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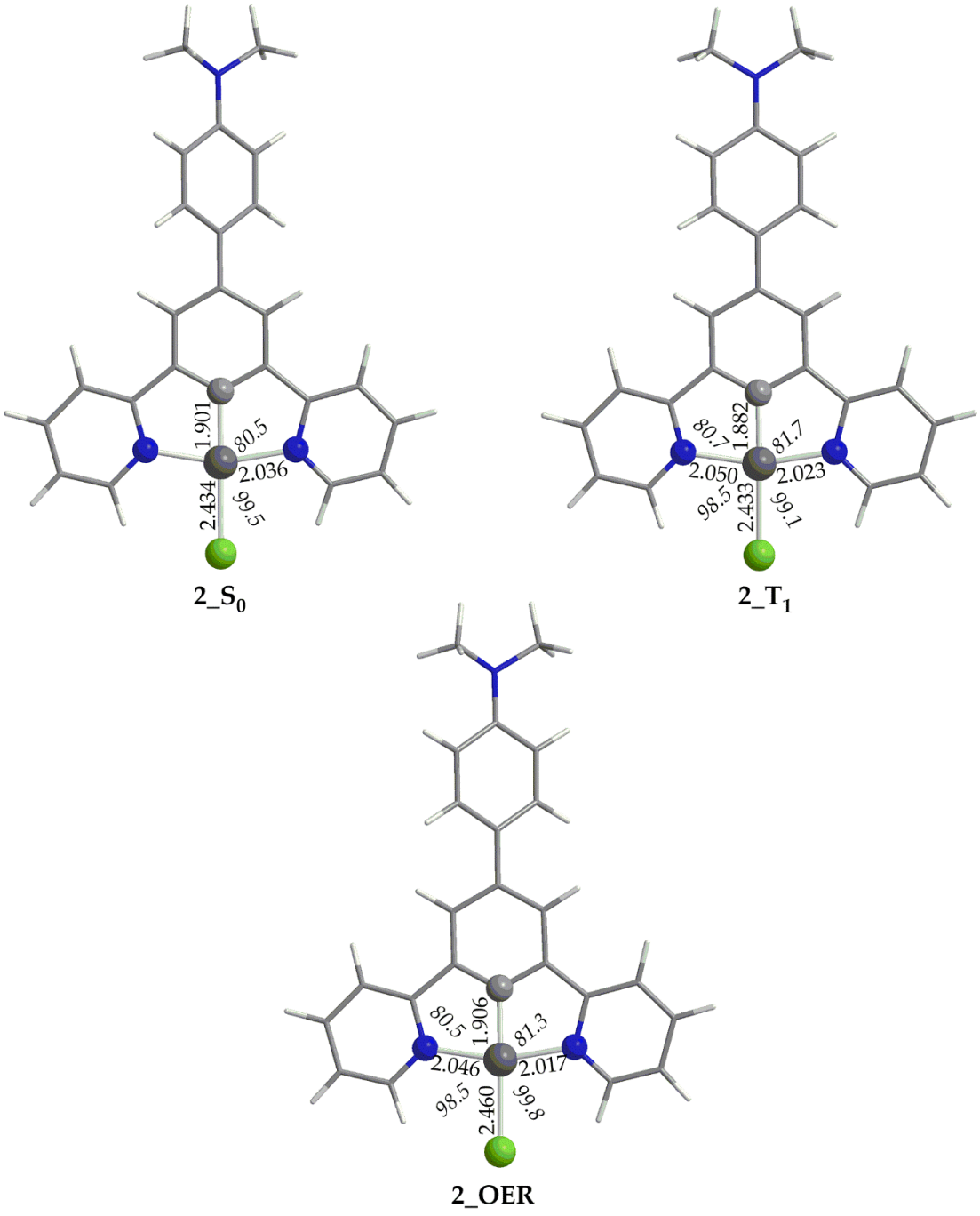
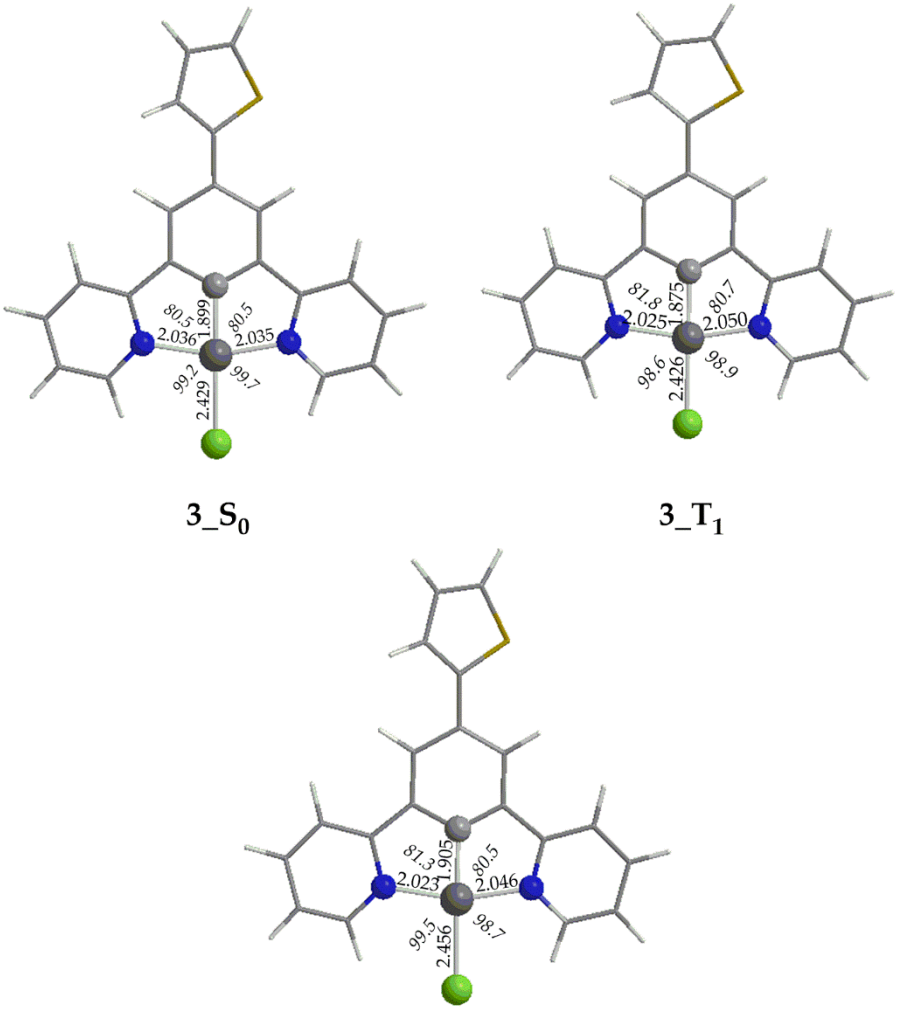


