222268000 1.900985000 -0.000010000

C -0.000006000 1.232065000 0.000025000

C 1.222254000 1.900988000 -0.000009000

C 1.216895000 3.293772000 0.000145000

C -0.000011000 3.972104000 0.000237000

C -2.357371000 0.983221000 -0.000085000

C 2.357361000 0.983230000 -0.000084000

C 3.695650000 1.345677000 -0.000377000

C 4.674794000 0.368754000 -0.000481000

C 4.300118000 -0.965686000 -0.000301000

C 2.954546000 -1.277455000 -0.000076000

N -2.007180000 -0.338722000 0.000004000

N 2.007180000 -0.338716000 0.000006000

C -2.954537000 -1.277470000 -0.000077000

C -4.300111000 -0.965714000 -0.000300000

C -4.674798000 0.368723000 -0.000479000

C -3.695664000 1.345656000 -0.000377000

H -2.141015000 3.861630000 0.000171000

H 2.140992000 3.861638000 0.000174000

H -0.000012000 5.055237000 0.000357000

H 3.960727000 2.394703000 -0.000534000

H 5.721590000 0.647140000 -0.000725000

H 5.032830000 -1.761291000 -0.000349000

H 2.595763000 -2.299300000 0.000008000

H -2.595745000 -2.299313000 0.000005000

H -5.032817000 -1.761325000 -0.000346000

H -5.721597000 0.647099000 -0.000723000

H -3.960750000 2.394679000 -0.000534000

Sum of electronic and zero-point Energies= -1304.604327

Sum of electronic and thermal Energies= -1304.588750

Sum of electronic and thermal Enthalpies= -1304.587806

Sum of electronic and thermal Free Energies= -1304.648026

**1\_T1**

Pt 0.000000000 0.657338000 0.000047000

Cl 0.000002000 3.058244000 -0.000277000

C -1.241109000 -3.289794000 -0.000018000

C -1.254378000 -1.878162000 -0.000001000

C 0.000000000 -1.215806000 0.000032000

C 1.254371000 -1.878163000 0.000024000

C 1.241105000 -3.289791000 0.000020000

C -0.000005000 -3.937323000 -0.000005000

C -2.361274000 -0.975761000 0.000004000

C 2.361273000 -0.975761000 0.000017000

C 3.714111000 -1.336736000 -0.000001000

C 4.687063000 -0.361944000 -0.000011000

C 4.317180000 0.982018000 -0.000004000

C 2.967624000 1.294322000 0.000017000

N -2.023488000 0.363059000 0.000033000

N 2.023491000 0.363056000 0.000029000

C -2.967620000 1.294326000 0.000039000

C -4.317176000 0.982026000 0.000017000

C -4.687064000 -0.361940000 -0.000012000

C -3.714116000 -1.336733000 -0.000018000

H -2.152228000 -3.873339000 -0.000032000

H 2.152224000 -3.873335000 0.000021000

H -0.000005000 -5.022874000 -0.000020000

H 3.979364000 -2.385761000 -0.000007000

H 5.733905000 -0.641232000 -0.000026000

H 5.050645000 1.776096000 -0.000014000

H 2.615627000 2.318647000 0.000021000

H -2.615622000 2.318652000 0.000057000

H -5.050638000 1.776106000 0.000021000

H -5.733906000 -0.641226000 -0.000031000

H -3.979374000 -2.385757000 -0.000041000

Sum of electronic and zero-point Energies= -1304.503025

Sum of electronic and thermal Energies= -1304.486879

Sum of electronic and thermal Enthalpies= -1304.485935

Sum of electronic and thermal Free Energies= -1304.548536

**1\_OER**

Pt 0.007126000 -0.670378000 0.000015000

Cl -0.026102000 -3.130343000 -0.000155000

C -1.242505000 3.302119000 -0.000020000

C -1.220132000 1.896244000 0.000057000

C -0.001200000 1.237349000 0.000040000

C 1.245372000 1.902467000 -0.000056000

C 1.203311000 3.313332000 -0.000151000

C -0.019519000 3.977130000 -0.000124000

C -2.352983000 0.981036000 0.000085000

C 2.352392000 1.008772000 -0.000032000

C 3.714501000 1.351762000 0.000054000

C 4.691471000 0.391407000 0.000119000

C 4.308156000 -0.976979000 0.000078000

C 2.972714000 -1.283366000 0.000001000

N -2.010808000 -0.344750000 0.000114000

N 1.998054000 -0.359024000 -0.000042000

C -2.966158000 -1.274360000 0.000072000

C -4.313424000 -0.956235000 0.000005000

C -4.679799000 0.379272000 -0.000002000

C -3.691570000 1.350430000 0.000047000

H -2.172300000 3.859376000 0.000037000

H 2.118939000 3.896766000 -0.000256000

H -0.020760000 5.062263000 -0.000192000

H 3.979415000 2.403533000 0.000091000

H 5.738229000 0.671839000 0.000219000

H 5.040584000 -1.773351000 0.000078000

H 2.625325000 -2.310528000 -0.000059000

H -2.613592000 -2.298775000 0.000103000

H -5.050200000 -1.748495000 -0.000023000

H -5.725051000 0.664920000 -0.000065000

H -3.947188000 2.401932000 0.000028000

Sum of electronic and zero-point Energies= -1304.694515

Sum of electronic and thermal Energies= -1304.678452

Sum of electronic and thermal Enthalpies= -1304.677508

Sum of electronic and thermal Free Energies= -1304.739261

**1\_ImΑ**

Pt -0.008118000 -0.912835000 0.000215000

C 1.251216000 3.011425000 -0.000284000

C 1.233263000 1.614549000 -0.000180000

C 0.005447000 0.969977000 -0.000110000

C -1.242436000 1.625895000 -0.000145000

C -1.191691000 3.030544000 -0.000242000

C 0.030082000 3.692564000 -0.000323000

C 2.365227000 0.694899000 -0.000161000

C -2.356881000 0.734721000 -0.000125000

C -3.713316000 1.074961000 -0.000264000

C -4.689709000 0.109882000 -0.000228000

C -4.297431000 -1.256065000 -0.000065000

C -2.965382000 -1.559341000 0.000040000

N 2.004832000 -0.625731000 -0.000001000

N -1.990800000 -0.626322000 0.000038000

C 2.957089000 -1.564215000 0.000104000

C 4.303615000 -1.256509000 -0.000018000

C 4.684363000 0.076823000 -0.000235000

C 3.702021000 1.055180000 -0.000280000

H 2.182366000 3.565875000 -0.000363000

H -2.106840000 3.613936000 -0.000297000

H 0.034811000 4.776688000 -0.000436000

H -3.981272000 2.125734000 -0.000368000

H -5.737192000 0.384407000 -0.000301000

H -5.026704000 -2.055298000 -0.000012000

H -2.625019000 -2.589342000 0.000203000

H 2.612061000 -2.590685000 0.000312000

H 5.033161000 -2.055325000 0.000064000

H 5.731517000 0.353023000 -0.000318000

H 3.965259000 2.104797000 -0.000407000

Sum of electronic and zero-point Energies= -844.435839

Sum of electronic and thermal Energies= -844.421708

Sum of electronic and thermal Enthalpies= -844.420764

Sum of electronic and thermal Free Energies= -844.478161

**1\_ImB**

Pt 0.000029000 -0.911260000 -0.004057000

C 1.224388000 3.013361000 -0.009246000

C 1.249637000 1.621537000 0.014324000

C -0.000023000 0.969855000 0.043637000

C -1.249541000 1.621483000 0.014141000

C -1.224622000 3.013264000 -0.009516000

C -0.000106000 3.689533000 -0.015570000

C 2.371438000 0.724040000 0.001859000

C -2.371474000 0.723865000 0.001738000

C -3.715040000 1.063172000 0.007561000

C -4.709061000 0.099857000 0.008954000

C -4.298252000 -1.256397000 0.006804000

C -2.969522000 -1.567119000 -0.003056000

N 1.974533000 -0.632678000 -0.009679000

N -1.974566000 -0.632691000 -0.009601000

C 2.969509000 -1.567084000 -0.003217000

C 4.298209000 -1.256434000 0.006651000

C 4.709051000 0.099945000 0.008949000

C 3.715133000 1.063223000 0.007690000

H 2.147069000 3.585566000 -0.028707000

H -2.147381000 3.585321000 -0.029047000

H -0.000120000 4.773825000 -0.036157000

H -3.972394000 2.117415000 0.013812000

H -5.756609000 0.371585000 0.013224000

H -5.022492000 -2.062564000 0.010327000

H -2.636331000 -2.599189000 -0.009719000

H 2.636307000 -2.599160000 -0.009920000

H 5.022438000 -2.062609000 0.010091000

H 5.756610000 0.371643000 0.013247000

H 3.972561000 2.117456000 0.014042000

Sum of electronic and zero-point Energies= -844.505298

Sum of electronic and thermal Energies= -844.490467

Sum of electronic and thermal Enthalpies= -844.489523

Sum of electronic and thermal Free Energies= -844.547806

**1\_ImC**

Pt -0.000011000 -0.621522000 0.000247000

C -1.219628000 3.413271000 0.004744000

C -1.217188000 2.019200000 0.005182000

C 0.000155000 1.347899000 0.000671000

C 1.217618000 2.018967000 -0.005262000

C 1.220300000 3.413036000 -0.007368000

C 0.000397000 4.090453000 -0.001876000

C -2.350801000 1.090354000 0.007559000

C 2.351082000 1.089928000 -0.007011000

C 3.686850000 1.463380000 -0.013874000

C 4.678748000 0.498227000 -0.013320000

C 4.315194000 -0.837862000 -0.003212000

C 2.970969000 -1.168135000 0.004384000

N -2.011890000 -0.239188000 0.000547000

N 2.011976000 -0.239570000 0.000367000

C -2.970996000 -1.167637000 -0.002695000

C -4.315172000 -0.837196000 0.005482000

C -4.678539000 0.498950000 0.015200000

C -3.686516000 1.463983000 0.014800000

C -0.000593000 -2.756475000 -0.001691000

O -1.098875000 -3.383458000 -0.129862000

O 1.097284000 -3.384423000 0.125313000

H -2.141394000 3.987092000 0.009004000

H 2.142168000 3.986682000 -0.012986000

H 0.000496000 5.174315000 -0.002905000

H 3.939404000 2.515904000 -0.019537000

H 5.722705000 0.789259000 -0.019364000

H 5.057290000 -1.625780000 -0.000265000

H 2.578615000 -2.189268000 0.024233000

H -2.578822000 -2.188826000 -0.022828000

H -5.057370000 -1.625019000 0.003282000

H -5.722454000 0.790116000 0.021689000

H -3.938930000 2.516543000 0.020124000

Sum of electronic and zero-point Energies= -1033.021665

Sum of electronic and thermal Energies= -1033.004495

Sum of electronic and thermal Enthalpies= -1033.003551

Sum of electronic and thermal Free Energies= -1033.067920

**1\_ImD**

Pt -0.002515000 -0.594341000 0.015933000

C -1.224016000 3.415176000 -0.078108000

C -1.221613000 2.022263000 -0.033615000

C -0.003117000 1.355530000 0.006262000

C 1.213069000 2.026280000 -0.002891000

C 1.212410000 3.419451000 -0.045166000

C -0.006613000 4.094116000 -0.081399000

C -2.355565000 1.098457000 -0.021759000

C 2.348735000 1.105559000 0.028269000

C 3.681447000 1.486809000 0.054384000

C 4.678014000 0.528926000 0.093369000

C 4.321928000 -0.809040000 0.102131000

C 2.981082000 -1.141874000 0.069449000

N -2.013425000 -0.228065000 0.015210000

N 2.012201000 -0.223813000 0.034105000

C -2.972797000 -1.154864000 0.053601000

C -4.316327000 -0.830443000 0.041771000

C -4.680732000 0.504506000 -0.009050000

C -3.690906000 1.470350000 -0.037320000

C -0.070195000 -2.687647000 -0.015461000

O -0.881230000 -3.420058000 0.535155000

H -2.147290000 3.983965000 -0.111634000

H 2.134288000 3.991362000 -0.053953000

H -0.008031000 5.176976000 -0.116050000

H 3.927425000 2.540512000 0.047380000

H 5.719779000 0.824848000 0.116566000

H 5.064280000 -1.595203000 0.131468000

H 2.650642000 -2.170823000 0.054640000

H -2.624717000 -2.178853000 0.111372000

H -5.054730000 -1.620314000 0.073105000

H -5.724863000 0.792798000 -0.022007000

H -3.944920000 2.521690000 -0.068956000

O 0.896117000 -3.316845000 -0.761608000

H 0.724929000 -4.271350000 -0.685061000

Sum of electronic and zero-point Energies= -1033.514038

Sum of electronic and thermal Energies= -1033.496508

Sum of electronic and thermal Enthalpies= -1033.495564

Sum of electronic and thermal Free Energies= -1033.560842

**1\_ImE**

Pt 0.001981000 -0.581907000 -0.021147000

C -1.238066000 3.417733000 0.051756000

C -1.230216000 2.024812000 0.008083000

C -0.009539000 1.365337000 -0.011679000

C 1.203659000 2.038365000 0.017371000

C 1.195583000 3.431211000 0.061730000

C -0.025091000 4.101210000 0.077057000

C -2.361818000 1.102055000 -0.015709000

C 2.345715000 1.128359000 0.001120000

C 3.676979000 1.513464000 0.002802000

C 4.675691000 0.557900000 -0.024781000

C 4.324708000 -0.781572000 -0.056239000

