Electronic Supplementary Information

Photocatalytic conversion of CO2 to CO by Ru(II) and Os(II) octahedral complexes: A DFT/TDDFT study.

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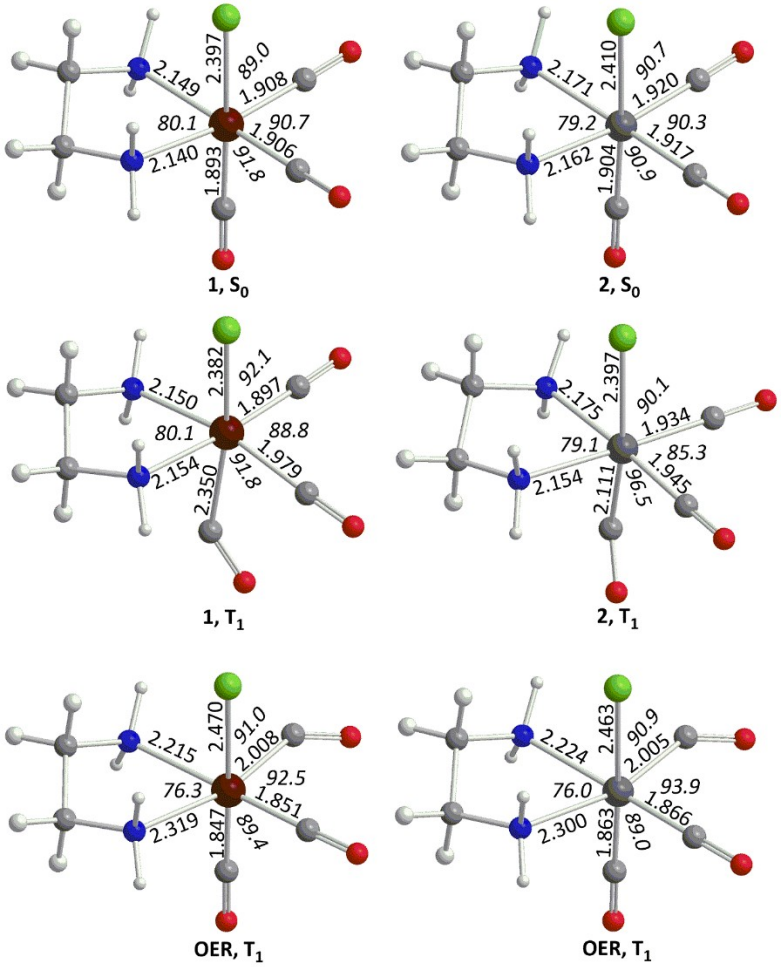

Fig. S1 Optimized geometries of **1** and **2** in their S_0 and T_1 states and respective OER species in DMF solvent at the PBE0/Def2-TZVP level.

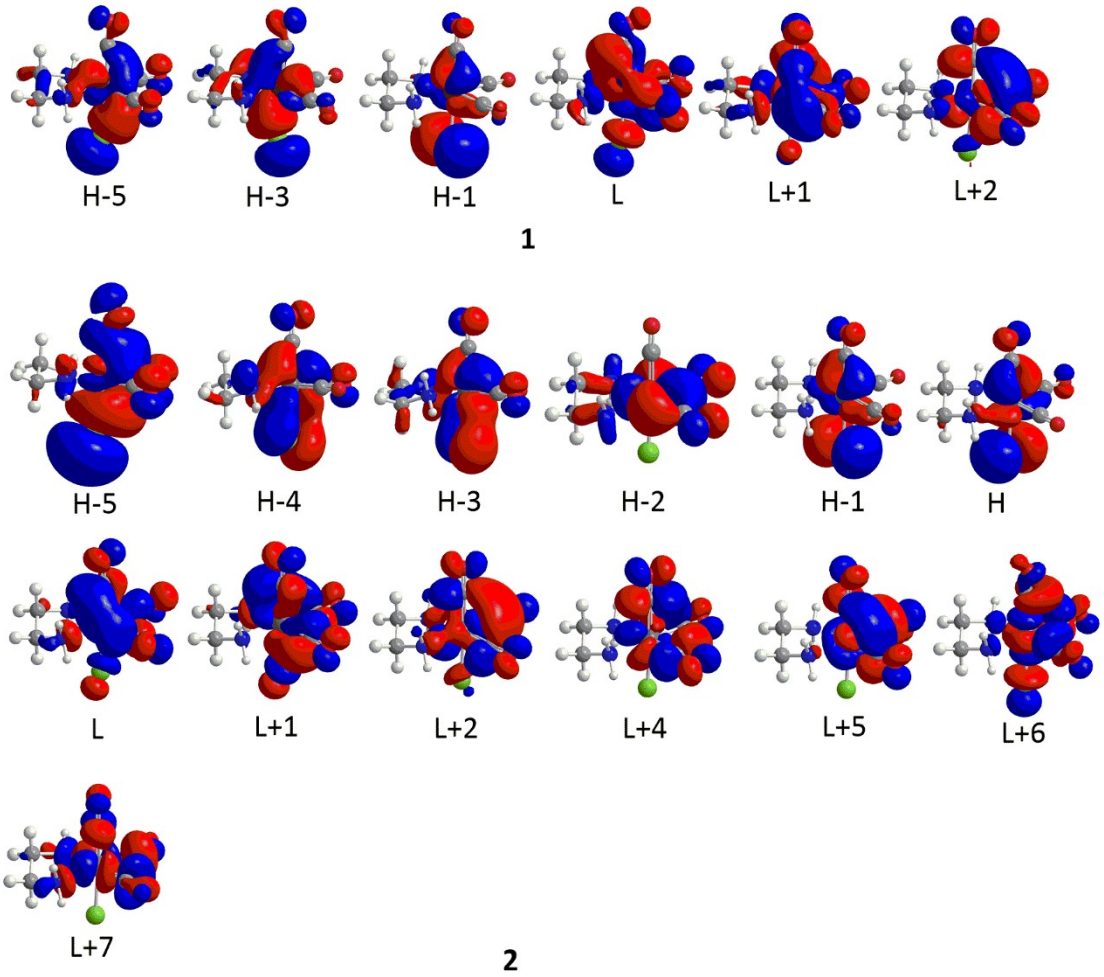

Fig. S2 3D surfaces of the MOs involved in the most relevant electronic excitations in the simulated absorption spectra of **1** and **2**.

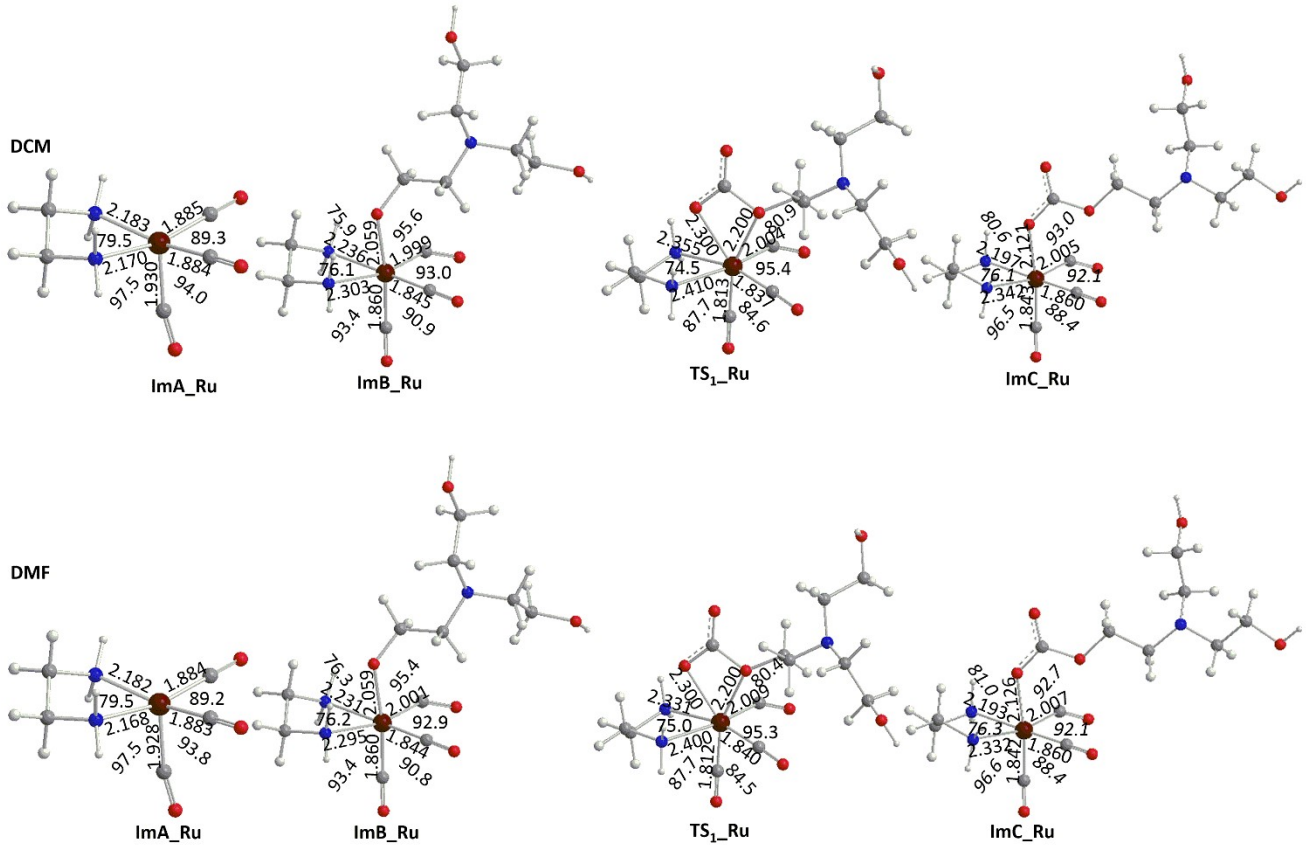

Fig. S3 Selected structural parameters of the various intermediates involved in *TEOA complex formation* step by **1**.

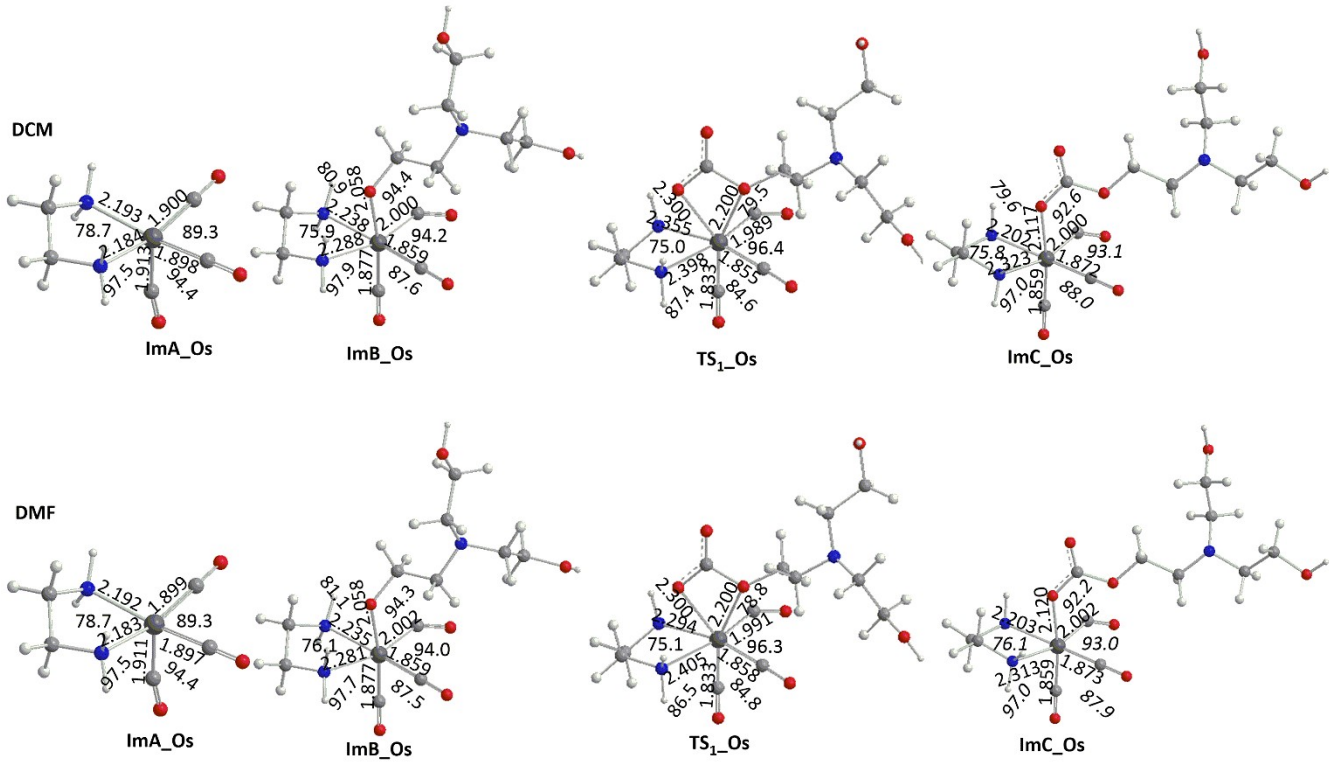

Fig. S4 Selected structural parameters of the various intermediates involved in *TEOA complex formation* step by **2**.

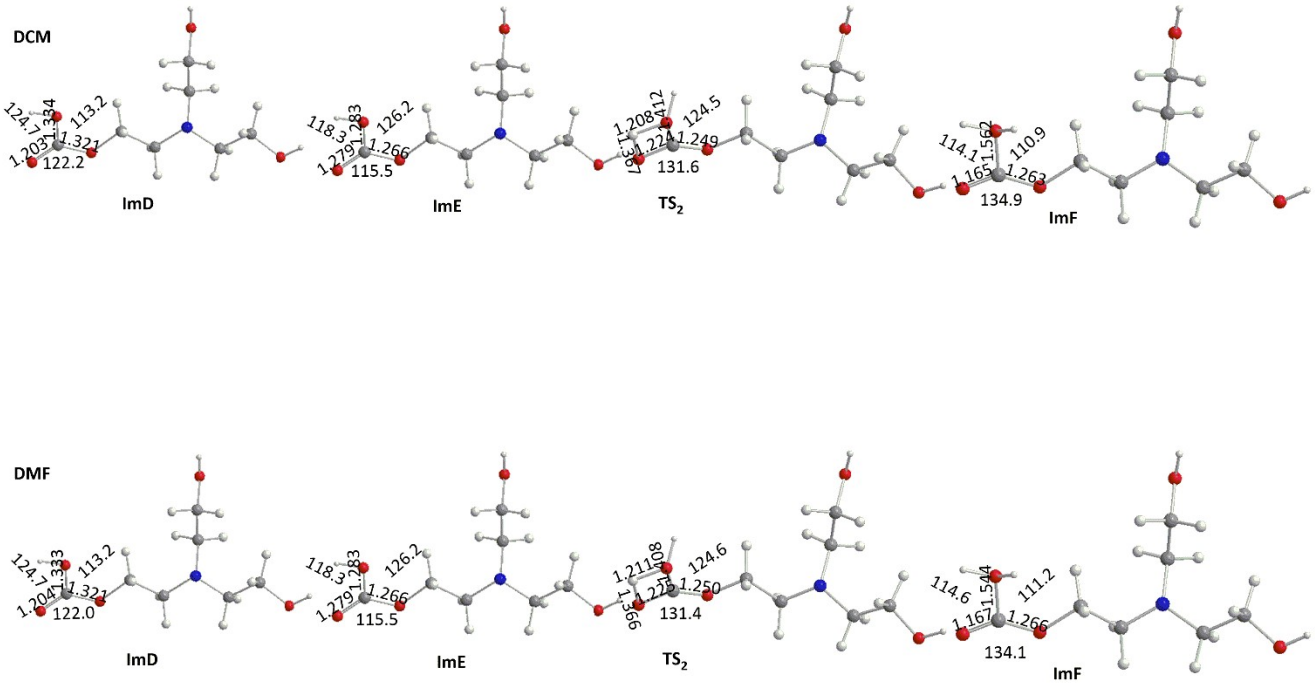

Fig. S5 Optimized geometries and selected structural parameters of the various intermediates involved in CO release step.