Figure S1: Optimized geometries of **2** in S_0 ground state, **2_S₀** in T_1 excited state, **2_T₁** and of One Electron Reduced form, **2_OER**, calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.



3_S$_0$ **3_T$_1$**

3_OER

Figure S2: Optimized geometries of **3** in S_0 ground state, **3_S$_0$** in T_1 excited state, **3_T$_1$** and of One Electron Reduced form, **3_OER**, calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

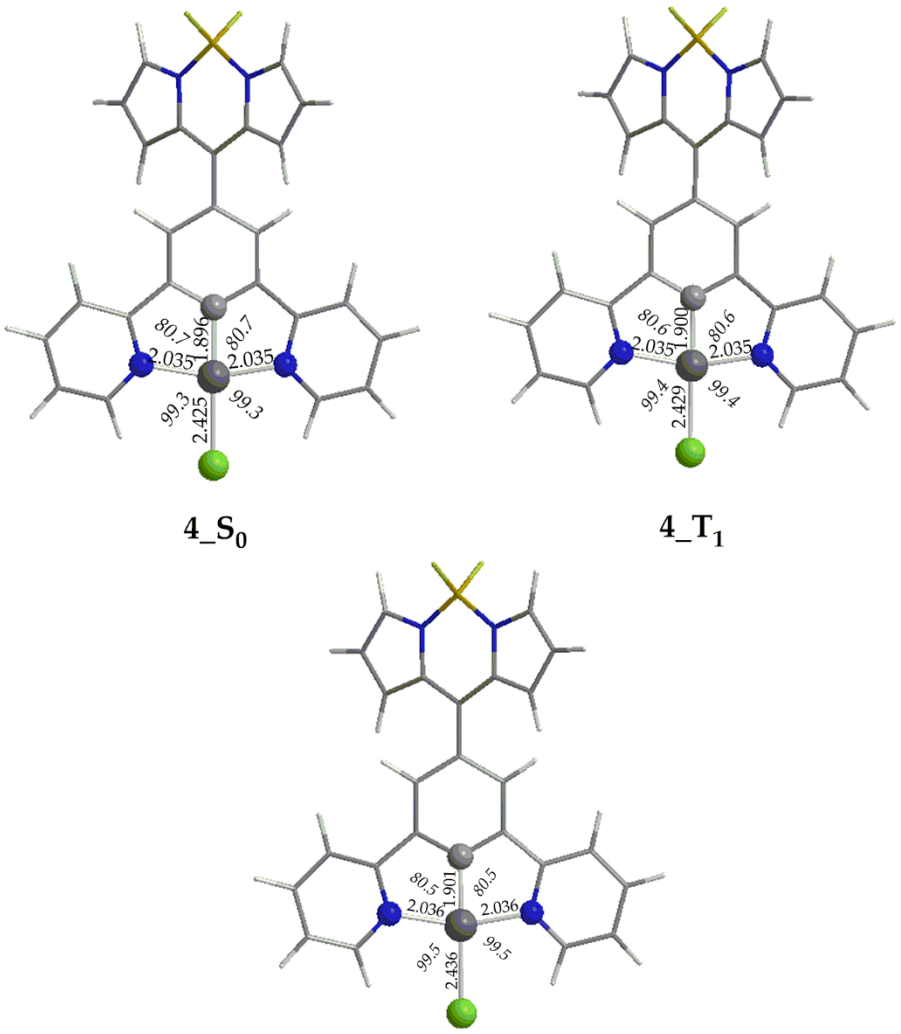


Figure S3: Optimized geometries of **4** in S_0 ground state, **4_S₀** in T_1 excited state, **4_T₁** and of One Electron Reduced form, **4_OER**, calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