C 2.985696000 -1.115892000 -0.053793000

N -2.016259000 -0.222361000 -0.035490000

N 2.014603000 -0.199528000 -0.022335000

C -2.978351000 -1.148316000 -0.072231000

C -4.320674000 -0.828019000 -0.085294000

C -4.685749000 0.507756000 -0.058313000

C -3.697036000 1.473326000 -0.023990000

C 0.025949000 -2.634322000 0.071016000

H -2.164754000 3.980512000 0.069428000

H 2.115802000 4.004195000 0.087217000

H -0.031242000 5.183679000 0.112643000

H 3.920534000 2.567280000 0.023208000

H 5.716842000 0.855926000 -0.023954000

H 5.069003000 -1.565619000 -0.081872000

H 2.672717000 -2.149929000 -0.080877000

H -2.655741000 -2.179576000 -0.093159000

H -5.056469000 -1.619856000 -0.116225000

H -5.729869000 0.795095000 -0.066145000

H -3.951437000 2.524615000 -0.006438000

O 0.228864000 -3.404532000 -0.951651000

H 0.215551000 -4.348614000 -0.703715000

O -0.142176000 -3.332042000 1.162858000

H -0.281998000 -2.733586000 1.911069000

Sum of electronic and zero-point Energies= -1033.933006

Sum of electronic and thermal Energies= -1033.915247

Sum of electronic and thermal Enthalpies= -1033.914303

Sum of electronic and thermal Free Energies= -1033.980394

**1\_TS**

Pt -0.000088000 -0.573257000 -0.024247000

C -1.166343000 3.448673000 0.045651000

C -1.184111000 2.055531000 0.018602000

C 0.024510000 1.375425000 0.019240000

C 1.250121000 2.024261000 0.043826000

C 1.267725000 3.417331000 0.073054000

C 0.059219000 4.109143000 0.073643000

C -2.333566000 1.154616000 -0.018680000

C 2.376017000 1.093623000 0.025946000

C 3.713292000 1.454713000 0.037685000

C 4.694642000 0.480689000 0.009307000

C 4.319433000 -0.851326000 -0.034570000

C 2.974199000 -1.162045000 -0.044452000

N -2.014906000 -0.176278000 -0.040716000

N 2.021577000 -0.227464000 -0.011715000

C -2.994583000 -1.082642000 -0.082447000

C -4.330262000 -0.734164000 -0.103591000

C -4.668352000 0.608273000 -0.079752000

C -3.660096000 1.553605000 -0.036705000

C 0.014225000 -2.596822000 -0.065491000

H -2.082168000 4.028990000 0.044498000

H 2.198067000 3.973790000 0.092897000

H 0.072920000 5.191935000 0.094473000

H 3.976043000 2.503612000 0.068122000

H 5.741007000 0.759649000 0.019607000

H 5.049507000 -1.648614000 -0.060669000

H 2.641552000 -2.189305000 -0.085009000

H -2.692970000 -2.119833000 -0.096412000

H -5.081729000 -1.510955000 -0.139171000

H -5.706224000 0.917065000 -0.095713000

H -3.892959000 2.609867000 -0.019257000

O 0.566212000 -3.500589000 -0.705763000

H -0.072648000 -4.200565000 0.200054000

O -0.772016000 -3.450953000 0.849429000

H -0.680198000 -3.256385000 1.797920000

Sum of electronic and zero-point Energies= -1033.872555

Sum of electronic and thermal Energies= -1033.854850

Sum of electronic and thermal Enthalpies= -1033.853906

Sum of electronic and thermal Free Energies= -1033.919398

**1\_ImF**

Pt -0.000002000 0.733407000 -0.000034000

C -1.217006000 -3.271562000 -0.000135000

C -1.218174000 -1.878367000 -0.000100000

C 0.000005000 -1.217760000 -0.000101000

C 1.218184000 -1.878364000 -0.000097000

C 1.217020000 -3.271559000 -0.000131000

C 0.000008000 -3.947116000 -0.000156000

C -2.357789000 -0.965148000 -0.000027000

C 2.357794000 -0.965141000 -0.000025000

C 3.688916000 -1.344923000 0.000047000

C 4.682848000 -0.382887000 0.000142000

C 4.325742000 0.954574000 0.000149000

C 2.985214000 1.283531000 0.000071000

N -2.021367000 0.359558000 -0.000008000

N 2.021366000 0.359563000 -0.000004000

C -2.985219000 1.283522000 0.000073000

C -4.325745000 0.954559000 0.000164000

C -4.682845000 -0.382904000 0.000158000

C -3.688909000 -1.344935000 0.000054000

C 0.000008000 2.693404000 0.000074000

O -0.000027000 3.822722000 0.000142000

H -2.140467000 -3.839042000 -0.000140000

H 2.140484000 -3.839036000 -0.000131000

H 0.000009000 -5.030070000 -0.000181000

H 3.937793000 -2.397499000 0.000031000

H 5.725386000 -0.675610000 0.000207000

H 5.065942000 1.742747000 0.000212000

H 2.669784000 2.317030000 0.000057000

H -2.669794000 2.317023000 0.000051000

H -5.065949000 1.742728000 0.000233000

H -5.725382000 -0.675631000 0.000232000

H -3.937781000 -2.397512000 0.000038000

Sum of electronic and zero-point Energies= -957.588276

Sum of electronic and thermal Energies= -957.572016

Sum of electronic and thermal Enthalpies= -957.571072

Sum of electronic and thermal Free Energies= -957.633427

**1\_ImG**

Pt -0.000002000 0.733407000 -0.000034000

C -1.217006000 -3.271562000 -0.000135000

C -1.218174000 -1.878367000 -0.000100000

C 0.000005000 -1.217760000 -0.000101000

C 1.218184000 -1.878364000 -0.000097000

C 1.217020000 -3.271559000 -0.000131000

C 0.000008000 -3.947116000 -0.000156000

C -2.357789000 -0.965148000 -0.000027000

C 2.357794000 -0.965141000 -0.000025000

C 3.688916000 -1.344923000 0.000047000

C 4.682848000 -0.382887000 0.000142000

C 4.325742000 0.954574000 0.000149000

C 2.985214000 1.283531000 0.000071000

N -2.021367000 0.359558000 -0.000008000

N 2.021366000 0.359563000 -0.000004000

C -2.985219000 1.283522000 0.000073000

C -4.325745000 0.954559000 0.000164000

C -4.682845000 -0.382904000 0.000158000

C -3.688909000 -1.344935000 0.000054000

C 0.000008000 2.693404000 0.000074000

O -0.000027000 3.822722000 0.000142000

H -2.140467000 -3.839042000 -0.000140000

H 2.140484000 -3.839036000 -0.000131000

H 0.000009000 -5.030070000 -0.000181000

H 3.937793000 -2.397499000 0.000031000

H 5.725386000 -0.675610000 0.000207000

H 5.065942000 1.742747000 0.000212000

H 2.669784000 2.317030000 0.000057000

H -2.669794000 2.317023000 0.000051000

H -5.065949000 1.742728000 0.000233000

H -5.725382000 -0.675631000 0.000232000

H -3.937781000 -2.397512000 0.000038000

Sum of electronic and zero-point Energies= -957.588276

Sum of electronic and thermal Energies= -957.572016

Sum of electronic and thermal Enthalpies= -957.571072

Sum of electronic and thermal Free Energies= -957.633427

**2\_S0**

Pt 2.555756000 0.004648000 0.004283000

Cl 4.989695000 0.011858000 0.008013000

C 3.166581000 -2.949107000 -0.091595000

C 2.856709000 -4.294199000 -0.144483000

C 1.522834000 -4.670177000 -0.165662000

C 0.544519000 -3.692896000 -0.133085000

C 0.904899000 -2.355156000 -0.080958000

N 2.226791000 -2.003483000 -0.060569000

C -0.014375000 -1.221301000 -0.043952000

C -1.404550000 -1.220038000 -0.057165000

C -2.114430000 -0.011278000 -0.018105000

C -1.413306000 1.202324000 0.028229000

C -0.023100000 1.213002000 0.029411000

C 0.655074000 -0.001856000 -0.003733000

C 3.145608000 2.962182000 0.106868000

C 2.826229000 4.305130000 0.157645000

C 1.489717000 4.672134000 0.166680000

C 0.518333000 3.688318000 0.124551000

C 0.888139000 2.353048000 0.075165000

N 2.212534000 2.010274000 0.066711000

C -3.587449000 -0.017549000 -0.026016000

C -4.318454000 -1.020200000 0.612713000

C -5.699856000 -1.035639000 0.612617000

C -6.437218000 -0.036006000 -0.047968000

C -5.702904000 0.985385000 -0.678012000

C -4.321502000 0.982378000 -0.665495000

N -7.806232000 -0.058487000 -0.080928000

C -8.521647000 1.090579000 -0.575619000

C -8.519083000 -1.013144000 0.729433000

H 4.187973000 -2.589432000 -0.073448000

H 3.653288000 -5.025466000 -0.168715000

H 1.245943000 -5.716548000 -0.207508000

H -0.504249000 -3.958719000 -0.148629000

H -1.959799000 -2.149627000 -0.118814000

H -1.975195000 2.128262000 0.083928000

H 4.169532000 2.609445000 0.097663000

H 3.617629000 5.041705000 0.189618000

H 1.205425000 5.716596000 0.206536000

H -0.532304000 3.947109000 0.130608000

H -3.795471000 -1.800915000 1.154618000

H -6.208913000 -1.828175000 1.143655000

H -6.214401000 1.786124000 -1.194281000

H -3.800889000 1.776758000 -1.189495000

H -9.589601000 0.885021000 -0.541599000

H -8.258910000 1.303372000 -1.615516000

H -8.325980000 1.995673000 0.015377000

H -9.586180000 -0.909605000 0.543336000

H -8.341673000 -0.871859000 1.804468000

H -8.236227000 -2.037589000 0.472594000

Sum of electronic and zero-point Energies= -1669.193769

Sum of electronic and thermal Energies= -1669.168855

Sum of electronic and thermal Enthalpies= -1669.167910

Sum of electronic and thermal Free Energies= -1669.249838

**2\_T1**

Pt -2.537275000 -0.002265000 0.001245000

Cl -4.970295000 0.020567000 0.005175000

C -3.168339000 -2.958241000 0.065805000

C -2.867392000 -4.299510000 0.094693000

C -1.510235000 -4.685994000 0.097177000

C -0.538451000 -3.723090000 0.070912000

C -0.879981000 -2.357468000 0.042879000

N -2.234579000 -2.002050000 0.040738000

C 0.015410000 -1.261100000 0.013120000

C 1.412942000 -1.233097000 0.007412000

C 2.116614000 -0.017239000 -0.007594000

C 1.409657000 1.236547000 -0.016684000

C 0.018275000 1.223253000 -0.022211000

C -0.655030000 0.007160000 -0.005460000

C -3.146991000 2.972172000 -0.059958000

C -2.826694000 4.319563000 -0.090392000

C -1.491740000 4.684022000 -0.097801000

C -0.519151000 3.697279000 -0.074971000

C -0.892409000 2.362043000 -0.046544000

N -2.216248000 2.022429000 -0.038846000

C 3.557258000 -0.011761000 -0.012151000

C 4.312067000 -1.161819000 -0.339527000

C 5.677607000 -1.165853000 -0.340621000

C 6.410225000 -0.000210000 0.002656000

C 5.667365000 1.159802000 0.330383000

C 4.299571000 1.146579000 0.311973000

N 7.755320000 0.002008000 0.011125000

C 8.484987000 1.206651000 0.344790000

C 8.495876000 -1.197675000 -0.317532000

H -4.191631000 -2.601739000 0.062109000

H -3.666385000 -5.027863000 0.114887000

H -1.239044000 -5.734802000 0.119594000

H 0.509581000 -3.997682000 0.071516000

H 1.967344000 -2.161288000 0.056002000

H 1.956570000 2.165801000 -0.077677000

H -4.171453000 2.620586000 -0.051882000

H -3.617817000 5.056918000 -0.107436000

H -1.206069000 5.728780000 -0.121108000

H 0.531753000 3.954545000 -0.078808000

H 3.803839000 -2.069938000 -0.634954000

H 6.197667000 -2.071099000 -0.620027000

H 6.177530000 2.071490000 0.606996000

H 3.782490000 2.053212000 0.595021000

H 9.550168000 1.004261000 0.281816000

H 8.256215000 1.538767000 1.361139000

H 8.246281000 2.017327000 -0.348706000

H 9.558626000 -0.993114000 -0.226385000

H 8.293393000 -1.520362000 -1.342524000

H 8.243304000 -2.015558000 0.362100000

Sum of electronic and zero-point Energies= -1669.117446

Sum of electronic and thermal Energies= -1669.092022

Sum of electronic and thermal Enthalpies= -1669.091077

Sum of electronic and thermal Free Energies= -1669.175280

**2\_OER**

C -1.413608000 -1.236917000 -0.071364000

C -0.009677000 -1.214586000 -0.055275000

C 0.652329000 -0.000033000 -0.012709000

C -0.018498000 1.241249000 0.019490000

C -1.426982000 1.197981000 0.013099000

C -2.114702000 -0.019669000 -0.035126000

Pt 2.558115000 0.010060000 0.008637000

C 0.903948000 -2.348174000 -0.086841000

C 0.871342000 2.350374000 0.068014000

C 0.523845000 3.711090000 0.108249000

C 1.481338000 4.689545000 0.154460000

C 2.850392000 4.311047000 0.160344000

C 3.160951000 2.976625000 0.118914000

N 2.230556000 -2.008355000 -0.062599000

N 2.240084000 2.000878000 0.073564000