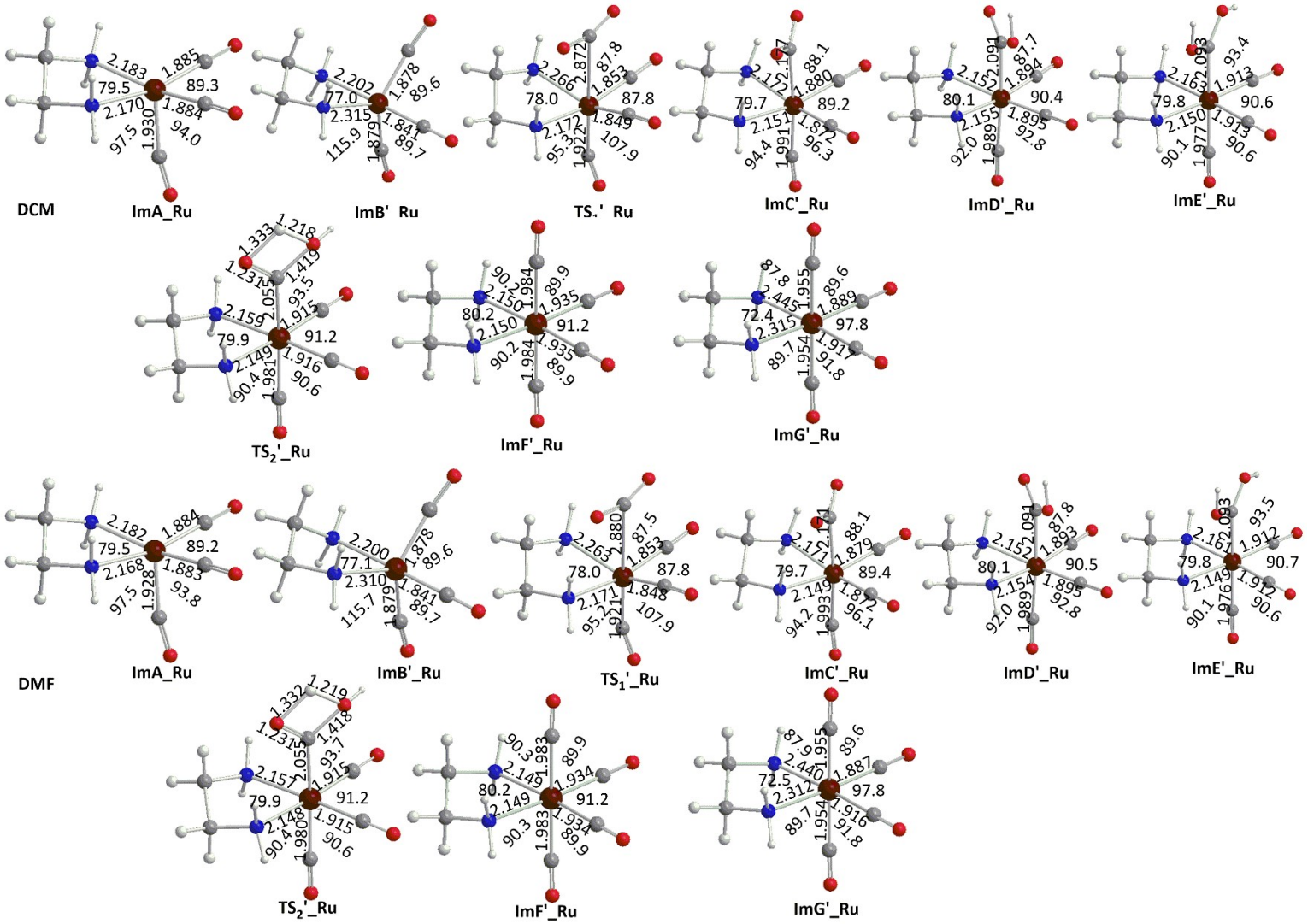

Fig. S6 Optimized geometries and selected structural parameters of the various intermediates involved in η^1-CO_2 *complex* formation catalytic cycle for the CO_2 to CO conversion by **1**.

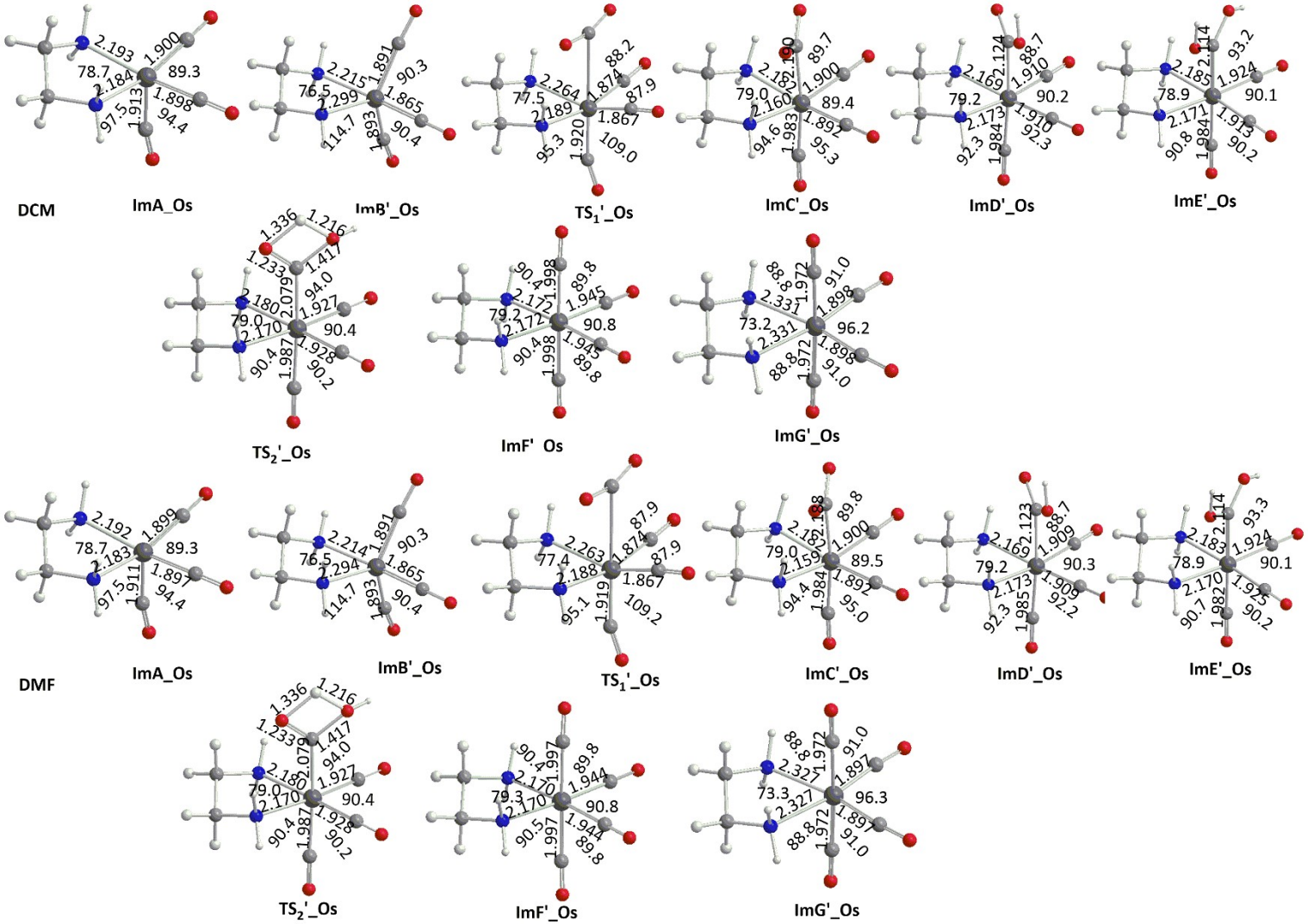

Fig. S7 Optimized geometries and selected structural parameters of the various intermediates involved in η^1-CO_2 *complex* formation catalytic cycle for the CO_2 to CO conversion by **2**.

Table S1 Gibbs free energies, *G* (in au) calculated at the PBE0/Def2-TZVP level for all species involved in the Born – Haber cycle employed for calculation of the redox potentials.

Species	***G*** (au)
[(en)Ru(CO)$_3$Cl], S_0 Gas	-1084.966129
[(en)Ru(CO)$_3$Cl], S_0 DCM	-1085.154581
[(en)Ru(CO)$_3$Cl], S_0 DMF	-1085.154581
[(en)Ru(CO)$_3$Cl]$^{\cdot-}$, OER Gas	-1085.154581
[(en)Ru(CO)$_3$Cl]$^{\cdot-}$, OER DCM	-1085.173077
[(en)Ru(CO)$_3$Cl]$^{\cdot-}$, OER DMF	-1085.175623
[(en)Os(CO)$_3$Cl], S_0 Gas	-1080.779082
[(en)Os(CO)$_3$Cl], S_0 DCM	-1080.956135
[(en)Os(CO)$_3$Cl], S_0 DMF	-1080.868122
[(en)Os(CO)$_3$Cl]$^{\cdot-}$, OER Gas	-1080.956135
[(en)Os(CO)$_3$Cl]$^{\cdot-}$, OER DCM	-1080.976766
[(en)Os(CO)$_3$Cl]$^{\cdot-}$, OER DMF	-1080.979599

Table S2 Parameters relevant to the Born – Haber cycle and redox potentials calculated at the PBE0/Def2-TZVP level.

Parameter	1		2	
	DCM	DMF	DCM	DMF
ΔG^{o}(gas,redox) (kcal/mol)	-118.255	-118.255	-111.102	-55.8734
ΔG^{o}(solv.,[(en)M(CO)$_3$Cl]$^{\cdot-}$) (kcal/mol)	-11.6064	-13.204	-12.9461	-14.7239
ΔG^{o}(solv.,[(en)M(CO)$_3$Cl], S_0) (kcal/mol)	-50.2371	-55.394	-50.8358	-125.826
ΔG^{o}(soln.,redox) (kcal/mol)	-79.6246	-76.0654	-73.2127	55.22895
E^{0}_{red} (V)	3.5	3.3	3.2	-2.4
$E_{0\text{-}0}$ (eV)	3	3	3.3	3.3
E^{0*}_{red} (V)	6.4	6.3	6.4	0.9
E^{0*}_{red} vs NHE (V)	2.1	1.9	2.1	-3.5

Table S3 Cartesian Coordinates and energetic data.

Initial Step

1_S_0 Gas

Ru	-0.221103000	0.085337000	-0.008120000
C	2.664229000	0.561956000	0.631241000
C	-1.554124000	-0.001022000	1.354662000
C	2.700428000	-0.247879000	-0.640080000
C	-0.389637000	1.972023000	-0.171798000
O	-0.494676000	3.094205000	-0.268814000
C	-1.555611000	-0.245420000	-1.336217000
O	-2.330518000	-0.467511000	-2.122217000
N	1.437130000	-0.041711000	-1.392809000
N	1.428978000	0.212553000	1.366225000
O	-2.327910000	-0.078782000	2.168881000
Cl	0.093011000	-2.251138000	0.199844000
H	2.640668000	1.633216000	0.417646000
H	3.551691000	0.361907000	1.236587000
H	2.762986000	-1.311076000	-0.404893000
H	3.565722000	0.019885000	-1.249396000
H	1.273647000	-0.854335000	-1.982686000
H	1.519874000	0.759986000	-2.011120000
H	1.306779000	0.828707000	2.164232000
H	1.496347000	-0.740887000	1.726012000

Sum of electronic and zero-point Energies= -1084.925171
Sum of electronic and thermal Energies= -1084.911559
Sum of electronic and thermal Enthalpies= -1084.910615
Sum of electronic and thermal Free Energies= -1084.966129

1_S_0 DCM

Ru	0.214572000	0.078688000	0.006575000
C	-2.664599000	0.557194000	-0.632517000
C	1.543315000	0.015880000	-1.358833000
C	-2.694086000	-0.241932000	0.643127000
C	0.380486000	1.957989000	0.165043000
O	0.498490000	3.078870000	0.261256000
C	1.542983000	-0.223701000	1.343577000
O	2.318456000	-0.429659000	2.136019000
N	-1.431580000	-0.016489000	1.387009000
N	-1.424673000	0.215053000	-1.363260000
O	2.319247000	-0.046007000	-2.174998000
Cl	-0.064340000	-2.289568000	-0.193434000
H	-2.651755000	1.628706000	-0.427045000
H	-3.543309000	0.340911000	-1.242832000
H	-2.752327000	-1.307041000	0.418631000
H	-3.554464000	0.029933000	1.255845000
H	-1.282396000	-0.791098000	2.027814000
H	-1.509582000	0.816441000	1.962964000
H	-1.290814000	0.853528000	-2.141161000
H	-1.507115000	-0.719158000	-1.761971000

Sum of electronic and zero-point Energies= -1085.005260
Sum of electronic and thermal Energies= -1084.991681
Sum of electronic and thermal Enthalpies= -1084.990736
Sum of electronic and thermal Free Energies= -1085.046187

1_S_0 DMF

Ru	-0.213756000	0.078009000	-0.006321000
C	2.665165000	0.556607000	0.632602000
C	-1.542666000	0.019278000	1.358853000
C	2.693720000	-0.241919000	-0.643206000
C	-0.379016000	1.956646000	-0.164905000
O	-0.498879000	3.077173000	-0.261193000
C	-1.540796000	-0.221108000	-1.344869000
O	-2.316129000	-0.426135000	-2.138093000
N	1.431220000	-0.014486000	-1.385996000
N	1.424491000	0.216160000	1.362867000
O	-2.319690000	-0.040829000	2.174516000
Cl	0.060111000	-2.294735000	0.193942000
H	2.654251000	1.628001000	0.427423000
H	3.542706000	0.338532000	1.243741000
H	2.751637000	-1.307192000	-0.419620000
H	3.553442000	0.030182000	-1.256570000
H	1.283234000	-0.785113000	-2.031723000
H	1.509056000	0.821166000	-1.958040000
H	1.289608000	0.857525000	2.138228000
H	1.508593000	-0.715398000	1.766898000

Sum of electronic and zero-point Energies= -1085.013486
Sum of electronic and thermal Energies= -1084.999909
Sum of electronic and thermal Enthalpies= -1084.998964
Sum of electronic and thermal Free Energies= -1085.054405

2_S_0 Gas

Os	-0.190860000	0.050813000	-0.004677000
C	2.695191000	0.681555000	0.626738000
C	-1.534290000	-0.070974000	1.362512000
C	2.775422000	-0.121729000	-0.646926000
C	-0.452476000	1.937118000	-0.169738000
O	-0.604069000	3.057655000	-0.268404000
C	-1.528473000	-0.316272000	-1.337374000
O	-2.300729000	-0.549551000	-2.126843000
N	1.495252000	0.004829000	-1.393581000
N	1.482600000	0.259140000	1.365995000
O	-2.310028000	-0.159633000	2.177807000
Cl	0.298058000	-2.273048000	0.200469000
H	2.607918000	1.750207000	0.417520000
H	3.593193000	0.530383000	1.229901000
H	2.907614000	-1.179412000	-0.416242000
H	3.616386000	0.203547000	-1.261565000
H	1.383839000	-0.817334000	-1.983454000
H	1.528443000	0.808190000	-2.015066000
H	1.326564000	0.873934000	2.159721000
H	1.615809000	-0.683221000	1.738047000

Sum of electronic and zero-point Energies= -1080.737826
Sum of electronic and thermal Energies= -1080.724350
Sum of electronic and thermal Enthalpies= -1080.723406
Sum of electronic and thermal Free Energies= -1080.779082

2_S_0 DCM

Os	0.184427000	0.048282000	0.004488000
C	-2.695598000	0.684198000	-0.623457000
C	1.523245000	-0.063685000	-1.363643000
C	-2.769071000	-0.118882000	0.647634000
C	0.454722000	1.927237000	0.162623000
O	0.630820000	3.044819000	0.256450000
C	1.515198000	-0.301196000	1.343823000
O	2.288829000	-0.523435000	2.138390000
N	-1.489896000	0.025587000	1.388517000
N	-1.477259000	0.274771000	-1.361488000
O	2.302417000	-0.147585000	-2.179450000
Cl	-0.273141000	-2.305558000	-0.199028000
H	-2.619205000	1.751819000	-0.412292000
H	-3.585091000	0.521710000	-1.233764000
H	-2.893663000	-1.177379000	0.419699000
H	-3.606830000	0.203350000	1.266323000
H	-1.389014000	-0.761888000	2.023954000
H	-1.521610000	0.855164000	1.974594000
H	-1.310454000	0.916904000	-2.130766000
H	-1.624608000	-0.643553000	-1.779575000

Sum of electronic and zero-point Energies= -1080.818838
Sum of electronic and thermal Energies= -1080.805375
Sum of electronic and thermal Enthalpies= -1080.804431
Sum of electronic and thermal Free Energies= -1080.860094

2_S_0 DMF

Os	-0.183539000	0.047991000	-0.004464000
C	2.695571000	0.683171000	0.623205000
C	-1.522127000	-0.057972000	1.364041000
C	2.768517000	-0.120638000	-0.647378000
C	-0.451303000	1.926487000	-0.164606000
O	-0.628420000	3.043746000	-0.259736000
C	-1.513312000	-0.299263000	-1.344767000
O	-2.287354000	-0.521106000	-2.139501000
N	1.489255000	0.023684000	-1.387883000
N	1.476652000	0.275325000	1.361008000
O	-2.301902000	-0.137640000	2.180123000
Cl	0.265722000	-2.310321000	0.201363000
H	2.620507000	1.750920000	0.412663000
H	3.584235000	0.519440000	1.234204000
H	2.893581000	-1.178926000	-0.418754000
H	3.605622000	0.201352000	-1.266926000
H	1.388337000	-0.762208000	-2.025129000
H	1.521354000	0.853569000	-1.973601000
H	1.308728000	0.920465000	2.127549000
H	1.625264000	-0.640239000	1.784176000

Sum of electronic and zero-point Energies= -1080.826867
Sum of electronic and thermal Energies= -1080.813404
Sum of electronic and thermal Enthalpies= -1080.812459
Sum of electronic and thermal Free Energies= -1080.868122

1_T_1 Gas

Ru	0.187926000	-0.077715000	0.003427000
C	-2.506784000	1.157278000	-0.510823000
C	1.702503000	0.177387000	-1.230035000
C	-2.734534000	0.202602000	0.634599000
C	0.571599000	2.061026000	0.750368000
O	1.369465000	2.828810000	0.492354000
C	1.407725000	-0.825018000	1.255868000
O	2.109858000	-1.299633000	2.001028000
N	-1.473514000	0.055538000	1.397834000
N	-1.358683000	0.678945000	-1.313466000
O	2.571582000	0.292655000	-1.933061000
Cl	-0.571173000	-2.204453000	-0.650896000
H	-2.262095000	2.154375000	-0.137830000
H	-3.408225000	1.241373000	-1.122338000
H	-3.006220000	-0.786055000	0.260244000
H	-3.542809000	0.558418000	1.277512000
H	-1.532809000	-0.754758000	2.008709000
H	-1.320156000	0.868048000	1.991440000
H	-1.079151000	1.395892000	-1.976556000
H	-1.632288000	-0.137835000	-1.859735000

Sum of electronic and zero-point Energies= -1084.818893
Sum of electronic and thermal Energies= -1084.803566
Sum of electronic and thermal Enthalpies= -1084.802622
Sum of electronic and thermal Free Energies= -1084.864038