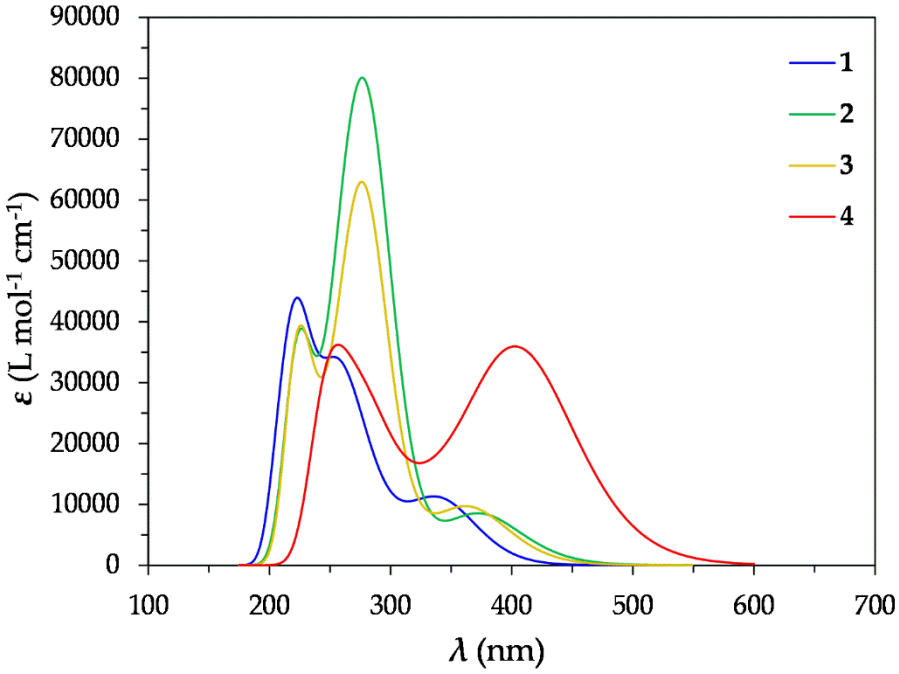


Figure S4: Simulated absorption spectra of **1** – **4** in DCM at the TDDFT/CAM-B3LYP/Def2-TZVP level.

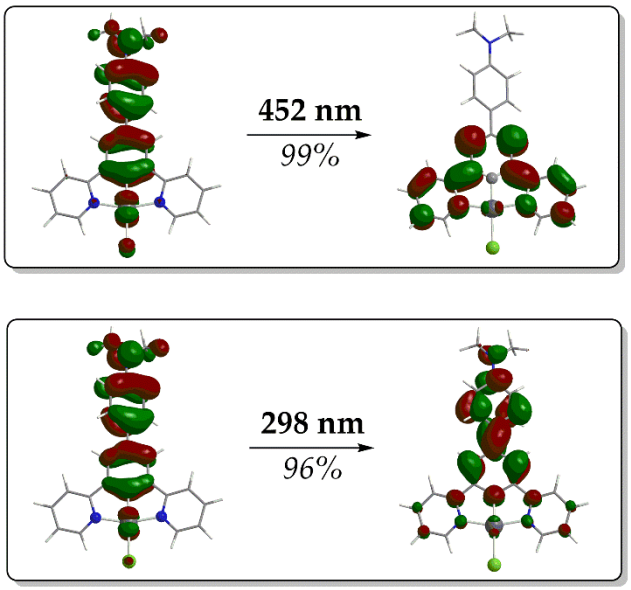


Figure S5: NTO pairs for the most significant electronic transitions of the simulated absorption spectra of **2** calculated at TDDFT/PBE0/Def2-TZVP level (hole, h^+ at the left, electron, e^- at the right).

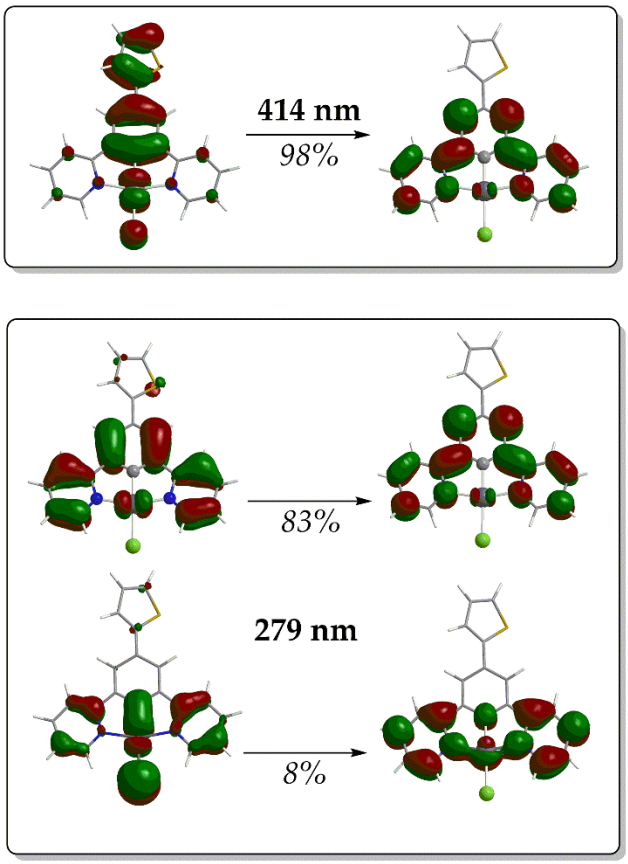


Figure S6: NTO pairs for the most significant electronic transitions of the simulated absorption spectra of **3** calculated at TDDFT/PBE0/Def2-TZVP level (hole, h^+ at the left, electron, e^- at the right).

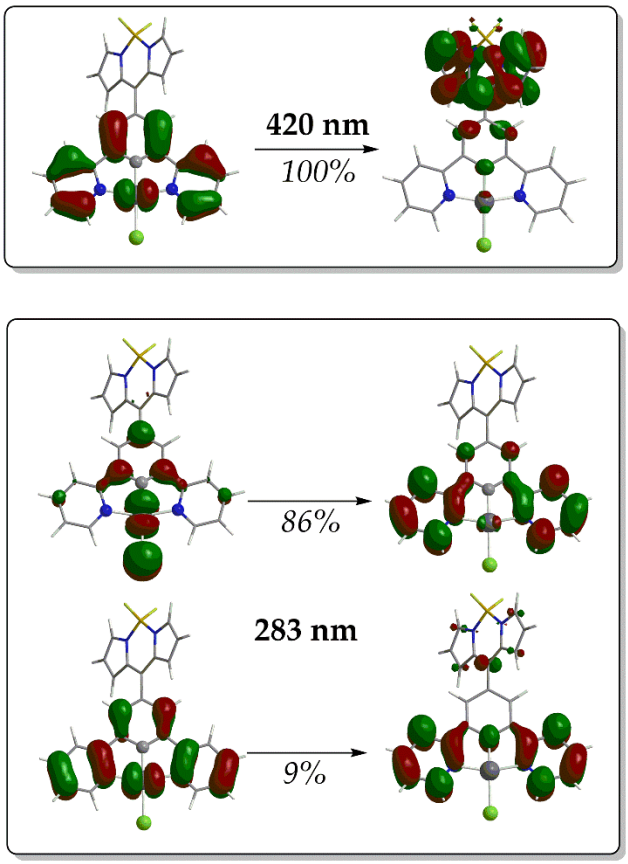


Figure S7: NTO pairs for the most significant electronic transitions of the simulated absorption spectra of **4** calculated at TDDFT/PBE0/Def2-TZVP level (hole, h^+ at the left, electron, e^- at the right).