C 3.158964000 -2.963749000 -0.088441000

C 2.839722000 -4.310147000 -0.139423000

C 1.503909000 -4.674224000 -0.163578000

C 0.533445000 -3.685756000 -0.136546000

Cl 5.017669000 -0.020891000 0.018915000

H -1.961333000 -2.169224000 -0.143421000

H -2.002311000 2.116225000 0.074280000

H -0.528591000 3.973108000 0.101666000

H 1.197516000 5.734978000 0.185397000

H 3.644087000 5.045423000 0.196345000

H 4.189089000 2.632182000 0.120855000

H 4.183705000 -2.612754000 -0.067143000

H 3.631148000 -5.047528000 -0.159089000

H 1.217331000 -5.718508000 -0.203105000

H -0.518281000 -3.939979000 -0.153321000

C -3.590614000 -0.026486000 -0.044226000

C -4.329781000 0.975397000 -0.675054000

C -4.324107000 -1.032442000 0.586670000

C -5.712712000 0.979258000 -0.683387000

H -3.808811000 1.774288000 -1.191587000

C -5.707243000 -1.047871000 0.589392000

H -3.798166000 -1.817501000 1.119276000

C -6.446151000 -0.045313000 -0.061187000

H -6.224011000 1.785687000 -1.191371000

H -6.214109000 -1.845629000 1.115156000

N -7.822353000 -0.070349000 -0.096358000

C -8.524654000 -0.991230000 0.760743000

H -9.594161000 -0.897755000 0.580358000

H -8.242968000 -2.024227000 0.542101000

H -8.337318000 -0.808152000 1.828790000

C -8.529751000 1.109031000 -0.526869000

H -8.262850000 1.376379000 -1.552309000

H -9.599256000 0.906797000 -0.509045000

H -8.332278000 1.981447000 0.112598000

Sum of electronic and zero-point Energies= -1669.283354

Sum of electronic and thermal Energies= -1669.258062

Sum of electronic and thermal Enthalpies= -1669.257118

Sum of electronic and thermal Free Energies= -1669.340235

**2\_ΙmΑ**

C -1.072833000 -1.239221000 -0.085220000

C 0.321233000 -1.224175000 -0.066286000

C 0.971907000 -0.001882000 -0.022982000

C 0.311971000 1.241398000 0.009232000

C -1.089390000 1.192213000 0.000870000

C -1.779338000 -0.022782000 -0.048817000

Pt 2.852750000 0.009156000 0.017564000

C 1.237731000 -2.359200000 -0.092778000

C 1.201558000 2.357217000 0.064410000

C 0.859267000 3.711947000 0.103579000

C 1.822777000 4.689300000 0.153287000

C 3.188819000 4.298205000 0.162629000

C 3.494328000 2.967077000 0.123933000

N 2.559505000 -2.002346000 -0.055325000

N 2.563009000 1.991763000 0.076876000

C 3.495570000 -2.956969000 -0.075802000

C 3.184920000 -4.301621000 -0.133953000

C 1.851111000 -4.678539000 -0.171380000

C 0.874969000 -3.693936000 -0.149586000

H -1.619142000 -2.172602000 -0.152367000

H -1.662582000 2.111556000 0.060452000

H -0.191876000 3.978280000 0.093394000

H 1.546730000 5.735931000 0.183810000

H 3.986816000 5.027937000 0.200167000

H 4.524759000 2.628229000 0.130447000

H 4.522642000 -2.615232000 -0.044061000

H 3.981966000 -5.033020000 -0.148948000

H 1.573073000 -5.724198000 -0.217132000

H -0.175240000 -3.953528000 -0.177274000

C -3.253976000 -0.030170000 -0.054823000

C -3.992740000 0.971732000 -0.686019000

C -3.984386000 -1.033851000 0.583052000

C -5.374861000 0.978694000 -0.686600000

H -3.473823000 1.767373000 -1.209687000

C -5.366787000 -1.045734000 0.594097000

H -3.458454000 -1.818554000 1.116288000

C -6.107063000 -0.041898000 -0.054676000

H -5.887678000 1.783710000 -1.195055000

H -5.872931000 -1.840146000 1.125345000

N -7.480248000 -0.060763000 -0.077490000

C -8.183600000 -0.990695000 0.769282000

H -7.908271000 -2.022100000 0.534735000

H -7.989934000 -0.822828000 1.838233000

H -9.253228000 -0.888739000 0.595759000

C -8.190414000 1.110074000 -0.527111000

H -7.933034000 1.355242000 -1.560719000

H -9.259759000 0.910256000 -0.494004000

H -7.985071000 1.994553000 0.092190000

Sum of electronic and zero-point Energies= -1209.024924

Sum of electronic and thermal Energies= -1209.001530

Sum of electronic and thermal Enthalpies= -1209.000586

Sum of electronic and thermal Free Energies= -1209.079581

**2\_ImB**

Pt -2.498408000 0.008229000 0.000377000

C 1.524848000 -1.229505000 -0.148204000

C 0.133454000 -1.218709000 -0.139739000

C -0.534090000 -0.001501000 -0.096083000

C 0.149744000 1.206515000 -0.045679000

C 1.541232000 1.198666000 -0.038702000

C 2.235916000 -0.020190000 -0.093262000

C -0.800940000 -2.348458000 -0.157704000

C -0.769671000 2.346428000 0.025301000

C -0.387282000 3.679019000 0.065150000

C -1.345578000 4.675866000 0.125107000

C -2.684098000 4.321091000 0.141074000

C -3.023538000 2.979756000 0.100234000

N -2.127332000 -2.004189000 -0.083253000

N -2.101616000 2.016048000 0.048202000

C -3.061259000 -2.957672000 -0.085056000

C -2.740681000 -4.301569000 -0.170554000

C -1.408221000 -4.670167000 -0.249907000

C -0.436818000 -3.684247000 -0.238806000

C -4.622784000 0.014887000 0.171682000

O -5.230857000 -1.070094000 0.435077000

O -5.261709000 1.102664000 0.013414000

H 2.084260000 -2.157999000 -0.207993000

H 2.112740000 2.118460000 0.038471000

H 0.666634000 3.925205000 0.045987000

H -1.047476000 5.717368000 0.156107000

H -3.466527000 5.067698000 0.184256000

H -4.047429000 2.595656000 0.098373000

H -4.076399000 -2.565632000 0.014704000

H -3.532587000 -5.039360000 -0.171183000

H -1.124703000 -5.714002000 -0.317495000

H 0.613123000 -3.941362000 -0.295537000

C 3.710090000 -0.031310000 -0.073935000

C 4.425418000 -1.030437000 0.587579000

C 4.462275000 0.964141000 -0.698852000

C 5.807155000 -1.046041000 0.623749000

H 3.887564000 -1.807734000 1.119717000

C 5.844501000 0.967257000 -0.673976000

H 3.954856000 1.757288000 -1.237554000

C 6.561825000 -0.050129000 -0.020477000

H 6.300886000 -1.836292000 1.172508000

H 6.368822000 1.767058000 -1.178871000

N 7.935683000 -0.073440000 -0.017309000

C 8.619026000 -0.994762000 0.854998000

H 9.692201000 -0.899123000 0.700495000

H 8.405652000 -0.812358000 1.917854000

H 8.344233000 -2.028044000 0.628565000

C 8.657116000 1.093548000 -0.458741000

H 9.725158000 0.890806000 -0.405408000

H 8.419291000 1.334715000 -1.497894000

H 8.443054000 1.981394000 0.152865000

Sum of electronic and zero-point Energies= -1397.610547

Sum of electronic and thermal Energies= -1397.584142

Sum of electronic and thermal Enthalpies= -1397.583198

Sum of electronic and thermal Free Energies= -1397.668898

**2\_ImC**

Pt 2.467511000 0.003451000 0.002980000

C -1.544424000 1.216788000 0.040696000

C -0.153413000 1.216314000 0.049298000

C 0.520857000 0.003086000 0.072440000

C -0.154269000 -1.208956000 0.093692000

C -1.545394000 -1.209157000 0.095577000

C -2.249214000 0.003810000 0.062772000

C 0.766040000 2.353030000 -0.005892000

C 0.764781000 -2.346697000 0.102789000

C 0.382807000 -3.678851000 0.141658000

C 1.340029000 -4.676853000 0.145094000

C 2.678084000 -4.322606000 0.110969000

C 3.011803000 -2.981968000 0.073484000

N 2.093627000 2.013918000 -0.046512000

N 2.094357000 -2.012024000 0.067318000

C 3.016362000 2.975234000 -0.116808000

C 2.687806000 4.317728000 -0.136332000

C 1.351982000 4.678928000 -0.086246000

C 0.389782000 3.687024000 -0.024555000

C 4.557044000 0.071058000 -0.151206000

O 5.225811000 0.855145000 -0.810757000

H -2.105514000 2.143500000 -0.015919000

H -2.107084000 -2.136405000 0.133251000

H -0.670971000 -3.923082000 0.169696000

H 1.043541000 -5.718286000 0.175519000

H 3.463708000 -5.066123000 0.114288000

H 4.040965000 -2.651078000 0.059792000

H 4.040727000 2.631219000 -0.179681000

H 3.475010000 5.057512000 -0.192151000

H 1.060258000 5.722114000 -0.098678000

H -0.662209000 3.938094000 0.009968000

O 5.263574000 -0.861430000 0.569605000

H 6.204496000 -0.696138000 0.386170000

C -3.722227000 0.005256000 0.029601000

C -4.438386000 -0.983928000 -0.646078000

C -4.470854000 0.996250000 0.665956000

C -5.818825000 -0.986376000 -0.697530000

H -3.902937000 -1.768418000 -1.169962000

C -5.851954000 1.011907000 0.627783000

H -3.962756000 1.768316000 1.233882000

C -6.570377000 0.025238000 -0.072166000

H -6.315559000 -1.777519000 -1.242280000

H -6.376029000 1.795459000 1.157630000

N -7.937464000 0.050976000 -0.147372000

C -8.674756000 0.997200000 0.650510000

H -9.735264000 0.898941000 0.427527000

H -8.533905000 0.841858000 1.728970000

H -8.380995000 2.024159000 0.416499000

C -8.639084000 -1.083658000 -0.692103000

H -9.707237000 -0.876482000 -0.686209000

H -8.344434000 -1.272032000 -1.728321000

H -8.463525000 -2.003370000 -0.117688000

Sum of electronic and zero-point Energies= -1398.103380

Sum of electronic and thermal Energies= -1398.076587

Sum of electronic and thermal Enthalpies= -1398.075643

Sum of electronic and thermal Free Energies= -1398.161875

**2\_ImD**

Pt 2.450459000 0.002523000 -0.009534000

C -1.552920000 -1.219575000 -0.126465000

C -0.162171000 -1.215522000 -0.120408000

C 0.506371000 -0.001877000 -0.080703000

C -0.170345000 1.207301000 -0.036906000

C -1.561151000 1.201919000 -0.028727000

C -2.262824000 -0.011378000 -0.074846000

C 0.754912000 -2.351924000 -0.150652000

C 0.739440000 2.348562000 0.023125000

C 0.355064000 3.679547000 0.058846000

C 1.311142000 4.677000000 0.107310000

C 2.650773000 4.325264000 0.115894000

C 2.984433000 2.986453000 0.080401000

N 2.080832000 -2.014060000 -0.102346000

N 2.067560000 2.016375000 0.039040000

C 3.002926000 -2.979805000 -0.134593000

C 2.677331000 -4.318819000 -0.211458000

C 1.339947000 -4.676277000 -0.256204000

C 0.378323000 -3.683588000 -0.225146000

C 4.500374000 0.014214000 0.162139000

H -2.108049000 -2.149102000 -0.184225000

H -2.122137000 2.127065000 0.041643000

H -0.698799000 3.923577000 0.046187000

H 1.013491000 5.717886000 0.135898000

H 3.435352000 5.068672000 0.149893000

H 4.018693000 2.672861000 0.082438000

H 4.035566000 -2.662913000 -0.099002000

H 3.466379000 -5.057867000 -0.235696000

H 1.048423000 -5.717527000 -0.316696000

H -0.674054000 -3.931542000 -0.262089000

O 5.310821000 0.222931000 -0.827868000

H 6.244492000 0.200687000 -0.543857000

O 5.154812000 -0.169642000 1.278292000

H 4.526204000 -0.315119000 2.000209000

C -3.734785000 -0.018071000 -0.055042000

C -4.481891000 0.989598000 -0.666990000

C -4.450571000 -1.027058000 0.591439000

C -5.862543000 0.994639000 -0.645162000

H -3.973320000 1.787902000 -1.196819000

C -5.830721000 -1.039606000 0.627696000

H -3.915806000 -1.813932000 1.112449000

C -6.582672000 -0.030276000 -0.002668000

H -6.386114000 1.799782000 -1.141973000

H -6.328122000 -1.836000000 1.163862000

N -7.949052000 -0.045954000 0.006321000

C -8.645735000 -1.023507000 0.803654000

H -8.435410000 -0.918675000 1.876431000

H -9.716811000 -0.905951000 0.653618000

H -8.378355000 -2.041054000 0.504908000

C -8.678234000 1.095936000 -0.485200000

H -8.448820000 1.291483000 -1.536638000

H -9.744742000 0.894267000 -0.412179000

H -8.461128000 2.008982000 0.084790000

Sum of electronic and zero-point Energies= -1398.523090

Sum of electronic and thermal Energies= -1398.496043

Sum of electronic and thermal Enthalpies= -1398.495099

Sum of electronic and thermal Free Energies= -1398.582381

**2\_ImE**

Pt 2.450459000 0.002523000 -0.009534000

C -1.552920000 -1.219575000 -0.126465000