1_T_1 DCM

Ru	-0.172466000	-0.081202000	-0.009861000
C	2.489054000	1.185942000	0.529501000
C	-1.685932000	0.120766000	1.247943000
C	2.725636000	0.263904000	-0.637477000
C	-0.615572000	2.092095000	-0.665509000
O	-1.464570000	2.812932000	-0.435723000
C	-1.383185000	-0.792803000	-1.287921000
O	-2.086267000	-1.247489000	-2.047994000
N	1.461097000	0.123166000	-1.394753000
N	1.349661000	0.669627000	1.318852000
O	-2.551377000	0.203643000	1.960367000
Cl	0.581578000	-2.249709000	0.613344000
H	2.230176000	2.187401000	0.181223000
H	3.385781000	1.264225000	1.146507000
H	3.012520000	-0.729819000	-0.290594000
H	3.518756000	0.647246000	-1.281460000
H	1.526751000	-0.660982000	-2.038017000
H	1.298917000	0.950634000	-1.964422000
H	1.045668000	1.373380000	1.984723000
H	1.645517000	-0.135788000	1.867952000

Sum of electronic and zero-point Energies= -1084.895957
Sum of electronic and thermal Energies= -1084.880524
Sum of electronic and thermal Enthalpies= -1084.879580
Sum of electronic and thermal Free Energies= -1084.941578

1_T_1 DMF

Ru	0.165784000	-0.095332000	0.004310000
C	-2.460093000	1.241847000	-0.532802000
C	1.681656000	0.089288000	-1.254335000
C	-2.713929000	0.345707000	0.650235000
C	0.676907000	2.109783000	0.637240000
O	1.560726000	2.794851000	0.441650000
C	1.367030000	-0.816909000	1.283405000
O	2.065925000	-1.278302000	2.044121000
N	-1.447400000	0.178400000	1.398760000
N	-1.344812000	0.677425000	-1.323141000
O	2.548023000	0.159213000	-1.967508000
Cl	-0.642565000	-2.256804000	-0.587540000
H	-2.166757000	2.239971000	-0.202950000
H	-3.359333000	1.337953000	-1.143409000
H	-3.033411000	-0.644073000	0.321306000
H	-3.488825000	0.762110000	1.295597000
H	-1.530521000	-0.593966000	2.054107000
H	-1.257359000	1.007997000	1.956541000
H	-1.025046000	1.360879000	-2.002504000
H	-1.670995000	-0.125762000	-1.858029000

Sum of electronic and zero-point Energies= -1084.904039
Sum of electronic and thermal Energies= -1084.888451
Sum of electronic and thermal Enthalpies= -1084.887507
Sum of electronic and thermal Free Energies= -1084.950569

2_T_1 Gas

Os	0.177461000	-0.018327000	0.006295000
C	-2.653389000	0.940276000	-0.483510000
C	1.661406000	0.306911000	-1.223859000
C	-2.799179000	-0.111667000	0.587671000
C	0.254352000	1.925297000	0.864052000
O	0.772562000	2.884039000	0.472171000
C	1.508459000	-0.648835000	1.240800000
O	2.283217000	-1.031819000	1.968044000
N	-1.532985000	-0.195280000	1.355246000
N	-1.444439000	0.636525000	-1.289397000
O	2.528971000	0.499255000	-1.915914000
Cl	-0.390290000	-2.218298000	-0.670067000
H	-2.517165000	1.929644000	-0.041724000
H	-3.543993000	0.972137000	-1.114363000
H	-2.975442000	-1.091918000	0.141542000
H	-3.638756000	0.121075000	1.245504000
H	-1.515285000	-1.062168000	1.887030000
H	-1.470633000	0.571397000	2.024332000
H	-1.219955000	1.434869000	-1.878008000
H	-1.636782000	-0.143533000	-1.917853000

Sum of electronic and zero-point Energies= -1080.620367
Sum of electronic and thermal Energies= -1080.605752
Sum of electronic and thermal Enthalpies= -1080.604808
Sum of electronic and thermal Free Energies= -1080.664635

2_T_1 DCM

Os	-0.167168000	0.002203000	-0.000957000
C	2.684592000	0.850489000	0.504540000
C	-1.627832000	0.298137000	1.250673000
C	2.798564000	-0.214448000	-0.553535000
C	-0.223023000	1.921938000	-0.878998000
O	-0.631692000	2.925791000	-0.460081000
C	-1.546624000	-0.546599000	-1.237642000
O	-2.357390000	-0.871041000	-1.954819000
N	1.537225000	-0.248201000	-1.330139000
N	1.450526000	0.603625000	1.291479000
O	-2.490280000	0.466250000	1.958719000
Cl	0.265465000	-2.282173000	0.567012000
H	2.599290000	1.840694000	0.054319000
H	3.558995000	0.846997000	1.155914000
H	2.929430000	-1.196272000	-0.097674000
H	3.648754000	-0.022961000	-1.208792000
H	1.483029000	-1.119825000	-1.850781000
H	1.526710000	0.500364000	-2.020302000
H	1.240833000	1.422246000	1.857474000
H	1.611437000	-0.154814000	1.953192000

Sum of electronic and zero-point Energies= -1080.698991
Sum of electronic and thermal Energies= -1080.684366
Sum of electronic and thermal Enthalpies= -1080.683421
Sum of electronic and thermal Free Energies= -1080.743468

2_T_1 DMF

Os	-0.165547000	0.005250000	0.000916000
C	2.689636000	0.838550000	0.507768000
C	-1.622440000	0.297740000	1.255372000
C	2.798634000	-0.227226000	-0.549513000
C	-0.222825000	1.920633000	-0.883739000
O	-0.617437000	2.930917000	-0.466259000
C	-1.551268000	-0.535246000	-1.235375000
O	-2.366191000	-0.853726000	-1.950500000
N	1.537833000	-0.253322000	-1.326997000
N	1.452078000	0.600131000	1.292088000
O	-2.484069000	0.462542000	1.965758000
Cl	0.248812000	-2.291458000	0.549831000
H	2.612242000	1.829154000	0.057342000
H	3.561722000	0.829108000	1.161891000
H	2.923545000	-1.209633000	-0.093475000
H	3.649981000	-0.040687000	-1.204452000
H	1.478636000	-1.124577000	-1.847613000
H	1.533743000	0.493873000	-2.018538000
H	1.245200000	1.421627000	1.855039000
H	1.608444000	-0.155289000	1.958313000

Sum of electronic and zero-point Energies= -1080.706971
Sum of electronic and thermal Energies= -1080.692330
Sum of electronic and thermal Enthalpies= -1080.691385
Sum of electronic and thermal Free Energies= -1080.751525

OER_Ru Gas

Ru	-0.274216000	0.051628000	-0.003379000
C	2.803196000	0.721509000	0.589326000
C	-1.571764000	-0.260914000	1.284835000
C	2.774149000	0.045890000	-0.765747000
C	-0.646973000	1.866168000	0.063266000
O	-0.866152000	2.989957000	0.095036000
C	-1.526989000	-0.244012000	-1.518905000
O	-2.616583000	-0.276480000	-1.889797000
N	1.476900000	0.265271000	-1.420590000
N	1.693820000	0.221278000	1.391049000
O	-2.384230000	-0.469525000	2.057368000
Cl	0.395908000	-2.279563000	0.057935000
H	2.680918000	1.803236000	0.475578000
H	3.782740000	0.552268000	1.053309000
H	2.882955000	-1.031883000	-0.631814000
H	3.606326000	0.398583000	-1.382539000
H	1.291840000	-0.474533000	-2.089237000
H	1.461027000	1.143810000	-1.925862000
H	1.587757000	0.729933000	2.258622000
H	1.792469000	-0.769795000	1.595002000

Sum of electronic and zero-point Energies= -1085.111018
Sum of electronic and thermal Energies= -1085.096055
Sum of electronic and thermal Enthalpies= -1085.095111
Sum of electronic and thermal Free Energies= -1085.154581

OER_Ru DCM

Ru	-0.237238000	0.046493000	-0.002917000
C	2.750312000	0.718611000	0.633387000
C	-1.551585000	-0.287813000	1.257618000
C	2.760070000	0.100553000	-0.745243000
C	-0.620864000	1.851172000	0.099515000
O	-0.873022000	2.965921000	0.157572000
C	-1.510772000	-0.206558000	-1.532616000
O	-2.630423000	-0.120243000	-1.830028000
N	1.461972000	0.330966000	-1.403123000
N	1.625953000	0.164447000	1.390719000
O	-2.366950000	-0.511696000	2.025376000
Cl	0.351658000	-2.345633000	-0.027411000
H	2.611433000	1.800358000	0.562508000
H	3.711887000	0.540285000	1.124854000
H	2.894683000	-0.978999000	-0.661510000
H	3.584109000	0.501983000	-1.339782000
H	1.325539000	-0.342352000	-2.149579000
H	1.443756000	1.247916000	-1.836825000
H	1.478229000	0.673678000	2.253126000
H	1.795366000	-0.808344000	1.629074000

Sum of electronic and zero-point Energies= -1085.129662
Sum of electronic and thermal Energies= -1085.114873
Sum of electronic and thermal Enthalpies= -1085.113929
Sum of electronic and thermal Free Energies= -1085.173077

OER_Ru DMF

Ru	-0.232965000	0.045861000	-0.003190000
C	2.744908000	0.718808000	0.638803000
C	-1.547595000	-0.291937000	1.255890000
C	2.758511000	0.108147000	-0.742509000
C	-0.620115000	1.849107000	0.103550000
O	-0.877650000	2.962200000	0.164273000
C	-1.510158000	-0.204686000	-1.531961000
O	-2.631388000	-0.101217000	-1.823593000
N	1.460372000	0.341454000	-1.400676000
N	1.617841000	0.159608000	1.390184000
O	-2.362687000	-0.518168000	2.023605000
Cl	0.347355000	-2.354555000	-0.038529000
H	2.605808000	1.800635000	0.573649000
H	3.703789000	0.537354000	1.133705000
H	2.895047000	-0.971615000	-0.665139000
H	3.581724000	0.514755000	-1.334269000
H	1.330529000	-0.321205000	-2.157826000
H	1.442225000	1.263723000	-1.823314000
H	1.464853000	0.669831000	2.251212000
H	1.794446000	-0.810492000	1.633854000

Sum of electronic and zero-point Energies= -1085.132194
Sum of electronic and thermal Energies= -1085.117418
Sum of electronic and thermal Enthalpies= -1085.116474
Sum of electronic and thermal Free Energies= -1085.175623

OER_Os Gas

Os	-0.233831000	0.026143000	-0.000211000
C	2.821226000	0.799097000	0.600072000
C	-1.533558000	-0.273380000	1.308709000
C	2.839171000	0.106220000	-0.746110000
C	-0.647497000	1.849650000	0.033616000
O	-0.884601000	2.973937000	0.050784000
C	-1.423940000	-0.300278000	-1.534286000
O	-2.492146000	-0.348828000	-1.982387000
N	1.535359000	0.259490000	-1.411066000
N	1.717536000	0.261224000	1.389674000
O	-2.347086000	-0.464033000	2.091440000
Cl	0.532324000	-2.282252000	0.085486000
H	2.654539000	1.872929000	0.472587000
H	3.796276000	0.675006000	1.085480000
H	2.996872000	-0.963769000	-0.599989000
H	3.656101000	0.491292000	-1.362746000
H	1.389092000	-0.492091000	-2.077293000
H	1.483287000	1.131163000	-1.927041000
H	1.563642000	0.790003000	2.238212000
H	1.869813000	-0.714608000	1.632595000

Sum of electronic and zero-point Energies= -1080.912505
Sum of electronic and thermal Energies= -1080.897790
Sum of electronic and thermal Enthalpies= -1080.896846
Sum of electronic and thermal Free Energies= -1080.956135

OER_Os DCM

Os	0.197729000	0.029821000	-0.001468000
C	-2.767473000	0.787687000	-0.634038000
C	1.527048000	-0.277637000	-1.274526000
C	-2.818676000	0.129680000	0.724324000
C	0.625854000	1.843384000	-0.039478000
O	0.903847000	2.957502000	-0.062460000
C	1.416912000	-0.291616000	1.554690000
O	2.541132000	-0.263305000	1.887490000
N	-1.515686000	0.291259000	1.399012000
N	-1.640501000	0.222477000	-1.386906000
O	2.348122000	-0.474122000	-2.050657000
Cl	-0.473433000	-2.335110000	-0.029156000
H	-2.599961000	1.862322000	-0.531367000
H	-3.719375000	0.646588000	-1.153477000
H	-2.994685000	-0.940789000	0.609694000
H	-3.628653000	0.547304000	1.325434000
H	-1.410594000	-0.411555000	2.124253000
H	-1.471477000	1.190255000	1.868331000
H	-1.461069000	0.760985000	-2.225817000
H	-1.846731000	-0.730360000	-1.675394000

Sum of electronic and zero-point Energies= -1080.933418
Sum of electronic and thermal Energies= -1080.918951
Sum of electronic and thermal Enthalpies= -1080.918007
Sum of electronic and thermal Free Energies= -1080.976766

OER_Os DMF

Os	-0.194152000	0.030421000	0.001049000
C	2.763479000	0.785353000	0.636858000
C	-1.523945000	-0.275107000	1.273960000
C	2.817241000	0.129173000	-0.721680000
C	-0.622126000	1.843600000	0.038316000
O	-0.904608000	2.956349000	0.060841000
C	-1.418378000	-0.292402000	-1.553745000
O	-2.546538000	-0.254713000	-1.878162000
N	1.514526000	0.293236000	-1.397856000
N	1.632829000	0.219970000	1.386088000
O	-2.345155000	-0.471357000	2.050397000
Cl	0.463850000	-2.342500000	0.024568000
H	2.597901000	1.860208000	0.535552000
H	3.712305000	0.641180000	1.160381000
H	2.993099000	-0.941494000	-0.609131000
H	3.627074000	0.548023000	-1.321736000
H	1.414480000	-0.403113000	-2.130041000
H	1.472508000	1.195545000	-1.861278000
H	1.450687000	0.761447000	2.222686000
H	1.843344000	-0.729699000	1.681744000

Sum of electronic and zero-point Energies= -1080.936257
Sum of electronic and thermal Energies= -1080.921812
Sum of electronic and thermal Enthalpies= -1080.920868
Sum of electronic and thermal Free Energies= -1080.979599

TEOA complex mechanism

ImA_Ru DCM

Ru	-0.180683000	0.021002000	-0.186387000
C	-0.516494000	-0.181775000	1.703269000
C	-1.475015000	-1.254876000	-0.683002000
O	-2.258264000	-2.034383000	-0.955688000
N	1.501210000	1.406291000	-0.050460000
C	-1.469737000	1.378377000	-0.407619000
O	-2.246689000	2.203048000	-0.514241000
O	-0.937660000	-0.301138000	2.753158000
C	2.746407000	0.701357000	-0.426222000
C	2.713820000	-0.692427000	0.143613000
N	1.485005000	-1.361977000	-0.329647000
H	1.581427000	1.770212000	0.893790000
H	1.376932000	2.217152000	-0.648121000
H	3.626073000	1.243656000	-0.074255000
H	2.788446000	0.660813000	-1.516457000
H	2.678795000	-0.662460000	1.234411000
H	3.604811000	-1.250168000	-0.152352000
H	1.596922000	-1.631724000	-1.303827000
H	1.340179000	-2.225913000	0.182544000

Sum of electronic and zero-point Energies= -624.877559
Sum of electronic and thermal Energies= -624.865085
Sum of electronic and thermal Enthalpies= -624.864141
Sum of electronic and thermal Free Energies= -624.917838

ImA_Ru DMF

Ru	-0.179421000	0.021747000	-0.187700000
C	-0.514409000	-0.184513000	1.699364000
C	-1.474491000	-1.252076000	-0.684325000
O	-2.260298000	-2.030495000	-0.955376000
N	1.502055000	1.405523000	-0.048890000
C	-1.467923000	1.379202000	-0.404826000
O	-2.247387000	2.202841000	-0.507493000
O	-0.945740000	-0.307997000	2.745463000
C	2.748423000	0.700449000	-0.419922000
C	2.712398000	-0.694029000	0.147547000
N	1.484383000	-1.360460000	-0.331426000
H	1.579396000	1.771358000	0.894734000
H	1.379167000	2.214823000	-0.648804000
H	3.626141000	1.242197000	-0.062645000
H	2.795229000	0.661157000	-1.509846000
H	2.673952000	-0.666411000	1.238197000
H	3.602939000	-1.252767000	-0.147594000
H	1.598090000	-1.624865000	-1.306844000
H	1.337955000	-2.226775000	0.176043000

Sum of electronic and zero-point Energies= -624.885730
Sum of electronic and thermal Energies= -624.873285
Sum of electronic and thermal Enthalpies= -624.872341
Sum of electronic and thermal Free Energies= -624.925939

ImA_Os DCM

Os	-0.150707000	0.013690000	-0.136602000
C	-0.454156000	-0.185204000	1.741989000
C	-1.456378000	-1.271501000	-0.631470000
O	-2.237720000	-2.052332000	-0.919418000
N	1.545955000	1.398836000	-0.019407000
C	-1.447809000	1.383261000	-0.360295000
O	-2.219820000	2.214765000	-0.483922000
O	-0.846612000	-0.299606000	2.808802000
C	2.789958000	0.707232000	-0.431747000
C	2.782397000	-0.688750000	0.132644000
N	1.538048000	-1.361847000	-0.301617000
H	1.651123000	1.760777000	0.923788000
H	1.404974000	2.213296000	-0.609280000
H	3.669760000	1.257802000	-0.095289000
H	2.804380000	0.675398000	-1.522737000
H	2.785521000	-0.665512000	1.223892000
H	3.660900000	-1.244156000	-0.199887000
H	1.631171000	-1.652819000	-1.271885000
H	1.407041000	-2.217016000	0.229882000

Sum of electronic and zero-point Energies= -620.678137
Sum of electronic and thermal Energies= -620.665894
Sum of electronic and thermal Enthalpies= -620.664950
Sum of electronic and thermal Free Energies= -620.718731