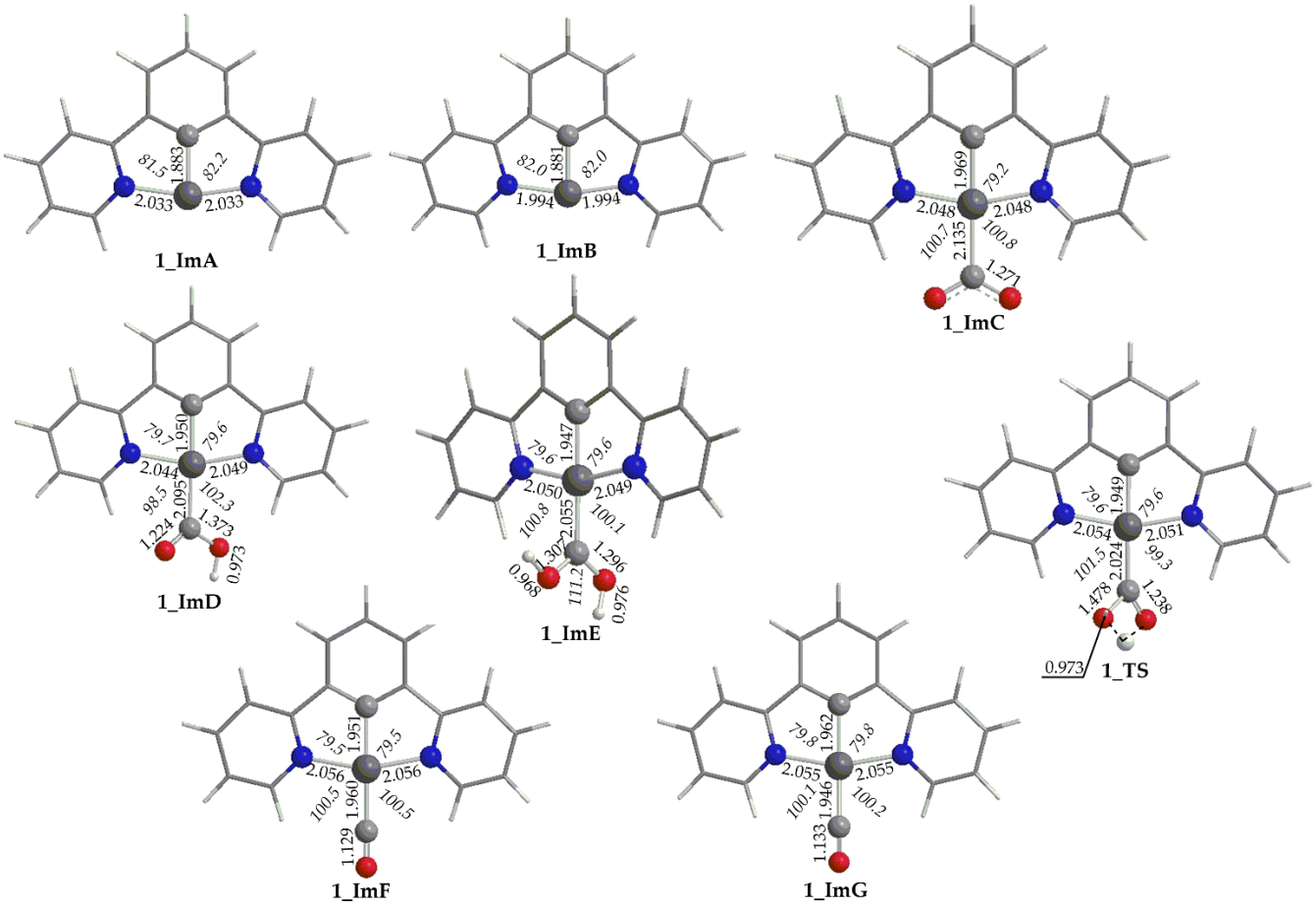


Figure S8: Optimized geometries of all species involved in the catalytic cycle of CO_2 to CO conversion by **1** calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