C -0.162171000 -1.215522000 -0.120408000

C 0.506371000 -0.001877000 -0.080703000

C -0.170345000 1.207301000 -0.036906000

C -1.561151000 1.201919000 -0.028727000

C -2.262824000 -0.011378000 -0.074846000

C 0.754912000 -2.351924000 -0.150652000

C 0.739440000 2.348562000 0.023125000

C 0.355064000 3.679547000 0.058846000

C 1.311142000 4.677000000 0.107310000

C 2.650773000 4.325264000 0.115894000

C 2.984433000 2.986453000 0.080401000

N 2.080832000 -2.014060000 -0.102346000

N 2.067560000 2.016375000 0.039040000

C 3.002926000 -2.979805000 -0.134593000

C 2.677331000 -4.318819000 -0.211458000

C 1.339947000 -4.676277000 -0.256204000

C 0.378323000 -3.683588000 -0.225146000

C 4.500374000 0.014214000 0.162139000

H -2.108049000 -2.149102000 -0.184225000

H -2.122137000 2.127065000 0.041643000

H -0.698799000 3.923577000 0.046187000

H 1.013491000 5.717886000 0.135898000

H 3.435352000 5.068672000 0.149893000

H 4.018693000 2.672861000 0.082438000

H 4.035566000 -2.662913000 -0.099002000

H 3.466379000 -5.057867000 -0.235696000

H 1.048423000 -5.717527000 -0.316696000

H -0.674054000 -3.931542000 -0.262089000

O 5.310821000 0.222931000 -0.827868000

H 6.244492000 0.200687000 -0.543857000

O 5.154812000 -0.169642000 1.278292000

H 4.526204000 -0.315119000 2.000209000

C -3.734785000 -0.018071000 -0.055042000

C -4.481891000 0.989598000 -0.666990000

C -4.450571000 -1.027058000 0.591439000

C -5.862543000 0.994639000 -0.645162000

H -3.973320000 1.787902000 -1.196819000

C -5.830721000 -1.039606000 0.627696000

H -3.915806000 -1.813932000 1.112449000

C -6.582672000 -0.030276000 -0.002668000

H -6.386114000 1.799782000 -1.141973000

H -6.328122000 -1.836000000 1.163862000

N -7.949052000 -0.045954000 0.006321000

C -8.645735000 -1.023507000 0.803654000

H -8.435410000 -0.918675000 1.876431000

H -9.716811000 -0.905951000 0.653618000

H -8.378355000 -2.041054000 0.504908000

C -8.678234000 1.095936000 -0.485200000

H -8.448820000 1.291483000 -1.536638000

H -9.744742000 0.894267000 -0.412179000

H -8.461128000 2.008982000 0.084790000

Sum of electronic and zero-point Energies= -1398.523090

Sum of electronic and thermal Energies= -1398.496043

Sum of electronic and thermal Enthalpies= -1398.495099

Sum of electronic and thermal Free Energies= -1398.582381

**2\_TS**

Pt 2.443224000 0.015641000 -0.022944000

C -1.555836000 -1.222922000 0.089016000

C -0.165469000 -1.214047000 0.068349000

C 0.496972000 0.002395000 0.036275000

C -0.182138000 1.210233000 0.018225000

C -1.572472000 1.200657000 0.027854000

C -2.269685000 -0.015874000 0.063769000

C 0.755116000 -2.348878000 0.072442000

C 0.722681000 2.356159000 -0.040813000

C 0.331818000 3.684567000 -0.076340000

C 1.283465000 4.685955000 -0.141907000

C 2.623550000 4.339399000 -0.173578000

C 2.964437000 3.001880000 -0.135333000

N 2.080139000 -2.008059000 0.026464000

N 2.051762000 2.030289000 -0.067707000

C 3.003474000 -2.972413000 0.017839000

C 2.678937000 -4.313879000 0.056652000

C 1.343054000 -4.674164000 0.107062000

C 0.380075000 -3.681798000 0.114019000

C 4.464254000 0.073654000 -0.106498000

H -2.107520000 -2.154797000 0.139760000

H -2.137007000 2.124862000 -0.021085000

H -0.722861000 3.924205000 -0.053554000

H 0.981012000 5.725469000 -0.169664000

H 3.404298000 5.085683000 -0.227238000

H 3.998884000 2.691122000 -0.165577000

H 4.034810000 -2.652980000 -0.018825000

H 3.468747000 -5.052445000 0.046505000

H 1.052879000 -5.717032000 0.139596000

H -0.671740000 -3.931869000 0.151146000

O 5.340282000 0.641028000 -0.772232000

H 6.075658000 0.024464000 0.118823000

O 5.360466000 -0.687681000 0.792928000

H 5.189194000 -0.586773000 1.744932000

C -3.741164000 -0.025989000 0.061237000

C -4.462473000 -1.029507000 -0.587975000

C -4.482850000 0.974020000 0.692466000

C -5.842680000 -1.043339000 -0.609742000

H -3.932499000 -1.809855000 -1.123438000

C -5.863376000 0.977120000 0.686123000

H -3.969741000 1.767084000 1.225715000

C -6.589055000 -0.041414000 0.039286000

H -6.345039000 -1.834316000 -1.149264000

H -6.382750000 1.775594000 1.197862000

N -7.954683000 -0.057577000 0.043077000

C -8.659694000 -1.031565000 -0.751349000

H -9.729119000 -0.914311000 -0.590135000

H -8.460083000 -0.921409000 -1.825500000

H -8.389434000 -2.050638000 -0.460245000

C -8.680499000 1.074259000 0.562117000

H -9.747400000 0.873282000 0.494042000

H -8.442284000 1.250778000 1.615065000

H -8.468589000 1.997501000 0.007075000

Sum of electronic and zero-point Energies= -1398.462909

Sum of electronic and thermal Energies= -1398.435864

Sum of electronic and thermal Enthalpies= -1398.434919

Sum of electronic and thermal Free Energies= -1398.522087

**2\_ImF**

Pt 2.633646000 0.000976000 0.001030000

C -1.370752000 -1.213919000 -0.027677000

C 0.018952000 -1.214259000 -0.017706000

C 0.685482000 -0.001095000 0.019539000

C 0.016986000 1.211108000 0.053023000

C -1.372715000 1.208753000 0.056956000

C -2.078093000 -0.003059000 0.012091000

C 0.930009000 -2.355337000 -0.062346000

C 0.926151000 2.353956000 0.089819000

C 0.542891000 3.682925000 0.145033000

C 1.502099000 4.679047000 0.178995000

C 2.840571000 4.326468000 0.155372000

C 3.173204000 2.987950000 0.098858000

N 2.255566000 -2.020768000 -0.055637000

N 2.252149000 2.022058000 0.066680000

C 3.178052000 -2.985117000 -0.093243000

C 2.847340000 -4.324471000 -0.140964000

C 1.509388000 -4.679641000 -0.149681000

C 0.548718000 -3.685187000 -0.109051000

C 4.591106000 0.004313000 -0.042920000

O 5.720507000 0.006816000 -0.078794000

H -1.925921000 -2.142490000 -0.091201000

H -1.929368000 2.136831000 0.113933000

H -0.510520000 3.927906000 0.162927000

H 1.206417000 5.719801000 0.223988000

H 3.626632000 5.068503000 0.180369000

H 4.207443000 2.675357000 0.079394000

H 4.211935000 -2.670907000 -0.085214000

H 3.634507000 -5.065154000 -0.170819000

H 1.215237000 -5.721112000 -0.187590000

H -0.504349000 -3.932199000 -0.113840000

C -3.548054000 -0.004622000 0.001473000

C -4.283061000 -1.023399000 0.611307000

C -4.275603000 1.013423000 -0.618496000

C -5.662788000 -1.034789000 0.606238000

H -3.765194000 -1.819853000 1.134675000

C -5.655143000 1.018954000 -0.640133000

H -3.751412000 1.816422000 -1.125245000

C -6.394757000 -0.013694000 -0.031009000

H -6.177824000 -1.839282000 1.112836000

H -6.163803000 1.828220000 -1.145630000

N -7.756909000 -0.024775000 -0.058550000

C -8.482876000 -1.056070000 0.638278000

H -8.301651000 -1.033245000 1.720213000

H -9.548310000 -0.916629000 0.470263000

H -8.213532000 -2.051672000 0.271661000

C -8.474285000 1.090131000 -0.623298000

H -8.226131000 1.234074000 -1.679899000

H -9.542377000 0.896829000 -0.555838000

H -8.262807000 2.028098000 -0.095183000

Sum of electronic and zero-point Energies= -1322.179305

Sum of electronic and thermal Energies= -1322.153563

Sum of electronic and thermal Enthalpies= -1322.152618

Sum of electronic and thermal Free Energies= -1322.237784

**2\_ImG**

Pt 2.633150000 0.003301000 0.002004000

C -1.365246000 -1.220977000 -0.021754000

C 0.024169000 -1.227285000 -0.011200000

C 0.697640000 -0.002747000 0.029909000

C 0.017780000 1.218468000 0.063241000

C -1.371557000 1.205472000 0.061499000

C -2.073268000 -0.009427000 0.015096000

C 0.926205000 -2.355415000 -0.058742000

C 0.913842000 2.351883000 0.098502000

C 0.539976000 3.688156000 0.152181000

C 1.491707000 4.686185000 0.183392000

C 2.841237000 4.319824000 0.158528000

C 3.172996000 2.990292000 0.104573000

N 2.264525000 -1.999513000 -0.056844000

N 2.253907000 2.003889000 0.073742000

C 3.188749000 -2.980876000 -0.096198000

C 2.863917000 -4.312486000 -0.139536000

C 1.516274000 -4.686710000 -0.143133000

C 0.559383000 -3.694047000 -0.101512000

C 4.569970000 0.011901000 -0.055690000

O 5.712503000 0.018403000 -0.104164000

H -1.922514000 -2.149318000 -0.085834000

H -1.933584000 2.131657000 0.113389000

H -0.515385000 3.929778000 0.170525000

H 1.199202000 5.727557000 0.226848000

H 3.630250000 5.059719000 0.181242000

H 4.208058000 2.677923000 0.085038000

H 4.222214000 -2.662691000 -0.092060000

H 3.656786000 -5.047966000 -0.170072000

H 1.229203000 -5.729941000 -0.177202000

H -0.494701000 -3.941821000 -0.101287000

C -3.545984000 -0.014060000 -0.004847000

C -4.285837000 -1.021519000 0.616668000

C -4.273934000 0.990745000 -0.644547000

C -5.667414000 -1.037542000 0.598661000

H -3.769697000 -1.806824000 1.158490000

C -5.655258000 0.993168000 -0.674722000

H -3.747611000 1.789823000 -1.155455000

C -6.397082000 -0.034133000 -0.064145000

H -6.182568000 -1.834800000 1.116720000

H -6.160232000 1.798316000 -1.190655000

N -7.766725000 -0.059289000 -0.118562000

C -8.488579000 -1.013471000 0.684194000

H -8.326535000 -0.869972000 1.761552000

H -9.553285000 -0.912789000 0.482893000

H -8.200134000 -2.037748000 0.433335000

C -8.475647000 1.096502000 -0.606633000

H -8.194712000 1.326630000 -1.637925000

H -9.543632000 0.888042000 -0.595784000

H -8.293094000 1.992736000 0.002202000

Sum of electronic and zero-point Energies= -1322.300221

Sum of electronic and thermal Energies= -1322.274498

Sum of electronic and thermal Enthalpies= -1322.273554

Sum of electronic and thermal Free Energies= -1322.358274

**3\_S0**

Pt 1.771945000 0.051636000 -0.000450000

Cl 4.197847000 0.169380000 -0.016104000

C -2.118259000 -1.373410000 0.023732000

C -0.731999000 -1.302709000 0.012082000

C -0.124578000 -0.049257000 0.022593000

C -0.861538000 1.131570000 0.049361000

C -2.248041000 1.052076000 0.076091000

C -2.882669000 -0.197986000 0.062886000

C 0.242364000 -2.390041000 -0.025138000

C -0.007509000 2.316247000 0.057509000

C -0.442475000 3.632002000 0.084523000

C 0.480026000 4.662853000 0.089195000

C 1.832373000 4.361239000 0.066218000

C 2.217067000 3.034710000 0.039306000

N 1.544071000 -1.971479000 -0.033598000

N 1.331579000 2.037889000 0.034762000

C 2.530045000 -2.868465000 -0.067778000

C 2.287469000 -4.228120000 -0.095650000

C 0.974530000 -4.671417000 -0.087289000

C -0.051545000 -3.744317000 -0.051383000

C -4.340532000 -0.294046000 0.093827000

C -5.117549000 -1.316150000 0.577475000

C -6.505354000 -1.076955000 0.442675000

C -6.775481000 0.124717000 -0.143130000

S -5.340323000 0.960252000 -0.536044000

H -2.629356000 -2.328613000 -0.014342000

H -2.856494000 1.949073000 0.125509000

H -1.504322000 3.839999000 0.101645000

H 0.145201000 5.692745000 0.110633000

H 2.587066000 5.136048000 0.069005000

H 3.256655000 2.732120000 0.021189000

H 3.531739000 -2.456873000 -0.072303000

H 3.119640000 -4.918496000 -0.123360000

H 0.750551000 -5.730956000 -0.108685000

H -1.085678000 -4.063092000 -0.044162000

H -4.703307000 -2.202308000 1.040454000

H -7.272780000 -1.763863000 0.774384000

H -7.736526000 0.563000000 -0.365183000

Sum of electronic and zero-point Energies= -1856.139329

Sum of electronic and thermal Energies= -1856.119150

Sum of electronic and thermal Enthalpies= -1856.118206