ImA_Os DMF

Os	-0.150365000	0.013920000	-0.136651000
C	-0.450664000	-0.187665000	1.739629000
C	-1.455887000	-1.269999000	-0.632152000
O	-2.239877000	-2.049770000	-0.919306000
N	1.545477000	1.398075000	-0.018345000
C	-1.446787000	1.383510000	-0.358461000
O	-2.220944000	2.214563000	-0.479888000
O	-0.847570000	-0.303865000	2.805566000
C	2.789829000	0.707069000	-0.430170000
C	2.781482000	-0.689100000	0.132884000
N	1.537178000	-1.360505000	-0.303488000
H	1.650020000	1.760123000	0.924752000
H	1.404763000	2.212334000	-0.608392000
H	3.668584000	1.257842000	-0.091722000
H	2.805140000	0.676047000	-1.520992000
H	2.783963000	-0.667477000	1.224043000
H	3.659130000	-1.245040000	-0.200638000
H	1.630329000	-1.647516000	-1.274911000
H	1.406485000	-2.217541000	0.224829000

Sum of electronic and zero-point Energies= -620.686661
Sum of electronic and thermal Energies= -620.674430
Sum of electronic and thermal Enthalpies= -620.673486
Sum of electronic and thermal Free Energies= -620.727250

ImB_Ru DCM

Ru	1.851590000	0.183463000	0.036423000
N	2.674351000	-1.187603000	-1.525998000
N	2.789570000	-1.536647000	1.246209000
C	3.650083000	-2.347310000	0.383665000
C	2.971820000	-2.511196000	-0.956807000
C	3.342491000	1.295833000	0.003161000
O	4.249191000	1.996981000	-0.022411000
C	0.950083000	1.299237000	-1.356412000
O	0.579135000	2.384616000	-1.572255000
C	1.187645000	1.203338000	1.422993000
O	0.790510000	1.853067000	2.278559000
N	-3.188214000	-0.190894000	0.081979000
C	-0.913169000	-1.068343000	-0.376740000
C	-1.800577000	-0.211176000	0.521120000
O	0.369704000	-1.244566000	0.109713000
C	-5.019768000	-1.747507000	-0.433232000
C	-3.929247000	-1.352038000	0.539876000
O	-5.736079000	-2.830384000	0.134017000
C	-3.565973000	2.134634000	-0.616881000
C	-3.859513000	1.055629000	0.404178000
O	-4.188816000	3.329055000	-0.176973000
H	3.491352000	-0.808346000	-1.992663000
H	1.946013000	-1.263430000	-2.227402000
H	1.926366000	-2.029939000	1.461786000
H	3.253432000	-1.296071000	2.112703000
H	3.861121000	-3.332413000	0.812790000
H	4.604113000	-1.826525000	0.267149000
H	3.591866000	-3.108584000	-1.629865000
H	2.019002000	-3.023179000	-0.819353000
H	-0.921253000	-0.610964000	-1.383220000
H	-1.387765000	-2.057525000	-0.489405000
H	-1.711725000	-0.566380000	1.562780000
H	-1.418725000	0.812968000	0.507775000
H	-4.561581000	-2.031137000	-1.388837000
H	-5.687419000	-0.897361000	-0.623402000
H	-4.374212000	-1.188384000	1.536278000
H	-3.241088000	-2.194691000	0.639027000
H	-6.427199000	-3.089905000	-0.480265000
H	-3.955790000	1.820155000	-1.593068000
H	-2.482971000	2.276280000	-0.720449000
H	-3.584200000	1.421565000	1.407919000
H	-4.939542000	0.888060000	0.418454000
H	-3.992093000	4.022689000	-0.811418000

Sum of electronic and zero-point Energies= -1141.882708

Sum of electronic and thermal Energies= -1141.856164

Sum of electronic and thermal Enthalpies= -1141.855220

Sum of electronic and thermal Free Energies= -1141.943658

ImB_Ru DMF

Ru	1.852251000	0.179195000	0.038513000
N	2.668414000	-1.179840000	-1.531232000
N	2.800943000	-1.532452000	1.238057000
C	3.662773000	-2.336602000	0.369429000
C	2.978145000	-2.503271000	-0.966961000
C	3.339684000	1.295552000	0.001906000
O	4.241648000	2.002716000	-0.024827000
C	0.941730000	1.301077000	-1.345650000
O	0.579102000	2.392726000	-1.551030000
C	1.191495000	1.193340000	1.430303000
O	0.795346000	1.839442000	2.289429000
N	-3.190018000	-0.190940000	0.076411000
C	-0.913237000	-1.069596000	-0.377013000
C	-1.802275000	-0.209153000	0.516462000
O	0.367263000	-1.247525000	0.113983000
C	-5.024343000	-1.748800000	-0.428507000
C	-3.929702000	-1.351323000	0.539161000
O	-5.739632000	-2.829214000	0.145221000
C	-3.571525000	2.132899000	-0.626297000
C	-3.862029000	1.055687000	0.397497000
O	-4.186660000	3.330434000	-0.183271000
H	3.481451000	-0.795467000	-2.000807000
H	1.939423000	-1.260375000	-2.231509000
H	1.948066000	-2.037657000	1.465720000
H	3.271470000	-1.286345000	2.099535000
H	3.882158000	-3.319929000	0.797731000
H	4.612290000	-1.809068000	0.248385000
H	3.598791000	-3.093433000	-1.645490000
H	2.030101000	-3.023037000	-0.825907000
H	-0.917039000	-0.613606000	-1.384329000
H	-1.390067000	-2.057812000	-0.489993000
H	-1.714868000	-0.560463000	1.559565000
H	-1.420698000	0.815083000	0.499838000
H	-4.570693000	-2.036706000	-1.384903000
H	-5.692333000	-0.899164000	-0.619150000
H	-4.370302000	-1.185147000	1.537141000
H	-3.240933000	-2.193606000	0.637232000
H	-6.431533000	-3.091727000	-0.467183000
H	-3.969241000	1.819853000	-1.599588000
H	-2.488708000	2.270565000	-0.737203000
H	-3.584387000	1.423384000	1.400021000
H	-4.941811000	0.886986000	0.414731000
H	-4.006379000	4.018248000	-0.829094000

Sum of electronic and zero-point Energies= -1141.885417

Sum of electronic and thermal Energies= -1141.858894

Sum of electronic and thermal Enthalpies= -1141.857950

Sum of electronic and thermal Free Energies= -1141.946405

ImB_Os DCM

Os	1.595737000	0.146537000	0.026245000
N	2.412274000	-1.272099000	-1.500614000
N	2.475072000	-1.562497000	1.267232000
C	3.356181000	-2.397204000	0.442841000
C	2.707106000	-2.589243000	-0.907528000
C	3.113812000	1.250110000	-0.002822000
O	4.033919000	1.941261000	-0.023683000
C	0.739836000	1.225886000	-1.423196000
O	0.360864000	2.308461000	-1.688123000
C	0.941244000	1.217017000	1.397765000
O	0.555455000	1.895599000	2.243105000
N	-3.443379000	-0.189862000	0.085798000
C	-1.184959000	-1.079792000	-0.404462000
C	-2.053428000	-0.227719000	0.514698000
O	0.104822000	-1.271235000	0.070548000
C	-5.293505000	-1.722935000	-0.433559000
C	-4.193414000	-1.347911000	0.536897000
O	-6.016945000	-2.804125000	0.127601000
C	-3.799282000	2.145934000	-0.590133000
C	-4.099732000	1.060880000	0.422521000
O	-4.411488000	3.341413000	-0.138626000
H	3.234301000	-0.901103000	-1.966386000
H	1.694257000	-1.362445000	-2.212120000
H	1.620481000	-2.064992000	1.498741000
H	2.930233000	-1.291784000	2.130029000
H	3.550940000	-3.369547000	0.904723000
H	4.312916000	-1.879864000	0.338628000
H	3.345840000	-3.186461000	-1.561548000
H	1.755839000	-3.107297000	-0.785112000
H	-1.192405000	-0.609111000	-1.403146000
H	-1.662677000	-2.064880000	-0.523915000
H	-1.958822000	-0.598962000	1.550087000
H	-1.662142000	0.792649000	0.512337000
H	-4.843888000	-2.001683000	-1.394648000
H	-5.953717000	-0.864385000	-0.611336000
H	-4.630820000	-1.189454000	1.537397000
H	-3.513457000	-2.198596000	0.623967000
H	-6.714604000	-3.050618000	-0.484653000
H	-4.193642000	1.842785000	-1.568087000
H	-2.715391000	2.279816000	-0.694958000
H	-3.816169000	1.414556000	1.428273000
H	-5.181325000	0.904389000	0.439978000
H	-4.205694000	4.040219000	-0.764466000

Sum of electronic and zero-point Energies= -1137.691350

Sum of electronic and thermal Energies= -1137.665114

Sum of electronic and thermal Enthalpies= -1137.664170

Sum of electronic and thermal Free Energies= -1137.752210

ImB_Os DMF

Os	1.597008000	0.143789000	0.025666000
N	2.414177000	-1.271987000	-1.497788000
N	2.478105000	-1.553172000	1.269359000
C	3.363556000	-2.387306000	0.447611000
C	2.715227000	-2.586858000	-0.901443000
C	3.113664000	1.248751000	-0.003907000
O	4.030247000	1.944684000	-0.024765000
C	0.739875000	1.224973000	-1.424464000
O	0.370954000	2.313859000	-1.684438000
C	0.940986000	1.216599000	1.394263000
O	0.554330000	1.897615000	2.237794000
N	-3.446600000	-0.189932000	0.081923000
C	-1.185773000	-1.076372000	-0.408533000
C	-2.056025000	-0.225162000	0.510083000
O	0.102009000	-1.270346000	0.069541000
C	-5.296097000	-1.725764000	-0.433652000
C	-4.193046000	-1.350499000	0.533343000
O	-6.017719000	-2.807176000	0.129916000
C	-3.812146000	2.145580000	-0.589398000
C	-4.105533000	1.058378000	0.422974000
O	-4.417113000	3.341729000	-0.129305000
H	3.235629000	-0.900294000	-1.964201000
H	1.698989000	-1.369185000	-2.211268000
H	1.630759000	-2.063445000	1.509550000
H	2.935174000	-1.275342000	2.129030000
H	3.561656000	-3.356254000	0.914485000
H	4.317751000	-1.866044000	0.341759000
H	3.356964000	-3.181306000	-1.554676000
H	1.766904000	-3.109985000	-0.778153000
H	-1.190065000	-0.603707000	-1.406476000
H	-1.664834000	-2.060472000	-0.531402000
H	-1.960997000	-0.595867000	1.545606000
H	-1.666680000	0.796001000	0.507374000
H	-4.850017000	-2.005084000	-1.396118000
H	-5.957423000	-0.867800000	-0.609592000
H	-4.626818000	-1.194135000	1.535785000
H	-3.510884000	-2.199783000	0.616517000
H	-6.714404000	-3.056475000	-0.482588000
H	-4.216182000	1.846622000	-1.564497000
H	-2.728879000	2.277363000	-0.703593000
H	-3.818496000	1.411078000	1.428156000
H	-5.186529000	0.898522000	0.444863000
H	-4.233793000	4.036410000	-0.766879000

Sum of electronic and zero-point Energies= -1137.694467

Sum of electronic and thermal Energies= -1137.668256

Sum of electronic and thermal Enthalpies= -1137.667312

Sum of electronic and thermal Free Energies= -1137.755312

ImC_Ru DCM

Ru	2.487016000	-0.371326000	0.119827000
C	3.522338000	-1.810675000	0.622353000
C	0.271770000	1.695867000	-0.618471000
C	1.357200000	-1.557317000	-0.760584000
O	0.673313000	-2.301264000	-1.291398000
O	-0.176822000	2.792475000	-0.916979000
N	3.845349000	1.120138000	0.989508000
C	1.410158000	-0.480769000	1.808081000
O	0.846396000	-1.224860000	2.499627000
O	4.152006000	-2.709229000	0.950249000
C	5.010004000	1.389643000	0.131722000
C	4.546660000	1.512316000	-1.301481000
N	3.819810000	0.298148000	-1.686471000
O	1.510651000	1.399369000	-0.521331000
N	-4.107868000	-0.203362000	-0.127754000
C	-1.949629000	0.911542000	-0.453143000
C	-2.668292000	-0.362860000	-0.061857000
O	-0.555516000	0.649284000	-0.357633000
C	-6.207866000	-1.308347000	-0.785274000
C	-4.807058000	-1.469033000	-0.232432000
O	-6.783882000	-2.599895000	-0.858662000
C	-5.254816000	1.930074000	0.355553000
C	-4.638984000	0.664016000	0.916859000
O	-5.743754000	2.692528000	1.443799000
H	4.139555000	0.907999000	1.936118000
H	3.253885000	1.946459000	1.040934000
H	5.706103000	0.554681000	0.237713000
H	5.529255000	2.300919000	0.440247000
H	5.401592000	1.708599000	-1.954717000
H	3.855357000	2.351751000	-1.390590000
H	3.209003000	0.483576000	-2.472958000
H	4.459525000	-0.435211000	-1.968754000
H	-2.209517000	1.743721000	0.205992000
H	-2.211848000	1.197746000	-1.475194000
H	-2.374739000	-1.149593000	-0.760792000
H	-2.327927000	-0.676132000	0.940445000
H	-6.152719000	-0.838943000	-1.775648000
H	-6.806397000	-0.656164000	-0.136785000
H	-4.866915000	-1.994950000	0.736734000
H	-4.251118000	-2.116700000	-0.915004000
H	-7.686564000	-2.510492000	-1.174265000
H	-6.062787000	1.669313000	-0.339732000
H	-4.498354000	2.487981000	-0.210418000
H	-3.848002000	0.942227000	1.623606000
H	-5.398788000	0.134879000	1.504543000
H	-6.116396000	3.508179000	1.099809000

Sum of electronic and zero-point Energies= -1330.359666

Sum of electronic and thermal Energies= -1330.330195

Sum of electronic and thermal Enthalpies= -1330.329251

Sum of electronic and thermal Free Energies= -1330.425201

ImC_Ru DMF

Ru	2.489454000	-0.366787000	0.118580000
C	3.517413000	-1.809134000	0.625364000
C	0.270012000	1.700796000	-0.617698000
C	1.357109000	-1.551128000	-0.760930000
O	0.672429000	-2.294776000	-1.291417000
O	-0.181275000	2.798820000	-0.912807000
N	3.852581000	1.113952000	0.989402000
C	1.408278000	-0.472205000	1.805649000
O	0.855490000	-1.223757000	2.500526000
O	4.138925000	-2.711752000	0.957090000
C	5.018089000	1.376456000	0.129277000
C	4.553451000	1.498374000	-1.303019000
N	3.817534000	0.287216000	-1.682671000
O	1.508039000	1.407305000	-0.519975000
N	-4.108997000	-0.203292000	-0.131350000
C	-1.951932000	0.913327000	-0.458447000
C	-2.669196000	-0.361976000	-0.067434000
O	-0.557414000	0.653301000	-0.361755000
C	-6.210415000	-1.311448000	-0.780816000
C	-4.806637000	-1.470138000	-0.234938000
O	-6.784096000	-2.604343000	-0.853661000
C	-5.262121000	1.925912000	0.356417000
C	-4.638913000	0.662487000	0.915499000
O	-5.743608000	2.690336000	1.446879000
H	4.149485000	0.896483000	1.934102000
H	3.271541000	1.947014000	1.047876000
H	5.710292000	0.538663000	0.236207000
H	5.540961000	2.285755000	0.436572000
H	5.408317000	1.684819000	-1.958816000
H	3.868373000	2.342593000	-1.394490000
H	3.214490000	0.472279000	-2.475344000
H	4.454107000	-0.451544000	-1.958391000
H	-2.214204000	1.744876000	0.200511000
H	-2.213928000	1.198464000	-1.480892000
H	-2.376078000	-1.148061000	-0.767252000
H	-2.327715000	-0.675601000	0.934393000
H	-6.161662000	-0.840692000	-1.770777000
H	-6.807762000	-0.662074000	-0.128685000
H	-4.860534000	-1.997259000	0.733959000
H	-4.252286000	-2.115456000	-0.921087000
H	-7.688526000	-2.515773000	-1.165015000
H	-6.075409000	1.662521000	-0.331351000
H	-4.511596000	2.484399000	-0.216864000
H	-3.845391000	0.943890000	1.618124000
H	-5.393593000	0.130250000	1.506980000
H	-6.131392000	3.498927000	1.102467000

Sum of electronic and zero-point Energies= -1330.363471

Sum of electronic and thermal Energies= -1330.334033

Sum of electronic and thermal Enthalpies= -1330.333089

Sum of electronic and thermal Free Energies= -1330.428955

ImC_Os DCM

Os	2.179771000	-0.308275000	0.098290000
C	3.252600000	-1.745517000	0.589203000
C	-0.064541000	1.739880000	-0.620145000
C	1.056770000	-1.528696000	-0.770829000
O	0.381252000	-2.292677000	-1.293614000
O	-0.511129000	2.835861000	-0.912848000
N	3.517923000	1.226582000	0.948366000
C	1.141961000	-0.401598000	1.805027000
O	0.576557000	-1.138607000	2.521120000
O	3.903238000	-2.640376000	0.901735000
C	4.671516000	1.513462000	0.076443000
C	4.186785000	1.620361000	-1.350119000
N	3.458972000	0.394279000	-1.709338000
O	1.182891000	1.452853000	-0.522154000
N	-4.421114000	-0.200168000	-0.132817000
C	-2.276050000	0.936574000	-0.461853000
C	-2.980089000	-0.345743000	-0.070462000
O	-0.877869000	0.687248000	-0.369095000
C	-6.511952000	-1.325345000	-0.785699000
C	-5.107709000	-1.472851000	-0.237968000
O	-7.074988000	-2.622568000	-0.859181000
C	-5.588576000	1.920537000	0.357277000
C	-4.958232000	0.659984000	0.914872000
O	-6.081969000	2.676298000	1.448089000
H	3.828948000	1.008859000	1.889028000
H	2.926317000	2.052062000	1.020785000
H	5.382431000	0.691340000	0.180576000
H	5.174283000	2.435390000	0.377431000
H	5.028405000	1.807401000	-2.021547000
H	3.489632000	2.454446000	-1.440189000
H	2.837832000	0.571467000	-2.490593000
H	4.101088000	-0.333740000	-2.001368000
H	-2.540799000	1.765403000	0.199190000
H	-2.540963000	1.221403000	-1.483400000
H	-2.680012000	-1.128310000	-0.771242000
H	-2.633585000	-0.656466000	0.930405000
H	-6.465122000	-0.853818000	-1.775492000
H	-7.114786000	-0.680381000	-0.133995000
H	-5.158833000	-2.001281000	0.730256000
H	-4.547410000	-2.113271000	-0.923783000
H	-7.979979000	-2.541856000	-1.170481000
H	-6.395858000	1.652589000	-0.336056000
H	-4.839581000	2.487058000	-0.210135000
H	-4.168283000	0.944996000	1.620064000
H	-5.710840000	0.122011000	1.503710000
H	-6.464726000	3.488234000	1.106427000