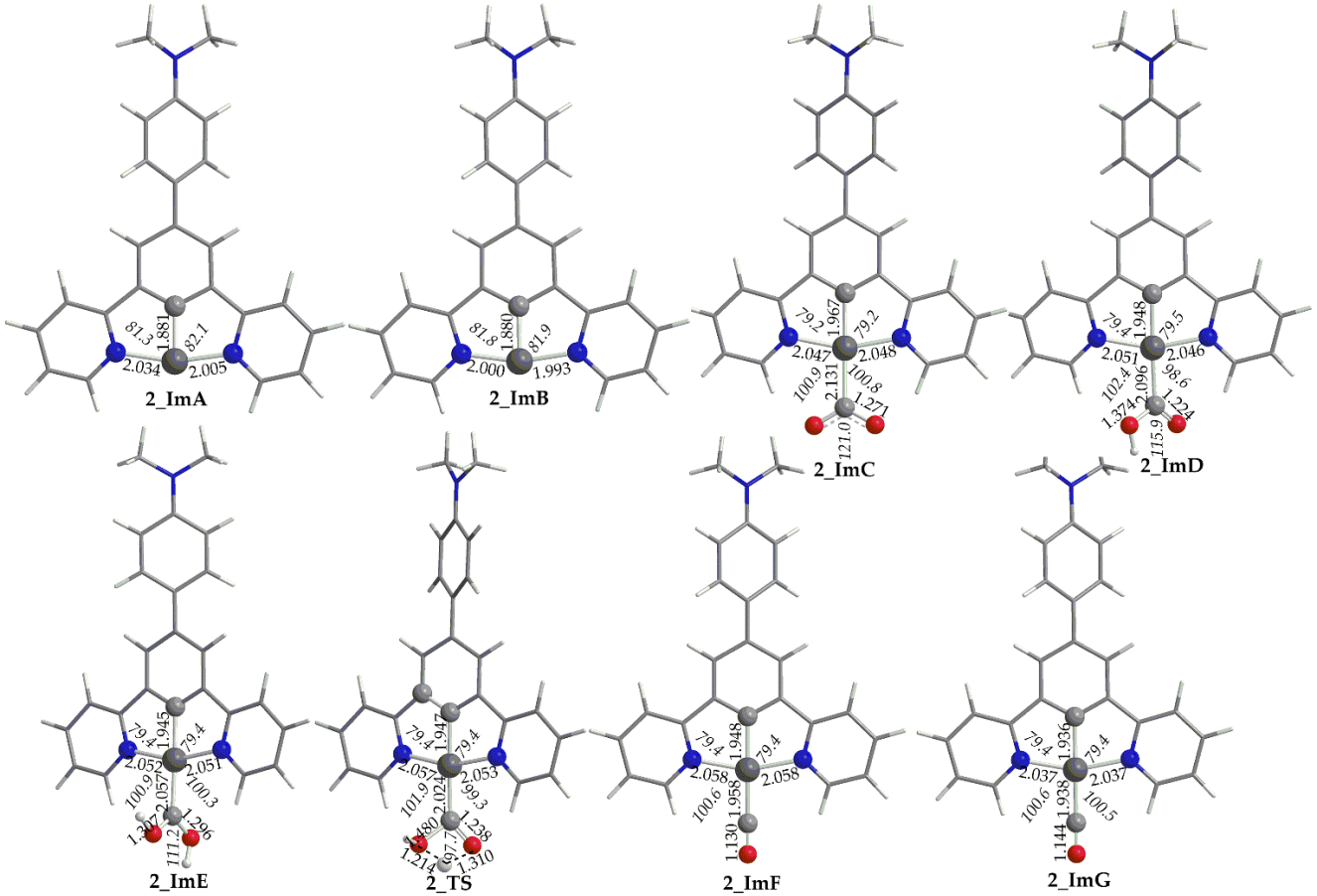


Figure S9: Optimized geometries of all species involved in the catalytic cycle of CO_2 to CO conversion by **2** calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