Sum of electronic and thermal Free Energies= -1856.190014

**3\_T1**

Pt 1.750354000 0.060195000 0.000010000

Cl 4.171399000 0.215428000 -0.000204000

C -2.098575000 -1.434322000 0.000025000

C -0.712527000 -1.366695000 0.000017000

C -0.121674000 -0.044495000 0.000015000

C -0.875853000 1.128481000 0.000020000

C -2.253450000 1.051376000 0.000027000

C -2.874194000 -0.265345000 0.000031000

C 0.254155000 -2.404828000 0.000008000

C -0.034076000 2.324651000 0.000021000

C -0.488445000 3.631653000 0.000026000

C 0.423993000 4.675994000 0.000024000

C 1.777142000 4.389809000 0.000018000

C 2.179232000 3.064488000 0.000013000

N 1.574678000 -1.956956000 0.000003000

N 1.305662000 2.061051000 0.000015000

C 2.571910000 -2.846794000 -0.000008000

C 2.357362000 -4.205752000 -0.000015000

C 1.034485000 -4.683260000 -0.000011000

C -0.000776000 -3.785578000 0.000000000

C -4.295046000 -0.361186000 0.000041000

C -5.105536000 -1.497109000 0.000117000

C -6.469352000 -1.204187000 0.000088000

C -6.720225000 0.150224000 -0.000020000

S -5.288964000 1.061312000 -0.000027000

H -2.599834000 -2.394028000 0.000018000

H -2.876636000 1.935752000 0.000039000

H -1.553074000 3.824898000 0.000030000

H 0.077055000 5.702029000 0.000028000

H 2.523204000 5.172965000 0.000017000

H 3.222882000 2.775619000 0.000009000

H 3.568764000 -2.423121000 -0.000010000

H 3.203427000 -4.879207000 -0.000024000

H 0.835042000 -5.747839000 -0.000018000

H -1.028395000 -4.127476000 0.000002000

H -4.713983000 -2.504553000 0.000195000

H -7.251065000 -1.951519000 0.000132000

H -7.678998000 0.646571000 -0.000072000

Sum of electronic and zero-point Energies= -1856.059350

Sum of electronic and thermal Energies= -1856.038631

Sum of electronic and thermal Enthalpies= -1856.037687

Sum of electronic and thermal Free Energies= -1856.111682

**3\_OER**

Pt 1.773218000 0.051827000 -0.002161000

Cl 4.222815000 0.221379000 -0.017390000

C -2.130524000 -1.388306000 0.028235000

C -0.718365000 -1.336593000 0.014835000

C -0.128993000 -0.054387000 0.025894000

C -0.861649000 1.119096000 0.058476000

C -2.270031000 1.052342000 0.090896000

C -2.884192000 -0.210703000 0.074109000

C 0.238186000 -2.385370000 -0.023193000

C -0.021822000 2.301499000 0.064176000

C -0.472999000 3.618312000 0.090961000

C 0.435141000 4.662114000 0.092217000

C 1.792402000 4.383132000 0.066213000

C 2.192101000 3.056886000 0.039132000

N 1.578158000 -1.961484000 -0.039059000

N 1.325317000 2.048196000 0.037965000

C 2.556918000 -2.871542000 -0.075983000

C 2.330369000 -4.227012000 -0.099487000

C 0.990757000 -4.682095000 -0.082570000

C -0.027460000 -3.768255000 -0.044612000

C -4.343177000 -0.309822000 0.102745000

C -5.133303000 -1.316336000 0.598673000

C -6.519971000 -1.072588000 0.447672000

C -6.781069000 0.119456000 -0.161516000

S -5.334153000 0.937895000 -0.559143000

H -2.651581000 -2.338256000 -0.022944000

H -2.878462000 1.946164000 0.166529000

H -1.538065000 3.809421000 0.108443000

H 0.084512000 5.687487000 0.113056000

H 2.536533000 5.168211000 0.066256000

H 3.236106000 2.768172000 0.018398000

H 3.560587000 -2.461506000 -0.086316000

H 3.166395000 -4.912530000 -0.129774000

H 0.771119000 -5.743595000 -0.099017000

H -1.060668000 -4.095897000 -0.029834000

H -4.725029000 -2.195063000 1.080558000

H -7.293287000 -1.749828000 0.787050000

H -7.738787000 0.558971000 -0.395495000

Sum of electronic and zero-point Energies= -1856.231641

Sum of electronic and thermal Energies= -1856.210950

Sum of electronic and thermal Enthalpies= -1856.210006

Sum of electronic and thermal Free Energies= -1856.283253

**3\_ImA**

Pt 2.043041000 0.107711000 -0.010213000

C -1.787959000 -1.401671000 0.036825000

C -0.385368000 -1.333666000 0.024075000

C 0.167952000 -0.035387000 0.035963000

C -0.579319000 1.127932000 0.064949000

C -1.973052000 1.031796000 0.094322000

C -2.568800000 -0.243796000 0.079042000

C 0.589704000 -2.369312000 -0.018999000

C 0.239794000 2.335383000 0.067347000

C -0.235139000 3.636023000 0.097988000

C 0.656196000 4.698172000 0.096372000

C 2.015711000 4.436328000 0.063129000

C 2.438093000 3.119721000 0.031799000

N 1.916183000 -1.899786000 -0.043129000

N 1.585390000 2.093458000 0.033520000

C 2.923889000 -2.791291000 -0.079188000

C 2.730867000 -4.145083000 -0.096414000

C 1.400797000 -4.643142000 -0.074987000

C 0.359936000 -3.752487000 -0.036389000

C -4.024869000 -0.374282000 0.102445000

C -4.788748000 -1.410914000 0.577278000

C -6.179999000 -1.200802000 0.424411000

C -6.469182000 -0.004772000 -0.164057000

S -5.044645000 0.860260000 -0.538377000

H -2.286852000 -2.363464000 -0.009679000

H -2.595452000 1.916749000 0.155085000

H -1.303157000 3.808344000 0.122130000

H 0.290731000 5.717448000 0.120569000

H 2.747937000 5.232560000 0.060406000

H 3.490050000 2.864495000 0.003876000

H 3.922354000 -2.367580000 -0.094779000

H 3.585148000 -4.807950000 -0.125974000

H 1.211976000 -5.709576000 -0.087762000

H -0.664892000 -4.105971000 -0.017109000

H -4.361296000 -2.288511000 1.044424000

H -6.936694000 -1.904288000 0.746687000

H -7.436762000 0.413901000 -0.395411000

Sum of electronic and zero-point Energies= -1395.972832

Sum of electronic and thermal Energies= -1395.954090

Sum of electronic and thermal Enthalpies= -1395.953146

Sum of electronic and thermal Free Energies= -1396.022122

**3\_ImB**

Pt 2.039919000 0.110743000 -0.006814000

C -1.769113000 -1.424375000 0.041950000

C -0.387543000 -1.332957000 0.058078000

C 0.171248000 -0.041228000 0.117032000

C -0.583352000 1.147559000 0.082988000

C -1.962883000 1.016855000 0.071255000

C -2.566976000 -0.258741000 0.064742000

C 0.594269000 -2.384469000 -0.004728000

C 0.221088000 2.340849000 0.052658000

C -0.228406000 3.651310000 0.073724000

C 0.652005000 4.718979000 0.057166000

C 2.034370000 4.421976000 0.020824000

C 2.452131000 3.121999000 -0.005303000

N 1.910683000 -1.887032000 -0.045713000

N 1.601342000 2.057571000 0.004752000

C 2.919376000 -2.802556000 -0.079969000

C 2.712420000 -4.152526000 -0.083328000

C 1.394644000 -4.664205000 -0.053073000

C 0.356641000 -3.749356000 -0.011359000

C -4.015602000 -0.390128000 0.061738000

C -4.788340000 -1.498507000 0.331501000

C -6.178789000 -1.261661000 0.225996000

C -6.473985000 0.023416000 -0.122304000

S -5.045635000 0.945565000 -0.330548000

H -2.253040000 -2.393156000 -0.017141000

H -2.595035000 1.900042000 0.077012000

H -1.299342000 3.822126000 0.106870000

H 0.296167000 5.740897000 0.073258000

H 2.777873000 5.210014000 0.007550000

H 3.506813000 2.873380000 -0.042807000

H 3.921233000 -2.389197000 -0.110715000

H 3.570898000 -4.812853000 -0.114130000

H 1.204593000 -5.729572000 -0.060211000

H -0.673704000 -4.087413000 0.020824000

H -4.367778000 -2.452653000 0.620037000

H -6.933667000 -2.015440000 0.411230000

H -7.441905000 0.479635000 -0.262295000

Sum of electronic and zero-point Energies= -1396.045100

Sum of electronic and thermal Energies= -1396.025630

Sum of electronic and thermal Enthalpies= -1396.024685

Sum of electronic and thermal Free Energies= -1396.094852

**3\_ImD**

Pt -1.719763000 -0.040176000 0.012387000

C 2.244780000 1.374329000 0.067796000

C 0.857295000 1.302448000 0.080970000

C 0.241730000 0.056193000 0.101626000

C 0.974931000 -1.124049000 0.105040000

C 2.363487000 -1.059015000 0.106128000

C 3.002023000 0.191231000 0.087686000

C -0.124097000 2.391537000 0.037507000

C 0.104498000 -2.304198000 0.099836000

C 0.543800000 -3.618916000 0.130856000

C -0.371656000 -4.657184000 0.128297000

C -1.723602000 -4.360080000 0.095810000

C -2.119833000 -3.034047000 0.063719000

N -1.434255000 1.987411000 -0.009198000

N -1.239554000 -2.030904000 0.062285000

C -2.407667000 2.899450000 -0.055575000

C -2.143212000 4.258266000 -0.050182000

C -0.827559000 4.686684000 -0.000634000

C 0.184526000 3.743177000 0.040066000

C 4.461280000 0.278800000 0.077176000

C 5.262583000 1.297652000 0.528007000

C 6.644130000 1.049378000 0.346291000

C 6.887861000 -0.156471000 -0.242252000

S 5.433390000 -0.984876000 -0.580655000

C -3.842332000 -0.143970000 -0.152767000

O -4.499431000 0.907291000 -0.432391000

O -4.430068000 -1.256296000 0.027214000

H 2.766192000 2.324426000 0.015553000

H 2.974307000 -1.956726000 0.131119000

H 1.607154000 -3.819585000 0.159525000

H -0.029894000 -5.685273000 0.153817000

H -2.473929000 -5.140134000 0.095287000

H -3.159177000 -2.693763000 0.043921000

H -3.405976000 2.459105000 -0.124463000

H -2.965544000 4.961002000 -0.087366000

H -0.588059000 5.743582000 0.004540000

H 1.222751000 4.047163000 0.077041000

H 4.869780000 2.189720000 0.998184000

H 7.426310000 1.733827000 0.647835000

H 7.838202000 -0.602404000 -0.493308000

Sum of electronic and zero-point Energies= -1584.558603

Sum of electronic and thermal Energies= -1584.536934

Sum of electronic and thermal Enthalpies= -1584.535990

Sum of electronic and thermal Free Energies= -1584.611493

**3\_ImD**

Pt -1.692301000 -0.037339000 -0.025982000

C 2.248484000 1.374977000 -0.034583000

C 0.861339000 1.304996000 -0.060835000

C 0.250078000 0.058406000 -0.110613000

C 0.980936000 -1.121367000 -0.127380000

C 2.369446000 -1.054181000 -0.118255000

C 3.007059000 0.194329000 -0.072255000

C -0.116499000 2.393812000 -0.016126000

C 0.115859000 -2.301373000 -0.149607000

C 0.556973000 -3.613907000 -0.216606000

C -0.354788000 -4.653078000 -0.250194000

C -1.708131000 -4.361016000 -0.216116000

C -2.100055000 -3.038643000 -0.142530000

N -1.424725000 1.985580000 -0.003841000

N -1.227622000 -2.028217000 -0.105942000

C -2.399528000 2.896965000 0.005384000

C -2.143585000 4.254708000 0.021980000

C -0.827260000 4.685016000 0.026572000

C 0.188061000 3.745704000 0.003660000

C -3.780666000 -0.081529000 0.146928000

O -4.599536000 0.459991000 -0.571658000

O -4.333050000 -0.779673000 1.208857000

C 4.466169000 0.282982000 -0.053902000

C 5.264654000 1.310921000 -0.487781000

C 6.645837000 1.061789000 -0.308526000

C 6.889528000 -0.153136000 0.261418000

S 5.437613000 -0.989720000 0.584354000

H 2.765812000 2.325054000 0.038854000

H 2.977886000 -1.952074000 -0.155413000

H 1.620500000 -3.811263000 -0.247910000

H -0.011894000 -5.678966000 -0.305526000

H -2.459757000 -5.138187000 -0.244220000

H -3.145497000 -2.764238000 -0.108562000

H -3.407709000 2.504295000 -0.012280000

H -2.970021000 4.952397000 0.030788000

H -0.591789000 5.742164000 0.042092000

H 1.225493000 4.053251000 -0.004301000

H -3.600819000 -1.107199000 1.744248000

H 4.871443000 2.209575000 -0.944909000

H 7.427653000 1.751737000 -0.597583000

H 7.839978000 -0.600935000 0.508778000

Sum of electronic and zero-point Energies= -1585.047561

Sum of electronic and thermal Energies= -1585.025450

Sum of electronic and thermal Enthalpies= -1585.024506

Sum of electronic and thermal Free Energies= -1585.100969

**3\_ImE**

Pt -1.675216000 -0.040517000 -0.019315000

C -2.367851000 2.911063000 0.027356000

C -2.106034000 4.266248000 0.041285000