Sum of electronic and zero-point Energies= -1326.164288

Sum of electronic and thermal Energies= -1326.135094

Sum of electronic and thermal Enthalpies= -1326.134150

Sum of electronic and thermal Free Energies= -1326.229802

ImC_Os DMF

Os	2.182026000	-0.304780000	0.097366000
C	3.247789000	-1.746007000	0.589301000
C	-0.065524000	1.743641000	-0.616812000
C	1.055916000	-1.522016000	-0.772435000
O	0.379135000	-2.284946000	-1.295518000
O	-0.514652000	2.840492000	-0.907650000
N	3.525021000	1.219311000	0.950411000
C	1.138233000	-0.397932000	1.803126000
O	0.582871000	-1.144778000	2.519699000
O	3.890185000	-2.645882000	0.904167000
C	4.678936000	1.501484000	0.076077000
C	4.192313000	1.609294000	-1.349173000
N	3.457007000	0.385718000	-1.704656000
O	1.180900000	1.459902000	-0.516190000
N	-4.422227000	-0.199807000	-0.136526000
C	-2.277586000	0.937097000	-0.467578000
C	-2.981112000	-0.345321000	-0.075436000
O	-0.879220000	0.690076000	-0.370681000
C	-6.515088000	-1.327397000	-0.780980000
C	-5.107952000	-1.473269000	-0.240252000
O	-7.076081000	-2.625809000	-0.853881000
C	-5.596469000	1.916716000	0.356242000
C	-4.958136000	0.659653000	0.912608000
O	-6.082362000	2.675263000	1.448766000
H	3.839359000	0.996244000	1.888840000
H	2.942669000	2.050548000	1.030062000
H	5.386772000	0.676932000	0.179676000
H	5.184678000	2.421517000	0.376934000
H	5.033347000	1.788522000	-2.023044000
H	3.500199000	2.447372000	-1.440313000
H	2.842497000	0.563221000	-2.491244000
H	4.097179000	-0.345978000	-1.992324000
H	-2.545832000	1.766439000	0.191352000
H	-2.540350000	1.219166000	-1.490462000
H	-2.681710000	-1.128226000	-0.776096000
H	-2.634150000	-0.655491000	0.925498000
H	-6.474552000	-0.854582000	-1.770331000
H	-7.116479000	-0.685086000	-0.125596000
H	-5.153372000	-2.002561000	0.727853000
H	-4.549652000	-2.111843000	-0.929480000
H	-7.982881000	-2.545714000	-1.160593000
H	-6.409124000	1.645207000	-0.329105000
H	-4.853750000	2.483455000	-0.219161000
H	-4.165536000	0.949072000	1.612985000
H	-5.705106000	0.118973000	1.506191000
H	-6.480933000	3.479356000	1.106148000

Sum of electronic and zero-point Energies= -1326.168423

Sum of electronic and thermal Energies= -1326.139264

Sum of electronic and thermal Enthalpies= -1326.138319

Sum of electronic and thermal Free Energies= -1326.233887

ImE DCM

C	-3.755251000	-0.366568000	0.075081000
O	-3.673493000	0.681623000	0.896949000
O	-4.783952000	-0.876463000	-0.283038000
N	1.049267000	-0.341994000	-0.121967000
C	-1.372639000	-0.171003000	0.135572000
C	-0.223447000	-0.908888000	-0.516638000
O	-2.575631000	-0.808790000	-0.322206000
C	3.357194000	-0.890378000	0.548130000
C	2.148857000	-1.274972000	-0.279835000
O	4.344549000	-1.881548000	0.332395000
C	1.417238000	2.060417000	0.323553000
C	1.308290000	0.964001000	-0.717445000
O	1.673092000	3.275341000	-0.355415000
H	-4.576490000	0.934359000	1.130441000
H	-1.395938000	0.882484000	-0.149380000
H	-1.307233000	-0.241738000	1.222645000
H	-0.259364000	-1.950169000	-0.189219000
H	-0.367754000	-0.905979000	-1.610350000
H	3.068436000	-0.837264000	1.605456000
H	3.731492000	0.097268000	0.250845000
H	2.460257000	-1.376463000	-1.334020000
H	1.816837000	-2.261108000	0.054089000
H	5.134567000	-1.632442000	0.818407000
H	2.224254000	1.822255000	1.027689000
H	0.483894000	2.116776000	0.898235000
H	0.511074000	1.228682000	-1.421990000
H	2.234758000	0.941056000	-1.303908000
H	1.738362000	3.979269000	0.294827000

Sum of electronic and zero-point Energies= -705.907873
Sum of electronic and thermal Energies= -705.892464
Sum of electronic and thermal Enthalpies= -705.891520
Sum of electronic and thermal Free Energies= -705.952801

ImE DMF

C	-3.755667000	-0.365371000	0.074403000
O	-3.675302000	0.680723000	0.896632000
O	-4.783777000	-0.877349000	-0.285475000
N	1.049122000	-0.341838000	-0.120535000
C	-1.372822000	-0.169841000	0.136104000
C	-0.223753000	-0.908485000	-0.515398000
O	-2.576266000	-0.807496000	-0.322671000
C	3.357233000	-0.891361000	0.548114000
C	2.148138000	-1.275524000	-0.278905000
O	4.344953000	-1.882570000	0.331290000
C	1.418607000	2.060597000	0.323721000
C	1.308685000	0.963916000	-0.716823000
O	1.674696000	3.275796000	-0.355506000
H	-4.577549000	0.934991000	1.132032000
H	-1.396140000	0.883424000	-0.149281000
H	-1.308910000	-0.240842000	1.223156000
H	-0.259907000	-1.949559000	-0.187360000
H	-0.367327000	-0.905727000	-1.609195000
H	3.070095000	-0.838865000	1.605783000
H	3.731796000	0.096101000	0.251169000
H	2.458357000	-1.377081000	-1.333486000

H	1.815281000	-2.261309000	0.055326000
H	5.135009000	-1.632623000	0.817135000
H	2.225984000	1.822942000	1.027421000
H	0.485673000	2.118083000	0.898719000
H	0.511164000	1.228193000	-1.421166000
H	2.234976000	0.939606000	-1.303534000
H	1.740673000	3.979111000	0.295571000

Sum of electronic and zero-point Energies= -705.909759
Sum of electronic and thermal Energies= -705.894344
Sum of electronic and thermal Enthalpies= -705.893400
Sum of electronic and thermal Free Energies= -705.954712

ImF DCM

C	-3.682368000	-0.266049000	0.116824000
O	-3.846638000	0.610175000	1.039351000
O	-4.720017000	-0.806480000	-0.398750000
N	1.072237000	-0.328872000	-0.169873000
C	-1.306627000	-0.125807000	0.152847000
C	-0.206522000	-0.842985000	-0.599317000
O	-2.573785000	-0.662017000	-0.348897000
C	3.349900000	-0.958207000	0.549846000
C	2.142130000	-1.303905000	-0.296086000
O	4.278023000	-2.012749000	0.388089000
C	1.603174000	2.038038000	0.324996000
C	1.394094000	0.976435000	-0.737688000
O	1.893830000	3.250659000	-0.339647000
H	-3.022281000	0.981999000	1.393468000
H	-5.541278000	-0.468703000	-0.003750000
H	-1.302320000	0.947822000	-0.043875000
H	-1.241905000	-0.334645000	1.221868000
H	-0.268097000	-1.905508000	-0.358753000
H	-0.379919000	-0.736342000	-1.681571000
H	3.040571000	-0.853317000	1.597654000
H	3.788947000	-0.005410000	0.229243000
H	2.466121000	-1.425675000	-1.343110000
H	1.768374000	-2.272805000	0.043275000
H	5.082834000	-1.784368000	0.860027000
H	2.422074000	1.743551000	0.992038000
H	0.696913000	2.129214000	0.938909000
H	0.590684000	1.308852000	-1.404903000
H	2.294827000	0.912275000	-1.360130000
H	2.084806000	3.923349000	0.319025000

Sum of electronic and zero-point Energies= -706.286887
Sum of electronic and thermal Energies= -706.271195
Sum of electronic and thermal Enthalpies= -706.270251
Sum of electronic and thermal Free Energies= -706.331914

ImF DMF

C	-3.681165000	-0.268926000	0.117404000
O	-3.849199000	0.619843000	1.025887000
O	-4.715945000	-0.821170000	-0.391441000
N	1.075009000	-0.329608000	-0.169566000
C	-1.306848000	-0.117039000	0.147669000
C	-0.205904000	-0.844035000	-0.593667000
O	-2.570683000	-0.668449000	-0.342384000
C	3.347580000	-0.961553000	0.556358000

C	2.144392000	-1.304123000	-0.297245000
O	4.286636000	-2.005995000	0.383689000
C	1.586554000	2.040650000	0.323032000
C	1.396460000	0.974965000	-0.738940000
O	1.899646000	3.250184000	-0.339269000
H	-3.027003000	0.998919000	1.377550000
H	-5.538472000	-0.480881000	-0.001232000
H	-1.308085000	0.952688000	-0.068210000
H	-1.239048000	-0.305816000	1.220027000
H	-0.270136000	-1.903419000	-0.340452000
H	-0.377043000	-0.749491000	-1.677422000
H	3.035090000	-0.873677000	1.604534000
H	3.780010000	-0.001028000	0.250465000
H	2.473363000	-1.419603000	-1.343671000
H	1.768666000	-2.274979000	0.034206000
H	5.083057000	-1.779988000	0.870941000
H	2.389274000	1.744591000	1.008977000
H	0.667972000	2.140489000	0.915966000
H	0.600815000	1.299477000	-1.419237000
H	2.306752000	0.912594000	-1.347523000
H	2.039659000	3.932432000	0.322516000

Sum of electronic and zero-point Energies= -706.295434
Sum of electronic and thermal Energies= -706.279768
Sum of electronic and thermal Enthalpies= -706.278824
Sum of electronic and thermal Free Energies= -706.340255

TS DCM

C	-3.675940000	-0.350784000	-0.012712000
O	-3.865256000	0.378917000	1.180794000
O	-4.794655000	-0.770526000	-0.279320000
N	1.079020000	-0.313170000	-0.203067000
C	-1.297608000	-0.033067000	0.010158000
C	-0.193554000	-0.786642000	-0.694927000
O	-2.570711000	-0.520978000	-0.570071000
C	3.306780000	-1.016589000	0.598434000
C	2.127890000	-1.313673000	-0.304662000
O	4.218539000	-2.086734000	0.446640000
C	1.633025000	2.031106000	0.361725000
C	1.458066000	0.993825000	-0.730727000
O	1.978697000	3.250777000	-0.262278000
H	-3.597222000	1.319360000	1.206636000
H	-4.961486000	0.010708000	0.830301000
H	-1.261829000	1.038272000	-0.184376000
H	-1.313443000	-0.241202000	1.078757000
H	-0.298085000	-1.847353000	-0.461229000
H	-0.311804000	-0.671828000	-1.783917000
H	2.957001000	-0.931459000	1.635233000
H	3.778337000	-0.065743000	0.321041000
H	2.492796000	-1.422226000	-1.339585000
H	1.715218000	-2.279155000	-0.002813000
H	5.007558000	-1.888696000	0.957372000
H	2.412076000	1.707278000	1.062149000
H	0.699337000	2.127670000	0.932224000
H	0.699671000	1.355448000	-1.434633000
H	2.389487000	0.919601000	-1.304619000
H	2.154380000	3.904796000	0.419080000

Sum of electronic and zero-point Energies= -706.212025
Sum of electronic and thermal Energies= -706.196482
Sum of electronic and thermal Enthalpies= -706.195538
Sum of electronic and thermal Free Energies= -706.256680

TS DMF

C	-3.673386000	-0.353287000	-0.010928000
O	-3.866335000	0.381257000	1.174501000
O	-4.789794000	-0.781339000	-0.277688000
N	1.081610000	-0.314346000	-0.200631000
C	-1.297947000	-0.026376000	0.006692000
C	-0.193083000	-0.789463000	-0.686821000
O	-2.567613000	-0.524594000	-0.568172000
C	3.306144000	-1.018004000	0.603046000
C	2.130736000	-1.313436000	-0.304992000
O	4.229405000	-2.078156000	0.441112000
C	1.614737000	2.034650000	0.359043000
C	1.458482000	0.992108000	-0.730986000
O	1.981898000	3.250377000	-0.262736000
H	-3.602375000	1.323282000	1.194910000
H	-4.962691000	0.005567000	0.824899000
H	-1.263465000	1.041918000	-0.202897000
H	-1.314341000	-0.218225000	1.078212000
H	-0.299858000	-1.847041000	-0.440469000
H	-0.309447000	-0.687060000	-1.777277000
H	2.954591000	-0.948375000	1.640136000
H	3.770090000	-0.060010000	0.338094000
H	2.498739000	-1.416364000	-1.339656000
H	1.717751000	-2.280772000	-0.009624000
H	5.010027000	-1.881893000	0.965426000
H	2.377029000	1.710161000	1.077561000
H	0.669928000	2.140490000	0.908171000
H	0.706971000	1.344844000	-1.446707000
H	2.398051000	0.919900000	-1.291749000
H	2.103142000	3.916475000	0.418927000

Sum of electronic and zero-point Energies= -706.221176
Sum of electronic and thermal Energies= -706.205639
Sum of electronic and thermal Enthalpies= -706.204695
Sum of electronic and thermal Free Energies= -706.265784

ImG DCM

C	-3.719237000	-0.493735000	-0.043542000
O	-3.716804000	0.789247000	0.846639000
O	-4.777020000	-0.818084000	-0.409206000
N	1.076705000	-0.353023000	-0.131252000
C	-1.307343000	-0.262747000	0.221185000
C	-0.180069000	-0.950341000	-0.517375000
O	-2.543606000	-0.919504000	-0.223261000
C	3.408601000	-0.835170000	0.528271000
C	2.195141000	-1.271157000	-0.266016000
O	4.390050000	-1.839072000	0.359329000
C	1.485094000	2.050658000	0.289078000
C	1.311184000	0.952043000	-0.741627000
O	1.687433000	3.261551000	-0.410589000
H	-4.638449000	1.040162000	1.047592000

H	-3.180218000	0.791985000	1.661596000
H	-1.381219000	0.795323000	-0.028013000
H	-1.214318000	-0.414518000	1.297078000
H	-0.180050000	-2.003738000	-0.232880000
H	-0.373742000	-0.898848000	-1.600403000
H	3.129881000	-0.720390000	1.583600000
H	3.780666000	0.132224000	0.169052000
H	2.491592000	-1.405459000	-1.319713000
H	1.886777000	-2.248842000	0.111869000
H	5.196714000	-1.552263000	0.794796000
H	2.336622000	1.820243000	0.940337000
H	0.591068000	2.103947000	0.925035000
H	0.475095000	1.221137000	-1.397142000
H	2.199368000	0.921427000	-1.384233000
H	1.862621000	3.958368000	0.227056000

Sum of electronic and zero-point Energies= -706.245414
Sum of electronic and thermal Energies= -706.229239
Sum of electronic and thermal Enthalpies= -706.228295
Sum of electronic and thermal Free Energies= -706.290470

ImG DMF

C	-3.719056000	-0.488050000	-0.038446000
O	-3.721069000	0.784590000	0.835550000
O	-4.772702000	-0.823689000	-0.411476000
N	1.077995000	-0.353815000	-0.129369000
C	-1.309141000	-0.257994000	0.222958000
C	-0.181256000	-0.950573000	-0.510152000
O	-2.542445000	-0.918342000	-0.218003000
C	3.407402000	-0.837981000	0.530266000
C	2.195311000	-1.271836000	-0.267147000
O	4.396705000	-1.833902000	0.351027000
C	1.475567000	2.051016000	0.289358000
C	1.311736000	0.950668000	-0.740958000
O	1.698650000	3.260121000	-0.409359000
H	-4.641737000	1.040627000	1.036674000
H	-3.179466000	0.797204000	1.647951000
H	-1.382616000	0.798363000	-0.033436000
H	-1.215648000	-0.400991000	1.299891000
H	-0.182470000	-2.002024000	-0.218661000
H	-0.374388000	-0.905735000	-1.593572000
H	3.129475000	-0.735927000	1.586850000
H	3.773868000	0.135093000	0.181155000
H	2.493027000	-1.401898000	-1.321312000
H	1.885800000	-2.250938000	0.106128000
H	5.197206000	-1.548994000	0.799159000
H	2.315273000	1.816859000	0.954666000
H	0.572129000	2.113038000	0.910009000
H	0.479540000	1.214970000	-1.403258000
H	2.205194000	0.921205000	-1.376469000
H	1.822377000	3.964109000	0.232618000

Sum of electronic and zero-point Energies= -706.254973
Sum of electronic and thermal Energies= -706.238845
Sum of electronic and thermal Enthalpies= -706.237900
Sum of electronic and thermal Free Energies= -706.300084

CO DCM

C	0.000000000	0.000000000	-0.641813000
O	0.000000000	0.000000000	0.481360000

Sum of electronic and zero-point Energies= -113.226422
Sum of electronic and thermal Energies= -113.224062
Sum of electronic and thermal Enthalpies= -113.223117
Sum of electronic and thermal Free Energies= -113.245536

CO DMF

C	0.000000000	0.000000000	-0.641790000
O	0.000000000	0.000000000	0.481342000

Sum of electronic and zero-point Energies= -113.226514
Sum of electronic and thermal Energies= -113.224153
Sum of electronic and thermal Enthalpies= -113.223209
Sum of electronic and thermal Free Energies= -113.245628