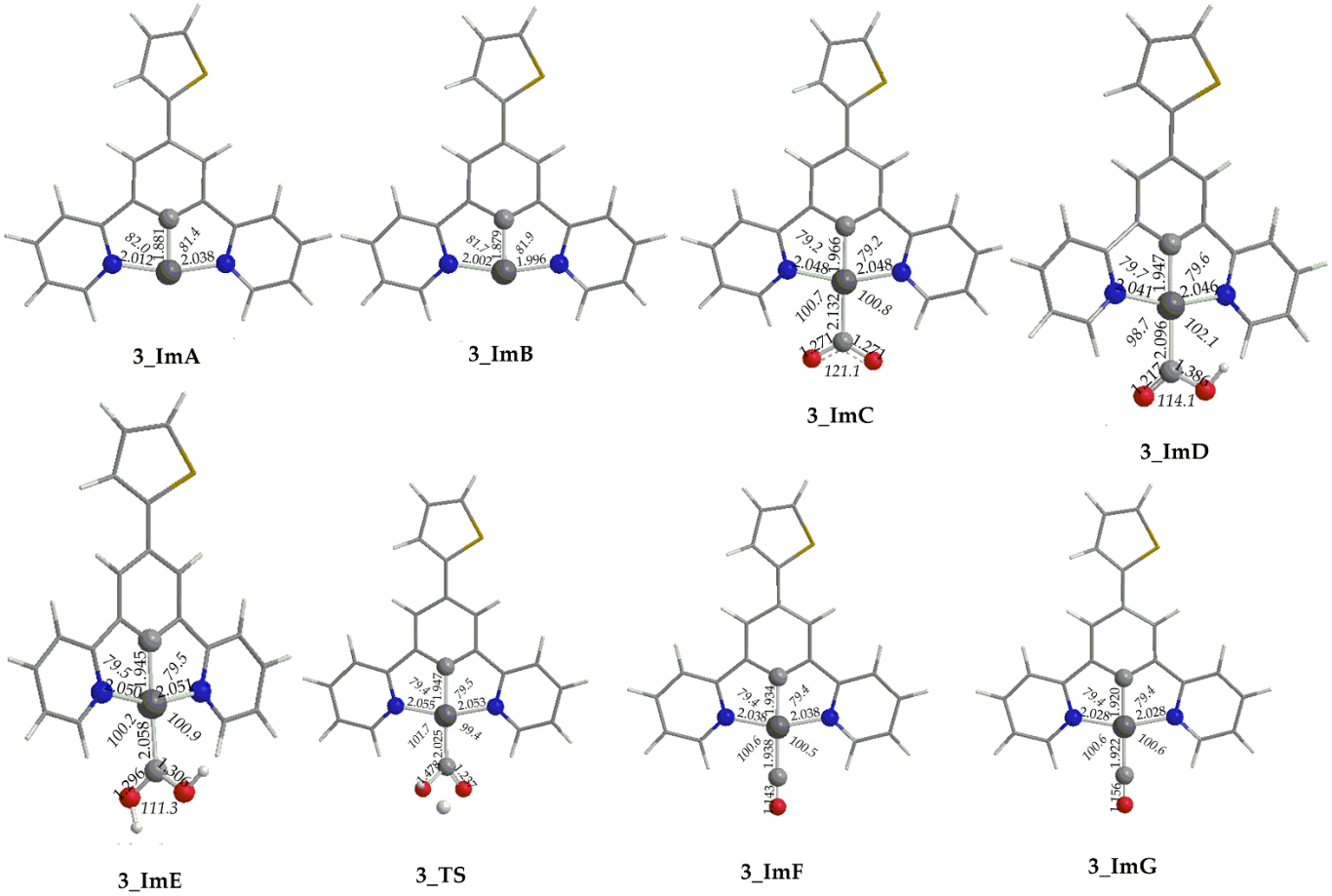


Figure S10: Optimized geometries of all species involved in the catalytic cycle of CO_2 to CO conversion by **3** calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

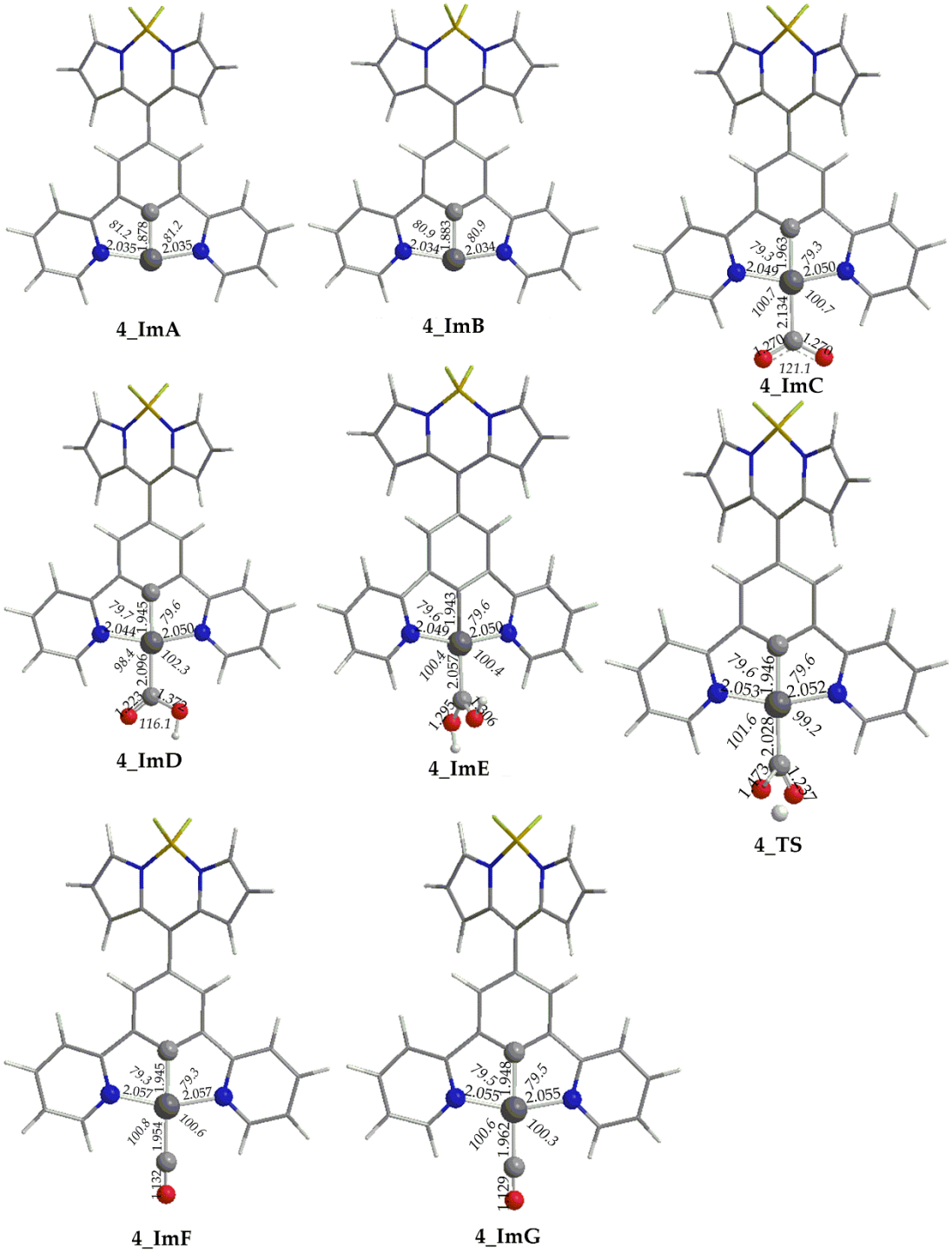


Figure S11: Optimized geometries of all species involved in the catalytic cycle of CO_2 to CO conversion by **4** calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

Table S1: Cartesian Coordinates and Energetic Data of the optimized geometries of all species calculated at the PBE0-GD3BJ/Def2-TZVP level, in DCM solvent.