C -0.787434000 4.689077000 0.029886000

C 0.220914000 3.743420000 0.000409000

C -0.092503000 2.394022000 -0.014325000

N -1.400320000 1.990910000 0.004083000

C 0.876900000 1.301384000 -0.055221000

C 2.264255000 1.371572000 -0.042772000

C 3.023893000 0.193133000 -0.076017000

C 2.384278000 -1.053626000 -0.109055000

C 0.996113000 -1.121848000 -0.104797000

C 0.265784000 0.056380000 -0.085036000

C -2.072191000 -3.048163000 -0.099795000

C -1.676761000 -4.369686000 -0.149175000

C -0.322673000 -4.658194000 -0.180556000

C 0.586242000 -3.616333000 -0.164812000

C 0.139881000 -2.305587000 -0.117617000

N -1.201681000 -2.035515000 -0.081567000

C -3.724065000 -0.132013000 0.146155000

O -4.538475000 0.049503000 -0.845569000

O -4.373048000 -0.359424000 1.256817000

H -3.383817000 2.542925000 0.031797000

H -2.929293000 4.967108000 0.060727000

H -0.545858000 5.744661000 0.041279000

H 1.260050000 4.043873000 -0.014360000

H 2.778164000 2.323902000 0.015861000

H 2.988618000 -1.953517000 -0.147908000

H -3.120077000 -2.784758000 -0.075315000

H -2.426367000 -5.148978000 -0.162718000

H 0.022826000 -5.683805000 -0.218907000

H 1.650186000 -3.810799000 -0.191937000

H -5.471617000 -0.018839000 -0.567105000

H -3.742387000 -0.480998000 1.981377000

C 4.482594000 0.281387000 -0.067884000

C 5.276155000 1.311469000 -0.505663000

S 5.458107000 -0.992784000 0.559191000

C 6.658135000 1.062390000 -0.337598000

H 4.879775000 2.211309000 -0.957654000

C 6.905610000 -0.153996000 0.228153000

H 7.437800000 1.753090000 -0.630093000

H 7.857892000 -0.601327000 0.469332000

Sum of electronic and zero-point Energies= -1585.468868

Sum of electronic and thermal Energies= -1585.446609

Sum of electronic and thermal Enthalpies= -1585.445665

Sum of electronic and thermal Free Energies= -1585.522811

**3\_TS**

Pt -1.667380000 -0.050996000 -0.016522000

C 2.267321000 1.377094000 0.032380000

C 0.880274000 1.301505000 0.022999000

C 0.275311000 0.054342000 0.046423000

C 1.007818000 -1.121436000 0.084962000

C 2.395110000 -1.047889000 0.113542000

C 3.030371000 0.201400000 0.084325000

C -0.092169000 2.391251000 -0.037667000

C 0.156846000 -2.309636000 0.086581000

C 0.608530000 -3.618108000 0.126628000

C -0.296721000 -4.663920000 0.115828000

C -1.650681000 -4.380824000 0.060363000

C -2.052253000 -3.060184000 0.021169000

N -1.399201000 1.986049000 -0.062247000

N -1.184949000 -2.045883000 0.036800000

C -2.366706000 2.904180000 -0.122251000

C -2.105131000 4.259399000 -0.160425000

C -0.787888000 4.684186000 -0.134072000

C 0.220662000 3.739935000 -0.071660000

C -3.684634000 -0.201612000 -0.109149000

H 2.778427000 2.331052000 -0.021970000

H 3.001712000 -1.945224000 0.169270000

H 1.672777000 -3.808742000 0.165712000

H 0.052598000 -5.688417000 0.148811000

H -2.396669000 -5.163589000 0.047206000

H -3.099601000 -2.799405000 -0.029502000

H -3.381891000 2.535405000 -0.137208000

H -2.928653000 4.958439000 -0.210378000

H -0.546799000 5.739558000 -0.162207000

H 1.259343000 4.041416000 -0.049713000

O -4.528419000 -0.820622000 -0.769475000

H -5.298805000 -0.214173000 0.100649000

O -4.618237000 0.541403000 0.763406000

H -4.451643000 0.474235000 1.719331000

C 4.488427000 0.294253000 0.100765000

C 5.271047000 1.332096000 0.540292000

S 5.478512000 -0.984986000 -0.492179000

C 6.656275000 1.084772000 0.400970000

H 4.864421000 2.236461000 0.973699000

C 6.917040000 -0.137950000 -0.145114000

H 7.428695000 1.781168000 0.699027000

H 7.874742000 -0.585302000 -0.363782000

Sum of electronic and zero-point Energies= -1585.408450

Sum of electronic and thermal Energies= -1585.386198

Sum of electronic and thermal Enthalpies= -1585.385254

Sum of electronic and thermal Free Energies= -1585.461943

**3\_ImF**

C -2.079743000 -1.385511000 0.037621000

C -0.694560000 -1.313748000 0.032689000

C -0.087643000 -0.052891000 0.048059000

C -0.831782000 1.131539000 0.068414000

C -2.216615000 1.044711000 0.085478000

C -2.848156000 -0.209364000 0.069434000

C 0.267578000 -2.392445000 -0.006922000

C 0.001848000 2.312242000 0.071261000

C -0.443388000 3.627234000 0.101042000

C 0.454312000 4.674455000 0.100570000

C 1.820732000 4.380371000 0.068758000

C 2.222835000 3.069392000 0.039183000

N 1.582919000 -1.964116000 -0.025825000

N 1.357363000 2.035846000 0.039278000

C 2.559418000 -2.892876000 -0.060048000

C 2.307603000 -4.241157000 -0.078109000

C 0.983338000 -4.688137000 -0.060057000

C -0.026615000 -3.749201000 -0.023722000

C -4.304810000 -0.306827000 0.081017000

C -5.091219000 -1.352854000 0.497004000

C -6.476954000 -1.104350000 0.357722000

C -6.739835000 0.128242000 -0.163569000

S -5.298189000 0.982608000 -0.490887000

H -2.587914000 -2.342142000 -0.005169000

H -2.827729000 1.940511000 0.125816000

H -1.509810000 3.813560000 0.125175000

H 0.107036000 5.699476000 0.124735000

H 2.569089000 5.161641000 0.066871000

H 3.272786000 2.812128000 0.014301000

H 3.573619000 -2.518210000 -0.072996000

H 3.139137000 -4.932666000 -0.105792000

H 0.753687000 -5.745938000 -0.073517000

H -1.065175000 -4.054879000 -0.007120000

H -4.685890000 -2.265336000 0.914179000

H -7.248787000 -1.808061000 0.640766000

H -7.697637000 0.580116000 -0.371881000

Pt 1.842863000 0.056907000 0.001000000

C 3.776746000 0.169923000 -0.064276000

O 4.916849000 0.238087000 -0.112830000

Sum of electronic and zero-point Energies= -1509.247660

Sum of electronic and thermal Energies= -1509.226758

Sum of electronic and thermal Enthalpies= -1509.225814

Sum of electronic and thermal Free Energies= -1509.299882

**3\_ImG**

C -2.067246000 -1.400595000 0.051502000

C -0.685079000 -1.328595000 0.057965000

C -0.070788000 -0.055502000 0.090921000

C -0.833980000 1.134248000 0.085148000

C -2.215105000 1.035770000 0.084135000

C -2.845585000 -0.224485000 0.071828000

C 0.268137000 -2.398891000 0.008018000

C -0.018078000 2.312787000 0.070194000

C -0.460978000 3.631775000 0.099032000

C 0.425235000 4.685670000 0.081443000

C 1.800541000 4.385559000 0.033709000

C 2.207417000 3.081441000 0.006981000

N 1.591603000 -1.949561000 -0.030736000

N 1.350319000 2.028280000 0.022606000

C 2.569982000 -2.890454000 -0.074133000

C 2.323980000 -4.234520000 -0.082703000

C 0.995476000 -4.700103000 -0.043490000

C -0.011691000 -3.761847000 0.002771000

C -4.297410000 -0.327120000 0.062191000

C -5.093640000 -1.410912000 0.356447000

C -6.478222000 -1.149411000 0.228827000

C -6.742380000 0.130290000 -0.160946000

S -5.294359000 1.016088000 -0.381205000

H -2.569840000 -2.360630000 0.002054000

H -2.830517000 1.930625000 0.101897000

H -1.529649000 3.809759000 0.136676000

H 0.076165000 5.710063000 0.105116000

H 2.549217000 5.167553000 0.016753000

H 3.259096000 2.829432000 -0.029366000

H 3.583326000 -2.512143000 -0.103005000

H 3.161757000 -4.919391000 -0.120174000

H 0.772983000 -5.759470000 -0.047888000

H -1.050808000 -4.068487000 0.036964000

H -4.694840000 -2.364148000 0.677217000

H -7.250567000 -1.881456000 0.428042000

H -7.699143000 0.601722000 -0.325387000

Pt 1.844337000 0.061758000 0.009919000

C 3.760404000 0.180167000 -0.074890000

O 4.911863000 0.252420000 -0.153260000

Sum of electronic and zero-point Energies= -1509.337601

Sum of electronic and thermal Energies= -1509.316530

Sum of electronic and thermal Enthalpies= -1509.315586

Sum of electronic and thermal Free Energies= -1509.389467

**4\_S0**

Pt 2.918305000 -0.000030000 -0.000001000

Cl 5.343221000 -0.000062000 0.000046000

C -1.035720000 1.203009000 -0.199953000

C 0.351040000 1.204385000 -0.207993000

C 1.022231000 -0.000011000 -0.000055000

C 0.351005000 -1.204377000 0.207886000

C -1.035765000 -1.202969000 0.199805000

C -1.728233000 0.000028000 -0.000088000

C 1.267715000 2.323375000 -0.412612000

C 1.267643000 -2.323384000 0.412579000

C 0.903225000 -3.639456000 0.645920000

C 1.880749000 -4.603006000 0.820561000

C 3.214537000 -4.232845000 0.758858000

C 3.527460000 -2.907951000 0.523567000

N 2.588731000 1.976233000 -0.354486000

N 2.588674000 -1.976279000 0.354493000

C 3.527549000 2.907890000 -0.523472000

C 3.214670000 4.232806000 -0.758700000

C 1.880894000 4.603007000 -0.820425000

C 0.903339000 3.639471000 -0.645880000

H -1.603752000 2.108710000 -0.376702000

H -1.603824000 -2.108651000 0.376537000

H -0.145805000 -3.901441000 0.688929000

H 1.602519000 -5.633728000 1.002935000

H 4.010031000 -4.953898000 0.889604000

H 4.549303000 -2.554623000 0.463231000

H 4.549381000 2.554535000 -0.463111000

H 4.010189000 4.953842000 -0.889383000

H 1.602697000 5.633749000 -1.002733000

H -0.145683000 3.901486000 -0.688910000

F -7.012763000 0.728838000 -0.870297000

F -7.011893000 -0.729603000 0.871306000

B -6.209310000 -0.000196000 0.000257000

N -5.279378000 0.944243000 0.797498000

N -5.279393000 -0.944179000 -0.797521000

C -3.440458000 1.854947000 1.739053000

C -4.559004000 2.464795000 2.280478000

C -5.672588000 1.869922000 1.676832000

C -5.672651000 -1.869550000 -1.677164000

C -4.559101000 -2.464168000 -2.281109000

C -3.440527000 -1.854501000 -1.739537000

C -3.193641000 0.000044000 -0.000041000

C -3.896844000 0.907510000 0.799332000

C -3.896867000 -0.907423000 -0.799436000

H -2.408588000 2.042512000 1.989839000

H -4.586233000 3.238513000 3.031222000

H -6.721838000 2.060430000 1.848021000

H -6.721904000 -2.060057000 -1.848321000

H -4.586355000 -3.237626000 -3.032121000

H -2.408656000 -2.041906000 -1.990453000

Sum of electronic and zero-point Energies= -1984.212650

Sum of electronic and thermal Energies= -1984.186059

Sum of electronic and thermal Enthalpies= -1984.185115

Sum of electronic and thermal Free Energies= -1984.271268

**4\_T1**

Pt 2.932722000 -0.000115000 0.000056000

Cl 5.361752000 -0.000396000 0.000040000

C -1.027941000 1.195099000 -0.219822000

C 0.361547000 1.201206000 -0.212963000

C 1.033190000 0.000098000 -0.000009000

C 0.361262000 -1.200864000 0.212934000

C -1.028209000 -1.194418000 0.219786000

C -1.727679000 0.000436000 -0.000017000

C 1.277859000 2.320034000 -0.416470000

C 1.277317000 -2.319889000 0.416542000

C 0.912437000 -3.636188000 0.651434000

C 1.888479000 -4.600906000 0.826212000

C 3.223037000 -4.232882000 0.763032000

C 3.536985000 -2.908600000 0.526107000

N 2.600144000 1.975197000 -0.356754000

N 2.599680000 -1.975341000 0.356919000

C 3.537663000 2.908256000 -0.525857000

C 3.224022000 4.232612000 -0.762772000

C 1.889548000 4.600927000 -0.826053000

C 0.913285000 3.636416000 -0.651380000

H -1.592100000 2.101485000 -0.411294000

H -1.592624000 -2.100675000 0.411184000

H -0.137040000 -3.896348000 0.695284000

H 1.608911000 -5.631117000 1.009822000

H 4.017705000 -4.954872000 0.893765000

H 4.559297000 -2.556644000 0.464467000

H 4.559892000 2.556074000 -0.464155000

H 4.018855000 4.954433000 -0.893429000

H 1.610221000 5.631201000 -1.009673000

H -0.136130000 3.896805000 -0.695320000

F -7.039176000 -0.749636000 0.852934000

F -7.041810000 0.747033000 -0.851041000