CO_2 DCM

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.156583000
O	0.000000000	0.000000000	-1.156583000

Sum of electronic and zero-point Energies= -188.456717
Sum of electronic and thermal Energies= -188.454108
Sum of electronic and thermal Enthalpies= -188.453164
Sum of electronic and thermal Free Energies= -188.477400

CO_2 DMF

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	1.156550000
O	0.000000000	0.000000000	-1.156550000

Sum of electronic and zero-point Energies= -188.457038
Sum of electronic and thermal Energies= -188.454427
Sum of electronic and thermal Enthalpies= -188.453483
Sum of electronic and thermal Free Energies= -188.477720

H DCM

H	0.000000000	0.000000000	0.000000000

Sum of electronic and zero-point Energies= -0.148025
Sum of electronic and thermal Energies= -0.146608
Sum of electronic and thermal Enthalpies= -0.145664
Sum of electronic and thermal Free Energies= -0.158024

H DMF

H	0.000000000	0.000000000	0.000000000

Sum of electronic and zero-point Energies= -0.162212
Sum of electronic and thermal Energies= -0.160796
Sum of electronic and thermal Enthalpies= -0.159852
Sum of electronic and thermal Free Energies= -0.172212

H_2O DCM

O	0.000000000	0.000000000	0.117524000
H	0.000000000	0.760075000	-0.470097000

H	0.000000000	-0.760075000	-0.470097000

Sum of electronic and zero-point Energies= -76.362241
Sum of electronic and thermal Energies= -76.359405
Sum of electronic and thermal Enthalpies= -76.358461
Sum of electronic and thermal Free Energies= -76.379881

H_2O DMF

O	0.000000000	0.000000000	0.117687000
H	0.000000000	0.759738000	-0.470747000
H	0.000000000	-0.759738000	-0.470747000

Sum of electronic and zero-point Energies= -76.363208
Sum of electronic and thermal Energies= -76.360372
Sum of electronic and thermal Enthalpies= -76.359428
Sum of electronic and thermal Free Energies= -76.380849

$TEOA^{\cdot+}$ DCM

N	0.028783000	-0.030698000	0.770576000
C	-0.804084000	-1.203546000	0.742418000
C	1.451126000	-0.170683000	0.787254000
C	-0.566687000	1.269744000	0.805942000
C	2.028901000	-0.672847000	-0.569047000
C	-1.662884000	-1.312245000	-0.520987000
O	-2.449933000	-2.454640000	-0.320921000
O	3.417667000	-0.724102000	-0.487974000
C	-0.378183000	2.063096000	-0.520759000
O	-0.918292000	3.337743000	-0.376013000
H	-0.177727000	-2.088893000	0.844937000
H	-1.478348000	-1.149795000	1.606131000
H	1.707226000	-0.906652000	1.556605000
H	1.906767000	0.786644000	1.035454000
H	-0.081067000	1.847017000	1.598253000
H	-1.628214000	1.167246000	1.029519000
H	1.774635000	0.043252000	-1.351402000
H	1.589130000	-1.640839000	-0.826505000
H	-1.018461000	-1.409401000	-1.402253000
H	-2.277877000	-0.412294000	-0.638457000
H	-2.996174000	-2.593295000	-1.099840000
H	3.687649000	-1.536061000	-0.047587000
H	-0.829263000	1.509709000	-1.349979000
H	0.687956000	2.183720000	-0.720031000
H	-1.872387000	3.301401000	-0.498533000

Sum of electronic and zero-point Energies= -517.246104
Sum of electronic and thermal Energies= -517.233075
Sum of electronic and thermal Enthalpies= -517.232131
Sum of electronic and thermal Free Energies= -517.286850

$TEOA^{\cdot+}$ DMF

N	0.017730000	-0.028689000	0.753728000
C	-0.910837000	-1.127864000	0.737031000
C	1.423447000	-0.289310000	0.779443000
C	-0.462908000	1.318675000	0.787979000
C	1.958194000	-0.864989000	-0.562303000
C	-1.779560000	-1.174989000	-0.521991000
O	-2.663580000	-2.244614000	-0.308956000

O	3.339409000	-1.029012000	-0.476552000
C	-0.185780000	2.101749000	-0.525412000
O	-0.584514000	3.428059000	-0.363167000
H	-0.358810000	-2.059938000	0.845297000
H	-1.574374000	-1.010202000	1.602165000
H	1.612650000	-1.029758000	1.563940000
H	1.958279000	0.629652000	1.014246000
H	0.059167000	1.845415000	1.592320000
H	-1.532315000	1.308557000	0.995313000
H	1.765322000	-0.149743000	-1.362482000
H	1.441506000	-1.799781000	-0.798919000
H	-1.150115000	-1.338801000	-1.403562000
H	-2.316174000	-0.227665000	-0.648116000
H	-3.205208000	-2.354060000	-1.096290000
H	3.538009000	-1.840346000	0.002263000
H	-0.695390000	1.614108000	-1.361697000
H	0.886435000	2.108224000	-0.726556000
H	-1.538956000	3.490064000	-0.473100000

Sum of electronic and zero-point Energies= -517.254596
Sum of electronic and thermal Energies= -517.241573
Sum of electronic and thermal Enthalpies= -517.240629
Sum of electronic and thermal Free Energies= -517.296349

TEOA DCM

N	-0.002830000	-0.002251000	0.086015000
C	0.297680000	1.358888000	0.494019000
C	-1.335957000	-0.424044000	0.478313000
C	1.021257000	-0.947794000	0.494393000
C	-2.397222000	0.054507000	-0.498115000
C	1.230805000	2.045802000	-0.480947000
O	1.545860000	3.320302000	0.048782000
O	-3.695957000	-0.349157000	-0.108422000
C	1.140790000	-2.112738000	-0.474460000
O	2.057773000	-3.090710000	-0.023633000
H	-0.631179000	1.932675000	0.536731000
H	0.737094000	1.396154000	1.504733000
H	-1.587792000	-0.077141000	1.496785000
H	-1.372295000	-1.515563000	0.506144000
H	0.841076000	-1.337174000	1.510334000
H	1.983459000	-0.427871000	0.525642000
H	-2.213703000	-0.392161000	-1.477812000
H	-2.345099000	1.144091000	-0.620453000
H	0.733081000	2.130491000	-1.454807000
H	2.140146000	1.447327000	-0.623163000
H	2.120636000	3.772918000	-0.573595000
H	-3.923879000	0.106804000	0.707009000
H	1.415505000	-1.732094000	-1.465931000
H	0.181463000	-2.625016000	-0.576726000
H	2.935772000	-2.698895000	-0.010031000

Sum of electronic and zero-point Energies= -517.454275
Sum of electronic and thermal Energies= -517.441384
Sum of electronic and thermal Enthalpies= -517.440440
Sum of electronic and thermal Free Energies= -517.494354

TEOA DMF

N	0.001850000	-0.011157000	0.078562000
C	-0.338154000	1.340064000	0.491274000
C	-1.005691000	-0.982126000	0.468614000
C	1.339132000	-0.400380000	0.492974000
C	-2.173269000	-1.014266000	-0.503343000
C	0.192492000	2.375383000	-0.477811000
O	-0.102025000	3.654992000	0.053073000
O	-3.176755000	-1.925861000	-0.097574000
C	1.971925000	-1.387627000	-0.473679000
O	3.231011000	-1.846928000	-0.019506000
H	-1.425483000	1.438657000	0.532146000
H	0.036436000	1.563654000	1.503964000
H	-1.381284000	-0.787469000	1.489190000
H	-0.555619000	-1.977314000	0.489148000
H	1.345319000	-0.830402000	1.508535000
H	1.968299000	0.493960000	0.528508000
H	-1.821822000	-1.354217000	-1.479912000
H	-2.590574000	-0.008419000	-0.637485000
H	-0.284537000	2.230486000	-1.454800000
H	1.274352000	2.250224000	-0.613568000
H	0.218480000	4.318693000	-0.562968000
H	-3.566146000	-1.600963000	0.719656000
H	2.048893000	-0.924368000	-1.464950000
H	1.346803000	-2.277733000	-0.576703000
H	3.837470000	-1.100603000	-0.006809000

Sum of electronic and zero-point Energies= -517.456379
Sum of electronic and thermal Energies= -517.443494
Sum of electronic and thermal Enthalpies= -517.442550
Sum of electronic and thermal Free Energies= -517.496382

TEOA$^{\cdot-}$ DCM

N	0.001079000	0.027259000	0.056844000
C	-0.387132000	1.376200000	0.461069000
C	-0.962233000	-0.976696000	0.462382000
C	1.348334000	-0.303491000	0.476233000
C	-2.126207000	-1.071373000	-0.509124000
C	0.100842000	2.510351000	-0.458565000
O	-0.232291000	3.731469000	-0.008210000
O	-3.121183000	-1.980124000	-0.067996000
C	2.022273000	-1.287609000	-0.464318000
O	3.306968000	-1.674085000	-0.006666000
H	-1.479860000	1.431264000	0.486020000
H	-0.040348000	1.592583000	1.488133000
H	-1.352786000	-0.777180000	1.478366000
H	-0.476769000	-1.955894000	0.506363000
H	1.376212000	-0.710421000	1.503509000
H	1.936727000	0.618651000	0.484300000
H	-1.769682000	-1.448185000	-1.470411000
H	-2.554030000	-0.077192000	-0.686073000
H	-0.312596000	2.250845000	-1.473684000
H	1.209088000	2.348814000	-0.591612000
H	-3.523777000	-1.616673000	0.726155000
H	2.072055000	-0.849275000	-1.468757000
H	1.442477000	-2.211035000	-0.538872000
H	3.862512000	-0.889485000	0.015566000

Sum of electronic and zero-point Energies= -516.942140
Sum of electronic and thermal Energies= -516.929943
Sum of electronic and thermal Enthalpies= -516.928999
Sum of electronic and thermal Free Energies= -516.981177

$TEOA^{\cdot-}$ DMF

N	0.000600000	0.031603000	0.060923000
C	-0.354435000	1.388063000	0.467712000
C	-0.986606000	-0.951471000	0.463652000
C	1.340315000	-0.333751000	0.479260000
C	-2.155103000	-1.014312000	-0.504836000
C	0.151663000	2.503520000	-0.463231000
O	-0.126913000	3.740449000	-0.009613000
O	-3.158869000	-1.918015000	-0.076049000
C	1.989466000	-1.327665000	-0.468678000
O	3.258494000	-1.759266000	-0.009150000
H	-1.445508000	1.466979000	0.505337000
H	0.008341000	1.598958000	1.490536000
H	-1.368002000	-0.748412000	1.482005000
H	-0.524361000	-1.941923000	0.499432000
H	1.356298000	-0.748324000	1.503181000
H	1.951781000	0.573111000	0.494817000
H	-1.805206000	-1.379007000	-1.473185000
H	-2.573013000	-0.012509000	-0.663043000
H	-0.293326000	2.259589000	-1.467665000
H	1.248778000	2.304509000	-0.619594000
H	-3.534872000	-1.579937000	0.742075000
H	2.059250000	-0.880159000	-1.467950000
H	1.380732000	-2.230891000	-0.556813000
H	3.841407000	-0.994846000	0.019631000

Sum of electronic and zero-point Energies= -516.953087
Sum of electronic and thermal Energies= -516.940805
Sum of electronic and thermal Enthalpies= -516.939861
Sum of electronic and thermal Free Energies= -516.992399

η^1-CO_2 complex mechanism

ImB'_M _Ru_DCM

Ru	-0.262420000	-0.000102000	0.026025000
C	-0.790336000	-1.595218000	0.867819000
C	-1.783151000	-0.056172000	-1.010086000
O	-2.727822000	-0.091313000	-1.667605000
N	1.619674000	0.062725000	1.166618000
C	-0.696938000	1.751305000	0.546549000
O	-1.086956000	2.755903000	0.974030000
O	-1.235140000	-2.474888000	1.477558000
C	2.747662000	0.376594000	0.273363000
C	2.642503000	-0.465953000	-0.974356000
N	1.351364000	-0.211721000	-1.620385000
H	1.780651000	-0.833263000	1.613540000
H	1.574896000	0.742384000	1.916835000
H	3.707741000	0.208282000	0.769371000
H	2.680133000	1.435769000	0.014458000
H	2.682085000	-1.525362000	-0.708533000
H	3.487950000	-0.256433000	-1.636773000
H	1.388307000	0.647206000	-2.156047000
H	1.128352000	-0.952065000	-2.273199000

Sum of electronic and zero-point Energies= -625.028848
Sum of electronic and thermal Energies= -625.016175
Sum of electronic and thermal Enthalpies= -625.015231
Sum of electronic and thermal Free Energies= -625.069555

ImB'_M _Ru_DMF

Ru	-0.262199000	0.000556000	0.029508000
C	-0.785947000	-1.598835000	0.865821000
C	-1.783122000	-0.054742000	-1.006104000
O	-2.728913000	-0.089281000	-1.662779000
N	1.621530000	0.062714000	1.164137000
C	-0.693185000	1.753233000	0.547685000
O	-1.082825000	2.760745000	0.970105000
O	-1.231529000	-2.483269000	1.468970000
C	2.747524000	0.375585000	0.267093000
C	2.636602000	-0.466902000	-0.979480000
N	1.341821000	-0.211677000	-1.619140000
H	1.785069000	-0.833222000	1.610403000
H	1.582444000	0.741701000	1.915344000
H	3.707955000	0.205183000	0.761164000
H	2.681205000	1.434886000	0.008777000
H	2.677502000	-1.526338000	-0.714480000
H	3.477505000	-0.256816000	-1.647061000
H	1.378271000	0.647750000	-2.154239000
H	1.118243000	-0.950471000	-2.273676000

Sum of electronic and zero-point Energies= -625.031376
Sum of electronic and thermal Energies= -625.018721
Sum of electronic and thermal Enthalpies= -625.017777
Sum of electronic and thermal Free Energies= -625.072074

ImB'_M_Os_DCM

Os	-0.214633000	0.002886000	0.026248000
C	-0.692414000	-1.614822000	0.885433000
C	-1.761456000	-0.075203000	-1.012984000
O	-2.710330000	-0.124112000	-1.668459000

N	1.701950000	0.090161000	1.133543000
C	-0.640651000	1.770162000	0.546099000
O	-1.008544000	2.789070000	0.972267000
O	-1.094377000	-2.513722000	1.505028000
C	2.823365000	0.381119000	0.220247000
C	2.682608000	-0.471122000	-1.016215000
N	1.370140000	-0.216613000	-1.624824000
H	1.870790000	-0.792060000	1.605177000
H	1.668092000	0.790218000	1.866023000
H	3.785729000	0.200523000	0.705425000
H	2.767204000	1.439121000	-0.044937000
H	2.726406000	-1.529034000	-0.746924000
H	3.502115000	-0.264831000	-1.709868000
H	1.397289000	0.634913000	-2.173610000
H	1.127140000	-0.963747000	-2.263320000

Sum of electronic and zero-point Energies= -620.829080
Sum of electronic and thermal Energies= -620.816638
Sum of electronic and thermal Enthalpies= -620.815694
Sum of electronic and thermal Free Energies= -620.869977

ImB'_M_Os_DMF

Os	0.214233000	0.002944000	-0.029241000
C	0.692571000	-1.620416000	-0.876961000
C	1.760267000	-0.068230000	1.011481000
O	2.709513000	-0.112729000	1.667506000
N	-1.703735000	0.081059000	-1.131521000
C	0.633910000	1.770988000	-0.551523000
O	1.002096000	2.791303000	-0.975627000
O	1.098452000	-2.524795000	-1.487104000
C	-2.823644000	0.376053000	-0.216579000
C	-2.677055000	-0.468786000	1.023577000
N	-1.361130000	-0.209093000	1.624199000
H	-1.874444000	-0.804350000	-1.596647000
H	-1.676260000	0.775631000	-1.869543000
H	-3.786032000	0.190301000	-0.699179000
H	-2.768930000	1.435696000	0.041814000
H	-2.721620000	-1.528293000	0.761362000
H	-3.491721000	-0.258252000	1.721197000
H	-1.388683000	0.645356000	2.168608000
H	-1.116736000	-0.951511000	2.267837000

Sum of electronic and zero-point Energies= -620.832112
Sum of electronic and thermal Energies= -620.819692
Sum of electronic and thermal Enthalpies= -620.818748
Sum of electronic and thermal Free Energies= -620.872981

ImC'_M_Ru_DCM

Ru	-0.307618000	0.141562000	-0.007636000
O	1.235694000	-2.018924000	1.241845000
O	0.785719000	-2.421742000	-0.917389000
C	0.708432000	-1.778346000	0.138787000
C	-1.077569000	1.970883000	-0.159448000
C	-1.416094000	-0.433233000	1.387179000
O	-2.075794000	-0.800863000	2.240789000
N	1.282709000	0.439131000	-1.457245000
C	-1.488175000	-0.649492000	-1.237821000
O	-2.191345000	-1.145795000	-1.982286000
O	-1.647547000	2.951605000	-0.208008000
C	2.573950000	0.594433000	-0.753759000
C	2.367187000	1.381049000	0.517276000

N	1.293642000	0.743040000	1.296386000
H	1.120082000	1.219044000	-2.084049000
H	1.302380000	-0.412232000	-2.013856000
H	3.314166000	1.080751000	-1.392184000
H	2.937104000	-0.406630000	-0.515888000
H	2.059951000	2.403855000	0.287826000
H	3.298082000	1.428193000	1.088320000
H	1.582955000	-0.174006000	1.661870000
H	1.025828000	1.331085000	2.077080000

Sum of electronic and zero-point Energies= -813.490106
Sum of electronic and thermal Energies= -813.474694
Sum of electronic and thermal Enthalpies= -813.473750
Sum of electronic and thermal Free Energies= -813.533728