1_S_0

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_T_1

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

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Sum of electronic and thermal Enthalpies= -1304.485935
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1_OER

Pt	0.007126000	-0.670378000	0.000015000
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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

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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_ImA

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

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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_S_0

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_T_1

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_ImA

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_S_0

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_T_1

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_T_1

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

TEOA in DCM

N	-0.001770000	-0.007522000	0.098609000
C	-0.107718000	1.382146000	0.501972000
C	-1.157847000	-0.793388000	0.485333000
C	1.250450000	-0.617101000	0.505450000
C	-2.298788000	-0.638513000	-0.504183000
C	0.587408000	2.299813000	-0.479778000
O	0.526280000	3.615232000	0.038820000
O	-3.444870000	-1.369940000	-0.115122000
C	1.696687000	-1.688769000	-0.473476000
O	2.859595000	-2.364236000	-0.036407000
H	-1.162400000	1.663614000	0.544221000
H	0.303634000	1.548591000	1.511197000
H	-1.507574000	-0.527647000	1.499107000
H	-0.879778000	-1.849058000	0.520733000
H	1.189048000	-1.049373000	1.517947000
H	2.021584000	0.158110000	0.542581000
H	-1.989968000	-1.035492000	-1.473344000
H	-2.539881000	0.422507000	-0.647465000
H	0.084634000	2.228855000	-1.451944000
H	1.629105000	1.983260000	-0.620351000
H	0.944650000	4.208349000	-0.589964000
H	-3.781329000	-0.990385000	0.701755000
H	1.842331000	-1.234714000	-1.461344000
H	0.924590000	-2.454557000	-0.577849000
H	3.584558000	-1.732979000	-0.015781000

Sum of electronic and zero-point Energies= -517.473018
Sum of electronic and thermal Energies= -517.460128

Sum of electronic and thermal Enthalpies= -517.459184
Sum of electronic and thermal Free Energies= -517.513101

TEOA in Gas phase

N	0.006421000	-0.006356000	0.113021000
C	-0.577225000	1.258365000	0.514296000
C	-0.802342000	-1.148539000	0.485915000
C	1.393488000	-0.143699000	0.510620000
C	-1.932899000	-1.389882000	-0.498901000
C	-0.267490000	2.353846000	-0.482344000
O	-0.789652000	3.560535000	0.032147000
O	-2.740021000	-2.484328000	-0.125672000
C	2.185176000	-0.981219000	-0.479090000
O	3.507151000	-1.215997000	-0.047341000
H	-1.662882000	1.153366000	0.572684000
H	-0.238968000	1.572805000	1.515213000
H	-1.216396000	-1.037020000	1.505982000
H	-0.176636000	-2.043483000	0.506233000
H	1.497201000	-0.578939000	1.518619000
H	1.842087000	0.854323000	0.555730000
H	-1.510740000	-1.633793000	-1.475527000
H	-2.532106000	-0.477647000	-0.624657000
H	-0.719668000	2.091596000	-1.447329000
H	0.818682000	2.425082000	-0.634947000
H	-0.643013000	4.258402000	-0.609150000
H	-3.165704000	-2.277000000	0.710081000
H	2.154891000	-0.496743000	-1.463743000
H	1.728690000	-1.967085000	-0.592370000
H	3.967542000	-0.374274000	-0.004009000

Sum of electronic and zero-point Energies= -517.460419
Sum of electronic and thermal Energies= -517.447528
Sum of electronic and thermal Enthalpies= -517.446583
Sum of electronic and thermal Free Energies= -517.500521

TEOA$^{\bullet+}$ in DCM

N	0.028783000	-0.030698000	0.770576000
C	-0.804085000	-1.203546000	0.742418000
C	1.451126000	-0.170684000	0.787254000
C	-0.566686000	1.269744000	0.805942000
C	2.028901000	-0.672848000	-0.569047000
C	-1.662885000	-1.312244000	-0.520987000
O	-2.449934000	-2.454639000	-0.320921000
O	3.417667000	-0.724104000	-0.487974000
C	-0.378182000	2.063096000	-0.520759000
O	-0.918290000	3.337744000	-0.376013000
H	-0.177728000	-2.088893000	0.844937000
H	-1.478349000	-1.149794000	1.606131000
H	1.707226000	-0.906653000	1.556605000
H	1.906767000	0.786643000	1.035454000
H	-0.081066000	1.847017000	1.598253000

H	-1.628213000	1.167247000	1.029519000
H	1.774635000	0.043251000	-1.351402000
H	1.589129000	-1.640840000	-0.826505000
H	-1.018462000	-1.409400000	-1.402253000
H	-2.277877000	-0.412293000	-0.638457000
H	-2.996175000	-2.593293000	-1.099840000
H	3.687648000	-1.536063000	-0.047587000
H	-0.829262000	1.509709000	-1.349979000
H	0.687957000	2.183720000	-0.720031000
H	-1.872385000	3.301402000	-0.498533000

Sum of electronic and zero-point Energies= -517.265783
Sum of electronic and thermal Energies= -517.252810
Sum of electronic and thermal Enthalpies= -517.251866
Sum of electronic and thermal Free Energies= -517.306319

TEOA$^{\bullet+}$ in Gas phase

N	-0.019779000	-0.008423000	0.827623000
C	-1.422294000	-0.321357000	0.783832000
C	0.940466000	-1.063592000	0.826028000
C	0.414871000	1.350821000	0.813550000
C	0.993826000	-1.839301000	-0.531336000
C	-2.096372000	0.071698000	-0.537105000
O	-3.423269000	-0.315243000	-0.365740000
O	2.084142000	-2.690152000	-0.520104000
C	1.074793000	1.774152000	-0.540172000
O	1.603358000	3.044658000	-0.401059000
H	-1.557617000	-1.389395000	0.951012000
H	-1.923743000	0.224555000	1.590884000
H	0.671617000	-1.777294000	1.612061000
H	1.931377000	-0.659112000	1.029258000
H	1.183578000	1.483805000	1.580706000
H	-0.432188000	2.001051000	1.031512000
H	1.145944000	-1.122481000	-1.340746000
H	0.042996000	-2.355641000	-0.699653000
H	-1.609667000	-0.449095000	-1.372552000
H	-1.995260000	1.153424000	-0.699239000
H	-3.921344000	-0.162554000	-1.173884000
H	1.854006000	-3.542930000	-0.139298000
H	0.339531000	1.697420000	-1.347730000
H	1.900954000	1.092939000	-0.756034000
H	0.962681000	3.715637000	-0.653221000

Sum of electronic and zero-point Energies= -517.188710
Sum of electronic and thermal Energies= -517.175571
Sum of electronic and thermal Enthalpies= -517.174627
Sum of electronic and thermal Free Energies= -517.229696