B -6.228952000 -0.000571000 0.000298000

N -5.297689000 -0.917557000 -0.810602000

N -5.298073000 0.918057000 0.809804000

C -3.469880000 -1.867866000 -1.758807000

C -4.583528000 -2.462806000 -2.299398000

C -5.705114000 -1.860231000 -1.703045000

C -5.706019000 1.860876000 1.701833000

C -4.584784000 2.464004000 2.298277000

C -3.470807000 1.869216000 1.758188000

C -3.196761000 0.000445000 -0.000035000

C -3.930927000 -0.889470000 -0.807845000

C -3.931276000 0.890372000 0.807419000

H -2.435883000 -2.061460000 -1.993374000

H -4.615605000 -3.239456000 -3.047186000

H -6.754712000 -2.045731000 -1.872072000

H -6.755719000 2.046214000 1.870407000

H -4.617282000 3.240923000 3.045767000

H -2.436950000 2.063352000 1.992918000

Sum of electronic and zero-point Energies= -1984.154943

Sum of electronic and thermal Energies= -1984.127910

Sum of electronic and thermal Enthalpies= -1984.126966

Sum of electronic and thermal Free Energies= -1984.215214

**4\_OER**

Pt 2.941361000 0.000052000 -0.000002000

Cl 5.377815000 0.000306000 0.000652000

C 3.540262000 2.913853000 -0.511518000

C 3.224762000 4.238886000 -0.740625000

C 1.888910000 4.604681000 -0.800790000

C 0.914843000 3.637669000 -0.631366000

C 1.280993000 2.319402000 -0.404566000

N 2.604815000 1.977625000 -0.347464000

C 0.366119000 1.199544000 -0.206704000

C -1.023611000 1.193902000 -0.211989000

C -1.733837000 -0.000287000 -0.000130000

C -1.023472000 -1.194368000 0.211662000

C 0.366288000 -1.199829000 0.206361000

C 1.040380000 -0.000117000 -0.000205000

C 3.540648000 -2.913711000 0.511162000

C 3.225329000 -4.238812000 0.740137000

C 1.889529000 -4.604802000 0.800216000

C 0.915330000 -3.637910000 0.630844000

C 1.281298000 -2.319579000 0.404141000

N 2.605080000 -1.977602000 0.347133000

F -7.046105000 0.657809000 -0.922965000

F -7.045793000 -0.657208000 0.923552000

B -6.205541000 0.000275000 0.000118000

N -5.299618000 1.000744000 0.715899000

N -5.299991000 -1.000332000 -0.715942000

C -3.489366000 2.013694000 1.575431000

C -4.637946000 2.656836000 2.068310000

C -5.728980000 2.009084000 1.523136000

C -5.729879000 -2.008824000 -1.522729000

C -4.639183000 -2.657237000 -2.067747000

C -3.490269000 -2.014445000 -1.575174000

C -3.197125000 -0.000252000 -0.000023000

C -3.920191000 0.982658000 0.726794000

C -3.920550000 -0.982933000 -0.726867000

H 4.563191000 2.563103000 -0.451901000

H 4.018174000 4.963031000 -0.867293000

H 1.607334000 5.635595000 -0.977896000

H -0.135468000 3.895119000 -0.672007000

H -1.586889000 2.101093000 -0.397123000

H -1.586583000 -2.101598000 0.397051000

H 4.563530000 -2.562808000 0.451655000

H 4.018840000 -4.962850000 0.866792000

H 1.608090000 -5.635772000 0.977214000

H -0.134945000 -3.895517000 0.671424000

H -2.463887000 2.247581000 1.814543000

H -4.672135000 3.496364000 2.746741000

H -6.783706000 2.192680000 1.660739000

H -6.784709000 -2.191820000 -1.660320000

H -4.673736000 -3.496923000 -2.745960000

H -2.464974000 -2.249009000 -1.814372000

Sum of electronic and zero-point Energies= -1984.339860

Sum of electronic and thermal Energies= -1984.313013

Sum of electronic and thermal Enthalpies= -1984.312069

Sum of electronic and thermal Free Energies= -1984.399234

**4\_ImA**

Pt 3.227529000 -0.000018000 0.000015000

C 3.853387000 2.914218000 -0.507742000

C 3.542023000 4.240387000 -0.733916000

C 2.206642000 4.608220000 -0.792322000

C 1.229497000 3.643462000 -0.624315000

C 1.595008000 2.325729000 -0.400713000

N 2.914758000 1.981163000 -0.345338000

C 0.684932000 1.203419000 -0.203302000

C -0.704188000 1.194154000 -0.206971000

C -1.416137000 -0.000034000 -0.000109000

C -0.704226000 -1.194182000 0.206729000

C 0.684934000 -1.203447000 0.203144000

C 1.349547000 -0.000029000 -0.000047000

C 3.853311000 -2.914333000 0.507889000

C 3.541884000 -4.240487000 0.734088000

C 2.206487000 -4.608272000 0.792379000

C 1.229390000 -3.643486000 0.624244000

C 1.594970000 -2.325771000 0.400630000

N 2.914739000 -1.981252000 0.345365000

F -6.722658000 0.639565000 -0.934846000

F -6.720837000 -0.640398000 0.936634000

B -5.884317000 -0.000065000 0.000300000

N -4.977211000 1.014643000 0.696828000

N -4.977335000 -1.014084000 -0.697381000

C -3.168230000 2.039940000 1.543476000

C -4.316587000 2.690400000 2.025035000

C -5.407001000 2.034285000 1.488018000

C -5.407326000 -2.033644000 -1.488540000

C -4.317036000 -2.690033000 -2.025490000

C -3.168544000 -2.039847000 -1.543870000

C -2.876182000 0.000019000 -0.000155000

C -3.598442000 0.996754000 0.709060000

C -3.598544000 -0.996565000 -0.709472000

H 4.879533000 2.573555000 -0.451624000

H 4.336527000 4.963181000 -0.859554000

H 1.927675000 5.640015000 -0.967042000

H 0.180062000 3.903860000 -0.663835000

H -1.263797000 2.103126000 -0.391397000

H -1.263787000 -2.103190000 0.391113000

H 4.879478000 -2.573719000 0.451853000

H 4.336355000 -4.963298000 0.859833000

H 1.927466000 -5.640050000 0.967118000

H 0.179945000 -3.903853000 0.663679000

H -2.143853000 2.276839000 1.784233000

H -4.351563000 3.539560000 2.691136000

H -6.461798000 2.219630000 1.622308000

H -6.462162000 -2.218667000 -1.622954000

H -4.352150000 -3.539115000 -2.691677000

H -2.144253000 -2.277066000 -1.784644000

Sum of electronic and zero-point Energies= -1524.070256

Sum of electronic and thermal Energies= -1524.045258

Sum of electronic and thermal Enthalpies= -1524.044314

Sum of electronic and thermal Free Energies= -1524.127411

**4\_ImB**

Pt 3.254146000 -0.000103000 0.000211000

C 3.865738000 2.941499000 -0.391206000

C 3.548927000 4.271854000 -0.567486000

C 2.209688000 4.638726000 -0.618254000

C 1.239515000 3.660483000 -0.490156000

C 1.606660000 2.334849000 -0.317560000

N 2.933421000 1.989777000 -0.269741000

C 0.699379000 1.206407000 -0.160041000

C -0.685067000 1.206432000 -0.158851000

C -1.434451000 0.000102000 -0.000730000

C -0.685229000 -1.206313000 0.157433000

C 0.699209000 -1.206499000 0.158558000

C 1.371500000 -0.000101000 -0.000894000

C 3.865317000 -2.941722000 0.392160000

C 3.548316000 -4.272061000 0.568189000

C 2.209016000 -4.638867000 0.617999000

C 1.238989000 -3.660577000 0.489203000

C 1.606315000 -2.334960000 0.316846000

N 2.933141000 -1.989951000 0.270017000

F -6.744206000 0.399785000 -1.059295000

F -6.743694000 -0.399532000 1.060616000

B -5.887130000 0.000111000 0.000454000

N -4.992281000 1.144315000 0.435163000

N -4.992525000 -1.144108000 -0.434716000

C -3.221771000 2.348118000 1.071882000

C -4.394542000 3.065593000 1.400951000

C -5.461431000 2.301601000 0.996932000

C -5.461915000 -2.301387000 -0.996287000

C -4.395207000 -3.065324000 -1.400899000

C -3.222316000 -2.347676000 -1.072681000

C -2.864402000 0.000186000 -0.000455000

C -3.611506000 1.143129000 0.464980000

C -3.611780000 -1.142756000 -0.465493000

H 4.894410000 2.606656000 -0.342526000

H 4.341652000 5.001950000 -0.661022000

H 1.926412000 5.675068000 -0.755146000

H 0.187328000 3.912458000 -0.520813000

H -1.223843000 2.125682000 -0.341663000

H -1.224121000 -2.125460000 0.340446000

H 4.894044000 -2.606929000 0.344263000

H 4.340937000 -5.002198000 0.662282000

H 1.925586000 -5.675194000 0.754676000

H 0.186769000 -3.912511000 0.519078000

H -2.215211000 2.658549000 1.297795000

H -4.447197000 4.035030000 1.875971000

H -6.522491000 2.484428000 1.070868000

H -6.523000000 -2.484334000 -1.069585000

H -4.448105000 -4.034814000 -1.875785000

H -2.215827000 -2.657804000 -1.299361000

Sum of electronic and zero-point Energies= -1524.159229

Sum of electronic and thermal Energies= -1524.133946

Sum of electronic and thermal Enthalpies= -1524.133002

Sum of electronic and thermal Free Energies= -1524.216832

**4\_ImC**

Pt -2.870260000 0.006551000 -0.011173000

C -3.423379000 -2.921367000 -0.518930000

C -3.094560000 -4.240938000 -0.778856000

C -1.760353000 -4.594297000 -0.883489000

C -0.793121000 -3.616564000 -0.724036000

C -1.166624000 -2.306628000 -0.469680000

N -2.493442000 -1.975803000 -0.370319000

C -0.237404000 -1.186965000 -0.284135000

C 1.148974000 -1.198772000 -0.261956000

C 1.844791000 0.005252000 -0.053871000

C 1.154070000 1.214730000 0.138122000

C -0.232808000 1.213435000 0.128052000

C -0.909044000 0.016776000 -0.091031000

C -3.413161000 2.936852000 0.491523000

C -3.079007000 4.263300000 0.705574000

C -1.743087000 4.624070000 0.740339000

C -0.779489000 3.646817000 0.557916000

C -1.157954000 2.331052000 0.344071000

N -2.486379000 1.992634000 0.316965000

F 7.141663000 -0.728489000 -0.819405000

F 7.117410000 0.662527000 0.975592000

B 6.323548000 -0.024528000 0.060801000

N 5.369174000 -0.987412000 0.801053000

N 5.422121000 0.957564000 -0.719869000

C 3.503932000 -1.908324000 1.674469000

C 4.606215000 -2.540654000 2.226549000

C 5.736531000 -1.938543000 1.665961000

C 5.847133000 1.909973000 -1.556530000

C 4.756110000 2.529196000 -2.173521000

C 3.618010000 1.906352000 -1.687002000

C 3.305736000 -0.003325000 -0.017808000

C 3.987287000 -0.941564000 0.770059000

C 4.040176000 0.927999000 -0.764979000

H -4.442240000 -2.544056000 -0.393544000

H -3.883450000 -4.973022000 -0.893470000

H -1.471522000 -5.618931000 -1.085839000

H 0.258558000 -3.861894000 -0.798341000

H 1.720809000 -2.104845000 -0.428575000

H 1.728479000 2.113287000 0.334464000

H -4.434933000 2.547160000 0.450650000

H -3.865208000 4.994472000 0.842411000

H -1.450218000 5.654156000 0.905878000

H 0.273251000 3.898058000 0.576472000

H 2.465442000 -2.092789000 1.898154000

H 4.609658000 -3.332979000 2.958212000

H 6.780407000 -2.138115000 1.858120000

H 6.902185000 2.098616000 -1.689596000

H 4.808813000 3.326994000 -2.897294000

H 2.595183000 2.105666000 -1.963941000

C -4.997485000 -0.018710000 0.155553000

O -5.626934000 1.075564000 0.293754000

O -5.612265000 -1.129342000 0.118624000

Sum of electronic and zero-point Energies= -1712.633109

Sum of electronic and thermal Energies= -1712.605009

Sum of electronic and thermal Enthalpies= -1712.604065

Sum of electronic and thermal Free Energies= -1712.693767

**4\_ImD**

Pt -2.837339000 0.011578000 -0.016152000

C -3.399197000 -2.917363000 -0.578126000

C -3.071856000 -4.230902000 -0.857442000

C -1.736307000 -4.581264000 -0.954133000

C -0.773153000 -3.605355000 -0.770945000

C -1.150194000 -2.300362000 -0.499040000

N -2.476576000 -1.968701000 -0.402227000

C -0.225828000 -1.184316000 -0.294688000

C 1.162022000 -1.195857000 -0.272959000

C 1.856099000 0.002095000 -0.048186000

C 1.168513000 1.207052000 0.159566000

C -0.219381000 1.209358000 0.148776000

C -0.893657000 0.016096000 -0.084482000

C -3.388387000 2.942166000 0.480112000

C -3.057243000 4.264702000 0.709385000

C -1.720511000 4.618613000 0.773857000

C -0.757630000 3.640481000 0.598071000

C -1.137168000 2.328309000 0.368209000

N -2.464435000 1.992840000 0.320993000

F 7.153104000 -0.754810000 -0.791583000

F 7.125774000 0.692693000 0.958898000

B 6.336544000 -0.024145000 0.065523000