ImC'_M_Ru_DMF

Ru	-0.300983000	0.144557000	-0.006525000
O	1.198324000	-2.053879000	1.228787000
O	0.696053000	-2.461039000	-0.915435000
C	0.658723000	-1.797979000	0.132800000
C	-1.030614000	1.993530000	-0.148055000
C	-1.419767000	-0.404035000	1.390305000
O	-2.084928000	-0.758600000	2.245316000
N	1.286840000	0.427192000	-1.459911000
C	-1.503808000	-0.606727000	-1.239807000
O	-2.220063000	-1.081340000	-1.986039000
O	-1.571458000	2.989947000	-0.191871000
C	2.584218000	0.549561000	-0.760917000
C	2.397591000	1.332819000	0.514701000
N	1.314060000	0.710694000	1.293697000
H	1.134668000	1.223615000	-2.068797000
H	1.293211000	-0.407490000	-2.040274000
H	3.331472000	1.023890000	-1.399844000
H	2.926861000	-0.460328000	-0.530199000
H	2.110039000	2.362812000	0.292676000
H	3.330363000	1.358106000	1.083635000
H	1.589691000	-0.211090000	1.656051000
H	1.059156000	1.301026000	2.077134000

Sum of electronic and zero-point Energies= -813.493879
Sum of electronic and thermal Energies= -813.478490
Sum of electronic and thermal Enthalpies= -813.477546
Sum of electronic and thermal Free Energies= -813.537544

ImC'_M_Os_DCM

Os	-0.267028000	0.095143000	-0.004838000
O	1.486972000	-1.938773000	1.246594000
O	1.005587000	-2.431324000	-0.882579000
C	0.896751000	-1.753333000	0.155508000
C	-1.117306000	1.878004000	-0.174571000
C	-1.377662000	-0.492705000	1.409856000
O	-2.028448000	-0.869049000	2.269277000
N	1.315738000	0.467972000	-1.459368000
C	-1.428574000	-0.756674000	-1.243294000
O	-2.108035000	-1.289628000	-1.987716000
O	-1.689039000	2.860086000	-0.239907000
C	2.605582000	0.701818000	-0.767201000
C	2.364662000	1.474673000	0.506052000
N	1.323055000	0.781904000	1.285875000
H	1.113577000	1.225495000	-2.102610000
H	1.383792000	-0.391065000	-2.002625000

H	3.303164000	1.232453000	-1.416742000
H	3.030051000	-0.275760000	-0.535273000
H	2.010620000	2.483401000	0.283377000
H	3.291810000	1.558366000	1.077621000
H	1.659644000	-0.128674000	1.644544000
H	1.032888000	1.354551000	2.070421000

Sum of electronic and zero-point Energies= -809.299575
Sum of electronic and thermal Energies= -809.284422
Sum of electronic and thermal Enthalpies= -809.283478
Sum of electronic and thermal Free Energies= -809.343349

ImC'_M_Os_DMF

Os	-0.260975000	0.098570000	-0.004355000
O	1.467923000	-1.971467000	1.222715000
O	0.892170000	-2.497107000	-0.871828000
C	0.846670000	-1.782002000	0.147008000
C	-1.074441000	1.901952000	-0.153289000
C	-1.377755000	-0.469899000	1.412717000
O	-2.032671000	-0.836468000	2.273460000
N	1.315273000	0.468325000	-1.466831000
C	-1.450587000	-0.709394000	-1.245423000
O	-2.147184000	-1.217526000	-1.991566000
O	-1.622187000	2.897684000	-0.202817000
C	2.615741000	0.662507000	-0.782106000
C	2.399088000	1.427123000	0.499789000
N	1.348917000	0.746543000	1.279483000
H	1.119078000	1.252298000	-2.080098000
H	1.368346000	-0.364038000	-2.049372000
H	3.320238000	1.184043000	-1.431309000
H	3.018655000	-0.327105000	-0.563519000
H	2.064053000	2.444760000	0.289447000
H	3.330737000	1.486437000	1.066652000
H	1.672621000	-0.172369000	1.628136000
H	1.074327000	1.317897000	2.070628000

Sum of electronic and zero-point Energies= -809.303941
Sum of electronic and thermal Energies= -809.288739
Sum of electronic and thermal Enthalpies= -809.287795
Sum of electronic and thermal Free Energies= -809.348102

ImD'_M_Ru_DCM

Ru	-0.245316000	0.174005000	-0.017960000
O	0.674796000	-2.453066000	-0.999785000
C	0.222828000	-1.864172000	-0.043804000
C	-0.582012000	2.133593000	-0.065651000
C	-1.597276000	-0.121907000	1.276995000
O	-2.397228000	-0.314710000	2.053669000
N	1.452272000	0.284358000	-1.336501000
C	-1.482681000	-0.170812000	-1.409730000
O	-2.209078000	-0.399628000	-2.246435000
O	-0.822234000	3.235133000	-0.098446000
C	2.709367000	0.208600000	-0.555558000
C	2.536265000	0.934410000	0.753018000
N	1.333567000	0.403322000	1.431425000
H	1.452363000	1.107084000	-1.930567000
H	1.394356000	-0.530229000	-1.945457000
H	3.542799000	0.626184000	-1.121986000
H	2.920419000	-0.847081000	-0.378335000
H	2.382190000	2.001939000	0.586587000
H	3.421344000	0.814190000	1.380539000

H	1.535551000	-0.502301000	1.847950000
H	1.081514000	1.009590000	2.205820000
O	0.051701000	-2.498482000	1.131801000
H	0.339902000	-3.421606000	1.023190000

Sum of electronic and zero-point Energies= -813.931409
Sum of electronic and thermal Energies= -813.915901
Sum of electronic and thermal Enthalpies= -813.914957
Sum of electronic and thermal Free Energies= -813.974995

ImD'_M_Ru_DMF

Ru	0.245341000	0.173071000	0.017770000
O	-0.655092000	-2.460829000	1.006272000
C	-0.222241000	-1.864932000	0.045199000
C	0.582857000	2.133067000	0.061046000
C	1.592973000	-0.124381000	-1.280345000
O	2.390957000	-0.319754000	-2.058909000
N	-1.447645000	0.290460000	1.340274000
C	1.485291000	-0.168725000	1.407089000
O	2.213866000	-0.396817000	2.242605000
O	0.824928000	3.234215000	0.090687000
C	-2.707031000	0.211951000	0.563382000
C	-2.537070000	0.935069000	-0.746812000
N	-1.336018000	0.402600000	-1.426946000
H	-1.444383000	1.118786000	1.926615000
H	-1.391293000	-0.516562000	1.958699000
H	-3.538265000	0.631232000	1.131596000
H	-2.918529000	-0.844055000	0.389040000
H	-2.382868000	2.002802000	-0.582717000
H	-3.423063000	0.812957000	-1.372415000
H	-1.540189000	-0.502420000	-1.843657000
H	-1.085016000	1.008695000	-2.201812000
O	-0.073359000	-2.493637000	-1.136809000
H	-0.364834000	-3.415703000	-1.028665000

Sum of electronic and zero-point Energies= -813.939269
Sum of electronic and thermal Energies= -813.923762
Sum of electronic and thermal Enthalpies= -813.922818
Sum of electronic and thermal Free Energies= -813.982851

ImD'_M_Os_DCM

Os	-0.227439000	0.110715000	-0.013298000
O	1.151577000	-2.341500000	-1.001592000
C	0.589581000	-1.849060000	-0.046059000
C	-0.869819000	1.987632000	-0.059578000
C	-1.531808000	-0.383525000	1.291594000
O	-2.292664000	-0.694555000	2.073482000
N	1.455671000	0.482402000	-1.330212000
C	-1.418841000	-0.409777000	-1.411997000
O	-2.110261000	-0.737319000	-2.249359000
O	-1.276652000	3.042513000	-0.093881000
C	2.714710000	0.595590000	-0.552424000
C	2.438565000	1.288879000	0.755560000
N	1.323651000	0.586652000	1.434367000
H	1.333608000	1.295676000	-1.925237000
H	1.525654000	-0.331932000	-1.940066000
H	3.471709000	1.133196000	-1.123891000
H	3.081122000	-0.416713000	-0.376619000
H	2.130800000	2.322738000	0.591226000
H	3.329600000	1.295351000	1.384862000
H	1.661098000	-0.274419000	1.858967000

H	0.985418000	1.154089000	2.205874000
O	0.506900000	-2.527457000	1.114997000
H	0.945558000	-3.387577000	0.994711000

Sum of electronic and zero-point Energies= -809.744471
Sum of electronic and thermal Energies= -809.729026
Sum of electronic and thermal Enthalpies= -809.728082
Sum of electronic and thermal Free Energies= -809.788718

ImD'_M_Os_DMF

Os	-0.229683000	-0.106810000	0.012668000
O	1.157052000	2.337719000	1.016695000
C	0.620604000	1.838044000	0.050067000
C	-0.906989000	-1.972052000	0.052235000
C	-1.516563000	0.412382000	-1.298675000
O	-2.267780000	0.739539000	-2.083885000
N	1.437031000	-0.517168000	1.338005000
C	-1.418752000	0.431951000	1.405396000
O	-2.108859000	0.771515000	2.239618000
O	-1.334802000	-3.018641000	0.082043000
C	2.699703000	-0.638092000	0.567556000
C	2.423152000	-1.324173000	-0.743685000
N	1.320169000	-0.607158000	-1.426406000
H	1.297922000	-1.339696000	1.916543000
H	1.516150000	0.281069000	1.966687000
H	3.447736000	-1.185129000	1.141658000
H	3.076513000	0.371230000	0.396994000
H	2.103409000	-2.354972000	-0.584008000
H	3.317020000	-1.337976000	-1.368510000
H	1.671327000	0.248916000	-1.849966000
H	0.977805000	-1.170293000	-2.199228000
O	0.591178000	2.499326000	-1.124218000
H	1.046374000	3.350644000	-1.003520000

Sum of electronic and zero-point Energies= -809.752565
Sum of electronic and thermal Energies= -809.737098
Sum of electronic and thermal Enthalpies= -809.736154
Sum of electronic and thermal Free Energies= -809.796821

ImE'_M_Ru_DCM

Ru	0.191982000	-0.198598000	-0.009690000
O	0.726902000	2.728080000	-0.859808000
C	0.226571000	1.894460000	-0.015432000
C	0.125163000	-2.171330000	0.103419000
C	1.438287000	-0.139181000	1.440557000
O	2.163878000	-0.096910000	2.300650000
N	-1.376660000	-0.208043000	-1.498341000
C	1.627622000	-0.337688000	-1.266075000
O	2.470723000	-0.445579000	-2.006652000
O	0.116666000	-3.291198000	0.183844000
C	-2.649136000	0.235480000	-0.878177000
C	-2.762555000	-0.386060000	0.487218000
N	-1.538278000	-0.064332000	1.259900000
O	-0.303284000	2.489164000	0.997676000
H	1.135185000	2.320981000	-1.636262000
H	-1.494516000	-1.145926000	-1.872914000
H	-1.179553000	0.367624000	-2.312034000
H	-3.496898000	-0.046066000	-1.504146000
H	-2.628393000	1.323995000	-0.809603000
H	-2.841832000	-1.471729000	0.412925000

H	-3.648120000	-0.020275000	1.008354000
H	-1.604224000	0.880526000	1.631929000
H	-1.481848000	-0.669800000	2.074087000
H	-0.237233000	3.463077000	0.948349000

Sum of electronic and zero-point Energies= -814.301027
Sum of electronic and thermal Energies= -814.285719
Sum of electronic and thermal Enthalpies= -814.284775
Sum of electronic and thermal Free Energies= -814.343647

ImE'_M_Ru_DMF

Ru	0.194085000	-0.195844000	-0.008963000
O	0.699479000	2.735807000	-0.860905000
C	0.203779000	1.897526000	-0.018838000
C	0.150856000	-2.167851000	0.111930000
C	1.440336000	-0.115435000	1.438554000
O	2.167822000	-0.060562000	2.296967000
N	-1.371593000	-0.226760000	-1.497903000
C	1.627752000	-0.325609000	-1.267317000
O	2.470076000	-0.431180000	-2.009547000
O	0.158708000	-3.287592000	0.198186000
C	-2.651038000	0.198496000	-0.880404000
C	-2.755940000	-0.419305000	0.487240000
N	-1.537173000	-0.076328000	1.258608000
O	-0.339353000	2.486114000	0.990484000
H	1.114336000	2.331557000	-1.635328000
H	-1.474674000	-1.165988000	-1.872947000
H	-1.180614000	0.352187000	-2.310663000
H	-3.493112000	-0.099715000	-1.506139000
H	-2.647820000	1.287286000	-0.815922000
H	-2.819475000	-1.506099000	0.417231000
H	-3.646406000	-0.063498000	1.006798000
H	-1.616173000	0.870141000	1.623753000
H	-1.472443000	-0.675232000	2.076882000
H	-0.290358000	3.460485000	0.937306000

Sum of electronic and zero-point Energies= -814.325467
Sum of electronic and thermal Energies= -814.310227
Sum of electronic and thermal Enthalpies= -814.309282
Sum of electronic and thermal Free Energies= -814.367900

ImE'_M_Os_DCM

Os	0.182884000	-0.140175000	-0.006466000
O	0.316973000	2.848193000	-0.828032000
C	-0.095637000	1.955343000	0.004012000
C	0.406312000	-2.109617000	0.071144000
C	1.421300000	0.064441000	1.454797000
O	2.136258000	0.189369000	2.319462000
N	-1.398346000	-0.339220000	-1.500846000
C	1.641180000	-0.049726000	-1.258382000
O	2.498014000	-0.012435000	-1.995099000
O	0.565087000	-3.222104000	0.128606000
C	-2.728394000	-0.118959000	-0.873629000
C	-2.740637000	-0.764525000	0.484852000
N	-1.577270000	-0.261000000	1.258601000
O	-0.748626000	2.468594000	0.989840000
H	0.810816000	2.490075000	-1.579252000
H	-1.376820000	-1.263334000	-1.925181000
H	-1.295954000	0.299489000	-2.285307000
H	-3.516412000	-0.528546000	-1.505913000
H	-2.886972000	0.957503000	-0.792614000

H	-2.652485000	-1.849081000	0.404705000
H	-3.669465000	-0.540770000	1.010373000
H	-1.791690000	0.662543000	1.630534000
H	-1.439008000	-0.849491000	2.076243000
H	-0.818278000	3.441793000	0.938593000

Sum of electronic and zero-point Energies= -810.115462
Sum of electronic and thermal Energies= -810.100157
Sum of electronic and thermal Enthalpies= -810.099213
Sum of electronic and thermal Free Energies= -810.158833

ImE'_M_Os_DMF

Os	0.186132000	-0.135870000	-0.006498000
O	0.254377000	2.856256000	-0.821284000
C	-0.144556000	1.952751000	0.005397000
C	0.456927000	-2.097941000	0.072548000
C	1.418170000	0.098268000	1.453970000
O	2.130986000	0.240316000	2.318498000
N	-1.387877000	-0.368906000	-1.501268000
C	1.641512000	-0.012125000	-1.258583000
O	2.498430000	0.041983000	-1.994612000
O	0.645908000	-3.205915000	0.132892000
C	-2.723125000	-0.181803000	-0.875630000
C	-2.720876000	-0.829298000	0.481706000
N	-1.570558000	-0.299014000	1.256290000
O	-0.818872000	2.446978000	0.986146000
H	0.761424000	2.508527000	-1.568531000
H	-1.344346000	-1.290819000	-1.928310000
H	-1.299157000	0.274526000	-2.283325000
H	-3.499436000	-0.610324000	-1.509594000
H	-2.908298000	0.890024000	-0.793197000
H	-2.606201000	-1.911033000	0.399553000
H	-3.654456000	-0.627585000	1.007535000
H	-1.806747000	0.619145000	1.627927000
H	-1.419158000	-0.884535000	2.073549000
H	-0.915565000	3.417561000	0.933485000

Sum of electronic and zero-point Energies= -810.140078
Sum of electronic and thermal Energies= -810.124815
Sum of electronic and thermal Enthalpies= -810.123871
Sum of electronic and thermal Free Energies= -810.183266

TS'_Ru_DCM

Ru	0.092638000	-0.260729000	-0.006567000
O	2.156114000	2.110545000	-0.125442000
C	0.819629000	1.660785000	0.031157000
C	-0.687872000	-2.081194000	0.044853000
C	1.310120000	-0.722631000	1.399370000
O	2.021179000	-0.984344000	2.231988000
N	-1.385743000	0.372801000	-1.446805000
C	1.346659000	-0.835444000	-1.334535000
O	2.070970000	-1.181465000	-2.125030000
O	-1.101129000	-3.123847000	0.083822000
C	-2.442110000	1.169588000	-0.771513000
C	-2.723546000	0.563762000	0.575933000
N	-1.443445000	0.451418000	1.317671000
O	0.269615000	2.724149000	0.318358000
H	2.694549000	1.839223000	-0.891601000
H	-1.808167000	-0.431778000	-1.901866000
H	-0.983731000	0.919159000	-2.203676000

H	-3.344188000	1.196366000	-1.383293000
H	-2.074664000	2.189797000	-0.663125000
H	-3.149395000	-0.435634000	0.476715000
H	-3.432805000	1.176299000	1.134392000
H	-1.185659000	1.367625000	1.678468000
H	-1.574566000	-0.136142000	2.136783000
H	1.515594000	3.128148000	0.068952000

Sum of electronic and zero-point Energies= -814.239802
Sum of electronic and thermal Energies= -814.224233
Sum of electronic and thermal Enthalpies= -814.223289
Sum of electronic and thermal Free Energies= -814.282990

TS'_Ru_DMF

Ru	0.095991000	-0.260387000	-0.005333000
O	2.121019000	2.140526000	-0.145776000
C	0.795434000	1.671361000	0.033624000
C	-0.660020000	-2.089904000	0.047066000
C	1.316540000	-0.701773000	1.402748000
O	2.030825000	-0.951506000	2.236851000
N	-1.383970000	0.352861000	-1.449733000
C	1.358683000	-0.821913000	-1.330393000
O	2.086545000	-1.164356000	-2.119489000
O	-1.059392000	-3.138207000	0.087661000
C	-2.448676000	1.141300000	-0.779364000
C	-2.729278000	0.534620000	0.567759000
N	-1.451141000	0.433056000	1.313565000
O	0.234830000	2.724686000	0.338086000
H	2.640400000	1.884005000	-0.929791000
H	-1.796702000	-0.457500000	-1.902932000
H	-0.983996000	0.900123000	-2.206880000
H	-3.348840000	1.159257000	-1.394053000
H	-2.090193000	2.164620000	-0.670870000
H	-3.146607000	-0.468055000	0.467644000
H	-3.444650000	1.142063000	1.123735000
H	-1.203156000	1.350539000	1.677670000
H	-1.579025000	-0.158234000	2.130278000
H	1.468248000	3.147483000	0.065725000