TEA in DCM

N	-0.000368000	-0.405317000	-0.262038000
C	0.000234000	0.997041000	-0.653396000
H	0.869909000	1.163877000	-1.293043000

H	-0.870009000	1.164913000	-1.292014000
C	1.190998000	-0.817386000	0.460256000
H	1.083570000	-1.888852000	0.656982000
H	1.259727000	-0.334373000	1.451956000
C	-1.191863000	-0.816176000	0.460642000
H	-1.084926000	-1.887489000	0.658443000
H	-1.260420000	-0.332198000	1.451866000
C	-2.482100000	-0.585556000	-0.300021000
H	-3.310484000	-1.065773000	0.225130000
H	-2.726734000	0.474446000	-0.393567000
H	-2.419848000	-1.012000000	-1.304255000
C	0.001506000	2.021713000	0.476135000
H	0.885364000	1.926203000	1.111281000
H	0.001304000	3.031750000	0.059742000
H	-0.881283000	1.926620000	1.112844000
C	2.481420000	-0.586767000	-0.300056000
H	2.726425000	0.473184000	-0.393070000
H	3.309487000	-1.067513000	0.225106000
H	2.419320000	-1.012791000	-1.304487000

Sum of electronic and zero-point Energies= -291.965566
Sum of electronic and thermal Energies= -291.956250
Sum of electronic and thermal Enthalpies= -291.955306
Sum of electronic and thermal Free Energies= -291.999289

$TEA^{\bullet+}$ in DCM

N	0.021760000	-0.308763000	-0.045015000
C	0.011237000	1.008119000	-0.621270000
H	0.935901000	1.153206000	-1.172699000
H	-0.824799000	1.060298000	-1.320192000
C	1.234906000	-1.060889000	0.176756000
H	1.117768000	-1.988698000	-0.401084000
H	1.205896000	-1.376580000	1.227644000
C	-1.196803000	-0.886480000	0.480189000
H	-1.020679000	-1.958217000	0.580723000
H	-1.303778000	-0.492067000	1.501466000
C	-2.441773000	-0.603471000	-0.331979000
H	-3.262768000	-1.168416000	0.109411000
H	-2.721258000	0.449775000	-0.318375000
H	-2.320921000	-0.931536000	-1.365267000
C	-0.145865000	2.080465000	0.460201000
H	0.680401000	2.046134000	1.170012000
H	-0.144970000	3.052408000	-0.032697000
H	-1.085304000	1.965872000	1.000808000
C	2.531589000	-0.370910000	-0.157828000
H	2.657171000	0.560714000	0.395007000
H	3.343986000	-1.038836000	0.129377000
H	2.631292000	-0.173714000	-1.225431000

Sum of electronic and zero-point Energies= -291.766698
Sum of electronic and thermal Energies= -291.757243
Sum of electronic and thermal Enthalpies= -291.756299
Sum of electronic and thermal Free Energies= -291.801226

TEA in Gas phase

N	-0.000336000	-0.400712000	-0.248921000
C	0.000333000	0.995808000	-0.650728000
H	0.869327000	1.157339000	-1.292679000
H	-0.868981000	1.158383000	-1.291986000
C	1.191753000	-0.816534000	0.464711000
H	1.081836000	-1.888104000	0.660177000
H	1.271545000	-0.336642000	1.458049000
C	-1.192612000	-0.815256000	0.465109000
H	-1.083171000	-1.886650000	0.661765000
H	-1.272256000	-0.334282000	1.457917000
C	-2.477322000	-0.590293000	-0.306721000
H	-3.308182000	-1.080189000	0.205402000
H	-2.730507000	0.468194000	-0.395588000
H	-2.397952000	-1.008837000	-1.312700000
C	0.001353000	2.028947000	0.471703000
H	0.884071000	1.936711000	1.108968000
H	0.001834000	3.037564000	0.051764000
H	-0.881200000	1.937852000	1.109383000
C	2.476669000	-0.591382000	-0.306686000
H	2.730283000	0.467073000	-0.394652000
H	3.307181000	-1.082009000	0.205307000
H	2.397481000	-1.009156000	-1.313004000

Sum of electronic and zero-point Energies= -291.963549
Sum of electronic and thermal Energies= -291.954252
Sum of electronic and thermal Enthalpies= -291.953308
Sum of electronic and thermal Free Energies= -291.997187

$TEA^{\bullet+}$ in Gas phase

N	-0.019939000	-0.307224000	-0.041331000
C	-0.014023000	1.009623000	-0.620281000
H	0.821855000	1.063832000	-1.320230000
H	-0.941290000	1.150469000	-1.169745000
C	1.204444000	-0.880040000	0.482503000
H	1.027876000	-1.950729000	0.602284000
H	1.322392000	-0.470071000	1.497480000
C	-1.236670000	-1.054108000	0.198915000
H	-1.111411000	-2.006878000	-0.336223000
H	-1.218556000	-1.326419000	1.263857000
C	-2.534368000	-0.385681000	-0.176364000
H	-3.348530000	-1.049264000	0.117241000
H	-2.679966000	0.560949000	0.345699000
H	-2.622827000	-0.222726000	-1.251234000
C	0.140720000	2.086171000	0.460390000
H	1.090442000	1.990729000	0.987202000
H	0.116420000	3.059725000	-0.029671000
H	-0.674788000	2.042201000	1.182769000
C	2.445662000	-0.610870000	-0.342474000
H	2.727374000	0.442028000	-0.347044000
H	3.271788000	-1.167158000	0.101145000
H	2.324210000	-0.956691000	-1.370348000

Sum of electronic and zero-point Energies=	-291.698548
Sum of electronic and thermal Energies=	-291.688926
Sum of electronic and thermal Enthalpies=	-291.687982
Sum of electronic and thermal Free Energies=	-291.733909