N 5.380929000 -0.965497000 0.835418000

N 5.432961000 0.932925000 -0.746863000

C 3.512639000 -1.872621000 1.720967000

C 4.613075000 -2.489725000 2.290571000

C 5.745539000 -1.896957000 1.720969000

C 5.853642000 1.866082000 -1.605299000

C 4.759234000 2.473019000 -2.231664000

C 3.623816000 1.863044000 -1.726678000

C 3.321841000 -0.006795000 -0.013227000

C 3.998980000 -0.922642000 0.798998000

C 4.050733000 0.903090000 -0.785942000

H -4.425860000 -2.597271000 -0.471240000

H -3.861368000 -4.957930000 -0.991813000

H -1.445490000 -5.602136000 -1.169530000

H 0.279200000 -3.847537000 -0.841034000

H 1.730635000 -2.101884000 -0.447165000

H 1.741226000 2.104822000 0.361424000

H -4.415191000 2.606268000 0.400983000

H -3.844705000 4.996027000 0.832510000

H -1.427913000 5.645874000 0.953786000

H 0.295127000 3.888445000 0.633641000

H 2.473281000 -2.056383000 1.941787000

H 4.616031000 -3.266959000 3.038152000

H 6.788774000 -2.092946000 1.920354000

H 6.907915000 2.053671000 -1.746055000

H 4.810079000 3.255090000 -2.972430000

H 2.599514000 2.059064000 -2.000977000

C -4.926950000 0.062348000 0.137640000

O -5.681746000 0.956944000 -0.217283000

O -5.516991000 -1.026136000 0.728339000

H -6.473744000 -0.850722000 0.738466000

Sum of electronic and zero-point Energies= -1713.122645

Sum of electronic and thermal Energies= -1713.094206

Sum of electronic and thermal Enthalpies= -1713.093262

Sum of electronic and thermal Free Energies= -1713.183541

**4\_ImE**

Pt -2.819620000 0.008363000 -0.015733000

C -3.380126000 -2.919393000 -0.574858000

C -3.056196000 -4.236484000 -0.831824000

C -1.719946000 -4.590996000 -0.908489000

C -0.755306000 -3.616160000 -0.730155000

C -1.131099000 -2.307457000 -0.477152000

N -2.455429000 -1.972448000 -0.397536000

C -0.212557000 -1.188323000 -0.278295000

C 1.176173000 -1.197518000 -0.261687000

C 1.869270000 0.000604000 -0.049551000

C 1.183186000 1.205338000 0.147338000

C -0.205721000 1.207718000 0.142058000

C -0.877325000 0.012653000 -0.073998000

C -3.362670000 2.948733000 0.491268000

C -3.030707000 4.271405000 0.705380000

C -1.692364000 4.623928000 0.746778000

C -0.733986000 3.642862000 0.569261000

C -1.117753000 2.329590000 0.354675000

N -2.444127000 1.994218000 0.321547000

F 7.167896000 -0.787253000 -0.760654000

F 7.133268000 0.737995000 0.923142000

B 6.350344000 -0.020633000 0.061152000

N 5.393943000 -0.929567000 0.871241000

N 5.444786000 0.897599000 -0.795542000

C 3.523946000 -1.806360000 1.786301000

C 4.623256000 -2.400166000 2.380055000

C 5.757044000 -1.827255000 1.790486000

C 5.862375000 1.796404000 -1.690084000

C 4.765430000 2.380585000 -2.335845000

C 3.631951000 1.793005000 -1.803387000

C 3.338163000 -0.007935000 -0.017332000

C 4.012061000 -0.889292000 0.831310000

C 4.062400000 0.868032000 -0.828578000

H -4.412069000 -2.605388000 -0.509698000

H -3.846716000 -4.961907000 -0.966685000

H -1.430604000 -5.615501000 -1.106775000

H 0.296545000 -3.862647000 -0.788141000

H 1.742560000 -2.106078000 -0.427835000

H 1.754239000 2.107139000 0.333509000

H -4.396697000 2.637213000 0.451599000

H -3.816820000 5.002470000 0.835457000

H -1.396724000 5.652299000 0.913152000

H 0.319320000 3.888885000 0.592276000

H 2.484206000 -1.985102000 2.009928000

H 4.626298000 -3.149898000 3.155158000

H 6.799905000 -2.016669000 1.998182000

H 6.916090000 1.979206000 -1.841138000

H 4.815071000 3.133783000 -3.105964000

H 2.606579000 1.981187000 -2.079647000

C -4.869996000 -0.015745000 0.144740000

O -5.674714000 0.047630000 -0.868261000

H -6.610617000 0.017660000 -0.592184000

O -5.526749000 -0.102905000 1.269731000

H -4.901896000 -0.155535000 2.007602000

Sum of electronic and zero-point Energies= -1713.539472

Sum of electronic and thermal Energies= -1713.510690

Sum of electronic and thermal Enthalpies= -1713.509746

Sum of electronic and thermal Free Energies= -1713.602145

**4\_TS**

Pt -2.814460000 0.001152000 -0.037093000

C 1.186398000 1.205725000 0.134648000

C -0.202632000 1.205898000 0.123321000

C -0.869459000 0.007266000 -0.082121000

C -0.204125000 -1.195347000 -0.268718000

C 1.184658000 -1.202641000 -0.243879000

C 1.874074000 -0.000697000 -0.043806000

C -1.116684000 2.330190000 0.317292000

C -1.119760000 -2.317793000 -0.464814000

C -0.740306000 -3.627316000 -0.704556000

C -1.703157000 -4.603870000 -0.886820000

C -3.039775000 -4.248954000 -0.829413000

C -3.368138000 -2.929986000 -0.584693000

N -2.442895000 1.995071000 0.282069000

N -2.444835000 -1.983904000 -0.401222000

C -3.361778000 2.951660000 0.433591000

C -3.029469000 4.277359000 0.630889000

C -1.691634000 4.629622000 0.675346000

C -0.732794000 3.645238000 0.516852000

C -4.838159000 -0.060418000 0.077464000

O -5.782835000 -0.537574000 -0.562985000

O -5.618632000 0.545689000 1.170466000

F 7.176255000 -0.798865000 -0.722301000

F 7.133325000 0.767562000 0.923158000

B 6.354944000 -0.013826000 0.077760000

N 5.397608000 -0.904569000 0.907225000

N 5.450100000 0.881274000 -0.804212000

C 3.525959000 -1.763900000 1.836149000

C 4.624308000 -2.342392000 2.446216000

C 5.759142000 -1.781011000 1.847180000

C 5.868039000 1.758674000 -1.719415000

C 4.771341000 2.327309000 -2.379723000

C 3.637647000 1.752554000 -1.834309000

C 3.343546000 -0.006600000 -0.007493000

C 4.015771000 -0.867296000 0.862625000

C 4.067739000 0.850674000 -0.837759000

H 1.755702000 2.110667000 0.310499000

H 1.753299000 -2.112314000 -0.395250000

H 0.312162000 -3.873742000 -0.749866000

H -1.411187000 -5.629689000 -1.074146000

H -3.828439000 -4.975366000 -0.969754000

H -4.400139000 -2.613212000 -0.537328000

H -4.395047000 2.638831000 0.396846000

H -3.815891000 5.010688000 0.745415000

H -1.395988000 5.659953000 0.829069000

H 0.320548000 3.890694000 0.542513000

H -6.412985000 -0.068237000 0.489977000

H -5.337040000 0.323419000 2.074530000

H 2.485733000 -1.939706000 2.060008000

H 4.626285000 -3.074830000 3.237677000

H 6.801637000 -1.964757000 2.061738000

H 6.921797000 1.938460000 -1.873804000

H 4.821540000 3.062078000 -3.167402000

H 2.612349000 1.934351000 -2.115201000

Sum of electronic and zero-point Energies= -1713.478764

Sum of electronic and thermal Energies= -1713.449976

Sum of electronic and thermal Enthalpies= -1713.449031

Sum of electronic and thermal Free Energies= -1713.541211

**4\_ImF**

Pt 2.995273000 -0.004279000 -0.000926000

C 3.550677000 2.930798000 -0.538261000

C 3.223190000 4.249129000 -0.785019000

C 1.886885000 4.601038000 -0.860353000

C 0.922675000 3.623546000 -0.688251000

C 1.301765000 2.315603000 -0.444494000

N 2.625327000 1.983350000 -0.370563000

C 0.387933000 1.192543000 -0.246982000

C -1.001283000 1.197567000 -0.238291000

C -1.690742000 -0.001716000 -0.029447000

C -1.005435000 -1.204712000 0.171613000

C 0.383894000 -1.205628000 0.172262000

C 1.047514000 -0.008034000 -0.039310000

C 3.541035000 -2.945595000 0.511806000

C 3.209136000 -4.267452000 0.732576000

C 1.871727000 -4.620067000 0.779182000

C 0.910817000 -3.640312000 0.601643000

C 1.294234000 -2.329440000 0.381642000

N 2.618912000 -1.995496000 0.341094000

F -6.979904000 0.802816000 -0.775945000

F -6.963987000 -0.768793000 0.865246000

B -6.172816000 0.013621000 0.033680000

N -5.225314000 0.900336000 0.879729000

N -5.256492000 -0.881042000 -0.838024000

C -3.364210000 1.760323000 1.830698000

C -4.469373000 2.338494000 2.427517000

C -5.597468000 1.776999000 1.814833000

C -5.661944000 -1.758709000 -1.758129000

C -4.556239000 -2.329088000 -2.402691000

C -3.430068000 -1.755448000 -1.841826000

C -3.162031000 0.003687000 -0.011120000

C -3.843043000 0.862986000 0.851783000

C -3.873776000 -0.851897000 -0.852246000

H 4.583570000 2.620528000 -0.471568000

H 4.012493000 4.976932000 -0.913129000

H 1.595817000 5.626315000 -1.051456000

H -0.129391000 3.869246000 -0.742905000

H -1.567962000 2.105027000 -0.407592000

H -1.574904000 -2.108540000 0.350966000

H 4.575014000 -2.634774000 0.468768000

H 3.996045000 -4.997266000 0.863934000

H 1.577284000 -5.647850000 0.950647000

H -0.142050000 -3.886960000 0.630731000

H -2.326653000 1.937023000 2.066228000

H -4.480897000 3.071260000 3.218554000

H -6.642326000 1.962096000 2.016381000

H -6.713502000 -1.938591000 -1.926809000

H -4.596216000 -3.064805000 -3.190039000

H -2.401047000 -1.939583000 -2.107336000

C 4.954676000 0.015089000 0.097979000

O 6.080282000 0.032639000 0.179555000

Sum of electronic and zero-point Energies= -1637.193285

Sum of electronic and thermal Energies= -1637.166064

Sum of electronic and thermal Enthalpies= -1637.165120

Sum of electronic and thermal Free Energies= -1637.253109

**4\_ImG**

Pt 3.017090000 -0.004105000 0.000017000

C 3.563480000 2.939607000 -0.507961000

C 3.234461000 4.259421000 -0.739625000

C 1.896150000 4.609672000 -0.810580000

C 0.934641000 3.629079000 -0.649160000

C 1.314280000 2.316904000 -0.420719000

N 2.639940000 1.987400000 -0.351129000

C 0.403820000 1.191885000 -0.233423000

C -0.983049000 1.195655000 -0.231722000

C -1.698713000 -0.001230000 -0.030402000

C -0.987330000 -1.201910000 0.163226000

C 0.399547000 -1.203887000 0.158741000

C 1.072867000 -0.007526000 -0.039611000

C 3.553120000 -2.952773000 0.491554000

C 3.219411000 -4.275096000 0.701211000

C 1.879931000 -4.625789000 0.741426000

C 0.921978000 -3.643544000 0.569439000

C 1.306220000 -2.329302000 0.361513000

N 2.633030000 -1.998570000 0.326528000

F -7.005504000 0.625115000 -0.918832000

F -6.989380000 -0.590921000 0.995305000

B -6.163796000 0.013143000 0.028800000

N -5.242221000 1.046031000 0.680843000

N -5.267060000 -1.028354000 -0.643965000

C -3.420573000 2.082539000 1.484238000

C -4.559067000 2.746190000 1.965177000

C -5.658279000 2.081312000 1.454669000

C -5.710807000 -2.065673000 -1.399405000

C -4.630396000 -2.738537000 -1.938883000

C -3.474955000 -2.077531000 -1.496134000

C -3.152731000 0.004071000 -0.013817000

C -3.863560000 1.024318000 0.675154000

C -3.888773000 -1.013335000 -0.679631000

H 4.596754000 2.629344000 -0.444324000

H 4.022394000 4.990195000 -0.859382000

H 1.603227000 5.636669000 -0.989948000

H -0.118568000 3.871375000 -0.698762000

H -1.541444000 2.105896000 -0.410648000

H -1.548512000 -2.108610000 0.351427000

H 4.587503000 -2.642156000 0.452568000

H 4.004758000 -5.007384000 0.828463000

H 1.583424000 -5.654590000 0.903762000

H -0.132028000 -3.886424000 0.592239000

H -2.393737000 2.319696000 1.712822000

H -4.583378000 3.608194000 2.614748000

H -6.710743000 2.271312000 1.600287000

H -6.768027000 -2.251579000 -1.512207000

H -4.678265000 -3.603935000 -2.582592000

H -2.456300000 -2.320841000 -1.753244000

C 4.968592000 0.011629000 0.088780000

O 6.098184000 0.025891000 0.161370000

Sum of electronic and zero-point Energies= -1637.332801

Sum of electronic and thermal Energies= -1637.305428

Sum of electronic and thermal Enthalpies= -1637.304484

Sum of electronic and thermal Free Energies= -1637.393159