Sum of electronic and zero-point Energies= -814.264357
Sum of electronic and thermal Energies= -814.248809
Sum of electronic and thermal Enthalpies= -814.247865
Sum of electronic and thermal Free Energies= -814.307526

TS'_Os_DCM

Os	0.102963000	-0.206754000	-0.006647000
O	1.899098000	2.399827000	-0.090488000
C	0.618689000	1.806612000	0.039137000
C	-0.494324000	-2.101461000	0.040815000
C	1.381120000	-0.566159000	1.391355000
O	2.124572000	-0.769693000	2.215968000
N	-1.460725000	0.293907000	-1.440597000
C	1.417626000	-0.651416000	-1.343670000
O	2.175802000	-0.919537000	-2.137043000
O	-0.805534000	-3.181471000	0.080648000
C	-2.605208000	0.956131000	-0.757579000
C	-2.807088000	0.315875000	0.588704000
N	-1.516499000	0.354404000	1.323785000
O	-0.053081000	2.806017000	0.302488000
H	2.489025000	2.176693000	-0.834004000
H	-1.791998000	-0.539525000	-1.919260000

H	-1.122819000	0.898807000	-2.184465000
H	-3.504376000	0.875113000	-1.368001000
H	-2.362040000	2.012997000	-0.647123000
H	-3.107908000	-0.728528000	0.490641000
H	-3.578883000	0.839169000	1.153970000
H	-1.365816000	1.296186000	1.680921000
H	-1.581039000	-0.236927000	2.148181000
H	1.149510000	3.342487000	0.076824000

Sum of electronic and zero-point Energies= -810.054100
Sum of electronic and thermal Energies= -810.038614
Sum of electronic and thermal Enthalpies= -810.037670
Sum of electronic and thermal Free Energies= -810.098048

TS'_Os_DMF

Os	0.102963000	-0.206754000	-0.006647000
O	1.899098000	2.399827000	-0.090488000
C	0.618689000	1.806612000	0.039137000
C	-0.494324000	-2.101461000	0.040815000
C	1.381120000	-0.566159000	1.391355000
O	2.124572000	-0.769693000	2.215968000
N	-1.460725000	0.293907000	-1.440597000
C	1.417626000	-0.651416000	-1.343670000
O	2.175802000	-0.919537000	-2.137043000
O	-0.805534000	-3.181471000	0.080648000
C	-2.605208000	0.956131000	-0.757579000
C	-2.807088000	0.315875000	0.588704000
N	-1.516499000	0.354404000	1.323785000
O	-0.053081000	2.806017000	0.302488000
H	2.489025000	2.176693000	-0.834004000
H	-1.791998000	-0.539525000	-1.919260000
H	-1.122819000	0.898807000	-2.184465000
H	-3.504376000	0.875113000	-1.368001000
H	-2.362040000	2.012997000	-0.647123000
H	-3.107908000	-0.728528000	0.490641000
H	-3.578883000	0.839169000	1.153970000
H	-1.365816000	1.296186000	1.680921000
H	-1.581039000	-0.236927000	2.148181000
H	1.149510000	3.342487000	0.076824000

Sum of electronic and zero-point Energies= -810.078845
Sum of electronic and thermal Energies= -810.063370
Sum of electronic and thermal Enthalpies= -810.062426
Sum of electronic and thermal Free Energies= -810.122750

ImF'_M_Ru_DCM

Ru	-0.198351000	0.000000000	0.000000000
C	-0.208886000	1.980286000	-0.118279000
C	-1.551906000	0.079866000	1.380220000
O	-2.330020000	0.124263000	2.187746000
N	1.446562000	-0.082825000	-1.382697000
C	-1.551895000	-0.079847000	-1.380240000
O	-2.330001000	-0.124262000	-2.187771000
O	-0.244004000	3.096628000	-0.188639000
C	2.704555000	-0.379796000	-0.649084000
C	2.704559000	0.379797000	0.649076000
N	1.446572000	0.082819000	1.382693000
H	1.543334000	0.799387000	-1.879205000
H	1.311436000	-0.775496000	-2.115197000
H	3.566614000	-0.105611000	-1.258180000
H	2.745946000	-1.455818000	-0.474865000

H	2.745942000	1.455819000	0.474853000
H	3.566621000	0.105620000	1.258169000
H	1.543348000	-0.799403000	1.879180000
H	1.311453000	0.775479000	2.115206000
C	-0.208936000	-1.980290000	0.118284000
O	-0.243990000	-3.096631000	0.188691000

Sum of electronic and zero-point Energies= -737.939135
Sum of electronic and thermal Energies= -737.924980
Sum of electronic and thermal Enthalpies= -737.924036
Sum of electronic and thermal Free Energies= -737.980447

ImF'_M_Ru_DMF

Ru	-0.198146000	0.000000000	0.000000000
C	-0.208129000	1.979740000	-0.115007000
C	-1.550679000	0.077302000	1.379985000
O	-2.329407000	0.120194000	2.187476000
N	1.445126000	-0.078729000	-1.382216000
C	-1.550666000	-0.077288000	-1.380005000
O	-2.329389000	-0.120209000	-2.187500000
O	-0.244183000	3.096289000	-0.183682000
C	2.703867000	-0.376274000	-0.651066000
C	2.703871000	0.376283000	0.651055000
N	1.445139000	0.078733000	1.382211000
H	1.539654000	0.804506000	-1.877016000
H	1.309560000	-0.769934000	-2.115808000
H	3.564150000	-0.095959000	-1.259644000
H	2.748135000	-1.452929000	-0.482928000
H	2.748134000	1.452938000	0.482912000
H	3.564159000	0.095976000	1.259629000
H	1.539672000	-0.804510000	1.876995000
H	1.309578000	0.769930000	2.115812000
C	-0.208173000	-1.979744000	0.115006000
O	-0.244145000	-3.096292000	0.183739000

Sum of electronic and zero-point Energies= -737.964344
Sum of electronic and thermal Energies= -737.950241
Sum of electronic and thermal Enthalpies= -737.949297
Sum of electronic and thermal Free Energies= -738.005566

ImF'_M_Os_DCM

Os	-0.162361000	0.000009000	-0.000001000
C	-0.177226000	1.994492000	-0.112286000
C	-1.527578000	0.075282000	1.382852000
O	-2.309199000	0.117489000	2.190909000
N	1.510552000	-0.075188000	-1.382775000
C	-1.527640000	-0.074834000	-1.382822000
O	-2.309197000	-0.116721000	-2.190956000
O	-0.220606000	3.112410000	-0.178884000
C	2.772239000	-0.375290000	-0.651986000
C	2.772255000	0.374629000	0.652051000
N	1.510499000	0.074699000	1.382788000
H	1.611550000	0.807381000	-1.878626000
H	1.377956000	-0.765263000	-2.118851000
H	3.631152000	-0.092527000	-1.260783000
H	2.816633000	-1.452694000	-0.487584000
H	2.816794000	1.452028000	0.487653000
H	3.631105000	0.091758000	1.260886000
H	1.611312000	-0.807943000	1.878550000
H	1.378020000	0.764737000	2.118923000
C	-0.177932000	-1.994449000	0.112748000

O	-0.221890000	-3.112393000	0.178493000

Sum of electronic and zero-point Energies= -733.752683
Sum of electronic and thermal Energies= -733.738725
Sum of electronic and thermal Enthalpies= -733.737780
Sum of electronic and thermal Free Energies= -733.794238

ImF'_M_Os_DMF

Os	-0.162228000	-0.000005000	-0.000008000
C	-0.176936000	-1.994035000	0.109101000
C	-1.526710000	-0.072586000	-1.382493000
O	-2.308425000	-0.113464000	-2.191195000
N	1.508878000	0.071281000	1.382221000
C	-1.526815000	0.072305000	1.382400000
O	-2.308393000	0.113052000	2.191239000
O	-0.219938000	-3.112166000	0.174279000
C	2.770952000	0.371965000	0.653663000
C	2.770961000	-0.371620000	-0.653688000
N	1.508869000	-0.070989000	-1.382237000
H	1.608052000	-0.812217000	1.876372000
H	1.375664000	0.759922000	2.119269000
H	3.628275000	0.083811000	1.261906000
H	2.817824000	1.449840000	0.494610000
H	2.817874000	-1.449494000	-0.494639000
H	3.628267000	-0.083429000	-1.261936000
H	1.607960000	0.812560000	-1.876317000
H	1.375722000	-0.759592000	-2.119333000
C	-0.177375000	1.993999000	-0.109545000
O	-0.220620000	3.112174000	-0.173807000

Sum of electronic and zero-point Energies= -733.778043
Sum of electronic and thermal Energies= -733.764131
Sum of electronic and thermal Enthalpies= -733.763186
Sum of electronic and thermal Free Energies= -733.819523

ImG'_M_Ru_DCM

Ru	-0.287175000	-0.000597000	-0.009731000
C	-0.246372000	-1.943803000	0.192476000
C	-1.552730000	-0.115985000	-1.445502000
O	-2.487702000	-0.169719000	-2.093224000
N	1.710766000	0.137844000	1.393607000
C	-1.524409000	0.108046000	1.413022000
O	-2.354151000	0.167372000	2.188662000
O	-0.229091000	-3.070042000	0.287335000
C	2.887686000	0.404259000	0.564546000
C	2.806852000	-0.426357000	-0.694754000
N	1.555946000	-0.120183000	-1.405194000
H	1.817280000	-0.734664000	1.900419000
H	1.583743000	0.859754000	2.093185000
H	3.821070000	0.189076000	1.091920000
H	2.892630000	1.466951000	0.310243000
H	2.800167000	-1.489409000	-0.443477000
H	3.678096000	-0.240307000	-1.327382000
H	1.647399000	0.760663000	-1.901907000
H	1.377733000	-0.817013000	-2.120185000
C	-0.257488000	1.951062000	-0.116662000
O	-0.245383000	3.077920000	-0.204311000

Sum of electronic and zero-point Energies= -738.106921
Sum of electronic and thermal Energies= -738.091247
Sum of electronic and thermal Enthalpies= -738.090303

Sum of electronic and thermal Free Energies= -738.151304

ImG'_M_Ru_DMF

Ru	-0.285484000	-0.000661000	-0.009695000
C	-0.244994000	-1.944114000	0.190356000
C	-1.549016000	-0.115429000	-1.445848000
O	-2.487908000	-0.168753000	-2.089392000
N	1.705939000	0.137148000	1.392760000
C	-1.522593000	0.106527000	1.411389000
O	-2.353848000	0.165093000	2.186279000
O	-0.229932000	-3.070510000	0.284143000
C	2.884716000	0.404374000	0.566491000
C	2.805956000	-0.424635000	-0.693798000
N	1.555142000	-0.118514000	-1.404104000
H	1.811842000	-0.735709000	1.898998000
H	1.577816000	0.858425000	2.092729000
H	3.816199000	0.187392000	1.096330000
H	2.890696000	1.467295000	0.313587000
H	2.800553000	-1.487987000	-0.444169000
H	3.676705000	-0.235900000	-1.326161000
H	1.646535000	0.762773000	-1.899986000
H	1.377408000	-0.814647000	-2.119860000
C	-0.257611000	1.951045000	-0.116072000
O	-0.248662000	3.077972000	-0.203602000

Sum of electronic and zero-point Energies= -738.114305
Sum of electronic and thermal Energies= -738.098657
Sum of electronic and thermal Enthalpies= -738.097712
Sum of electronic and thermal Free Energies= -738.158623

ImG'_M_Os_DCM

Os	-0.228784000	0.000008000	-0.000004000
C	-0.177858000	1.967393000	-0.128869000
C	-1.496142000	0.090479000	1.410402000
O	-2.343258000	0.139048000	2.172715000
N	1.642339000	-0.092201000	-1.386452000
C	-1.496129000	-0.090379000	-1.410422000
O	-2.343278000	-0.138918000	-2.172699000
O	-0.142561000	3.102033000	-0.204649000
C	2.876070000	-0.395374000	-0.642926000
C	2.876105000	0.395194000	0.642923000
N	1.642362000	0.092100000	1.386456000
H	1.735549000	0.794906000	-1.873029000
H	1.484912000	-0.785004000	-2.110878000
H	3.764696000	-0.163815000	-1.233587000
H	2.887765000	-1.466317000	-0.429787000
H	2.887867000	1.466135000	0.429783000
H	3.764724000	0.163580000	1.233575000
H	1.735518000	-0.795014000	1.873032000
H	1.484981000	0.784914000	2.110881000
C	-0.177960000	-1.967379000	0.128871000
O	-0.142881000	-3.102023000	0.204680000

Sum of electronic and zero-point Energies= -733.913577
Sum of electronic and thermal Energies= -733.898364
Sum of electronic and thermal Enthalpies= -733.897420
Sum of electronic and thermal Free Energies= -733.957541

ImG'_M_Os_DMF

Os	-0.227610000	0.000007000	-0.000003000
C	-0.177833000	1.967586000	-0.126319000
C	-1.493715000	0.088181000	1.410364000
O	-2.341523000	0.135331000	2.173175000
N	1.639518000	-0.089531000	-1.385585000
C	-1.493713000	-0.088093000	-1.410375000
O	-2.341532000	-0.135195000	-2.173177000
O	-0.146468000	3.102582000	-0.200650000
C	2.874077000	-0.393496000	-0.643930000
C	2.874101000	0.393326000	0.643932000
N	1.639524000	0.089437000	1.385587000
H	1.732252000	0.798231000	-1.870890000
H	1.481798000	-0.781061000	-2.111105000
H	3.761168000	-0.158267000	-1.235246000
H	2.887502000	-1.464914000	-0.434115000
H	2.887592000	1.464743000	0.434118000
H	3.761179000	0.158044000	1.235249000
H	1.732204000	-0.798330000	1.870893000
H	1.481843000	0.780978000	2.111105000
C	-0.177940000	-1.967575000	0.126318000
O	-0.146772000	-3.102574000	0.200682000

Sum of electronic and zero-point Energies= -733.921289
Sum of electronic and thermal Energies= -733.906107
Sum of electronic and thermal Enthalpies= -733.905163
Sum of electronic and thermal Free Energies= -733.965159

ImD_H^+_DCM

C	-3.71923700	-0.49373500	-0.04354200
O	-3.71680400	0.78924700	0.84663900
O	-4.77702000	-0.81808400	-0.40920600
N	1.07670500	-0.35302300	-0.13125200
C	-1.30734300	-0.26274700	0.22118500
C	-0.18006900	-0.95034100	-0.51737500
O	-2.54360600	-0.91950400	-0.22326100
C	3.40860100	-0.83517000	0.52827100
C	2.19514100	-1.27115700	-0.26601600
O	4.39005000	-1.83907200	0.35932900
C	1.48509400	2.05065800	0.28907800
C	1.31118400	0.95204300	-0.74162700
O	1.68743300	3.26155100	-0.41058900
H	-4.63844900	1.04016200	1.04759200
H	-3.18021800	0.79198500	1.66159600
H	-1.38121900	0.79532300	-0.02801300
H	-1.21431800	-0.41451800	1.29707800
H	-0.18005000	-2.00373800	-0.23288000
H	-0.37374200	-0.89884800	-1.60040300
H	3.12988100	-0.72039000	1.58360000
H	3.78066600	0.13222400	0.16905200
H	2.49159200	-1.40545900	-1.31971300
H	1.88677700	-2.24884200	0.11186900
H	5.19671400	-1.55226300	0.79479600
H	2.33662200	1.82024300	0.94033700
H	0.59106800	2.10394700	0.92503500
H	0.47509500	1.22113700	-1.39714200
H	2.19936800	0.92142700	-1.38423300
H	1.86262100	3.95836800	0.22705600

Sum of electronic and zero-point Energies=	-706.245414
Sum of electronic and thermal Energies=	-706.229239
Sum of electronic and thermal Enthalpies=	-706.228295
Sum of electronic and thermal Free Energies=	-706.290470

ImD_H$^+$_DMF

C	-3.71905600	-0.48805000	-0.03844600
O	-3.72106900	0.78459000	0.83555000
O	-4.77270200	-0.82368900	-0.41147600
N	1.07799500	-0.35381500	-0.12936900
C	-1.30914100	-0.25799400	0.22295800
C	-0.18125600	-0.95057300	-0.51015200
O	-2.54244500	-0.91834200	-0.21800300
C	3.40740200	-0.83798100	0.53026600
C	2.19531100	-1.27183600	-0.26714700
O	4.39670500	-1.83390200	0.35102700
C	1.47556700	2.05101600	0.28935800
C	1.31173600	0.95066800	-0.74095800
O	1.69865000	3.26012100	-0.40935900
H	-4.64173700	1.04062700	1.03667400
H	-3.17946600	0.79720400	1.64795100
H	-1.38261600	0.79836300	-0.03343600
H	-1.21564800	-0.40099100	1.29989100
H	-0.18247000	-2.00202400	-0.21866100
H	-0.37438800	-0.90573500	-1.59357200
H	3.12947500	-0.73592700	1.58685000
H	3.77386800	0.13509300	0.18115500
H	2.49302700	-1.40189800	-1.32131200
H	1.88580000	-2.25093800	0.10612800
H	5.19720600	-1.54899400	0.79915900
H	2.31527300	1.81685900	0.95466600
H	0.57212900	2.11303800	0.91000900
H	0.47954000	1.21497000	-1.40325800
H	2.20519400	0.92120500	-1.37646900
H	1.82237700	3.96410900	0.23261800

Sum of electronic and zero-point Energies=	-706.254973
Sum of electronic and thermal Energies=	-706.238845
Sum of electronic and thermal Enthalpies=	-706.237900
Sum of electronic and thermal Free Energies=	-706.300084