

ELECTRONIC SUPPLEMENTARY INFORMATION

DFT Insights on the Photocatalytic CO₂ to CO reduction by Re(I) complexes: The Crucial Role of Triethanolamine“Magic” Sacrificial Electron Donor

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Table S1. Cartesian coordinates of reactants, intermediates and products involved in the catalytic cycles.	S3

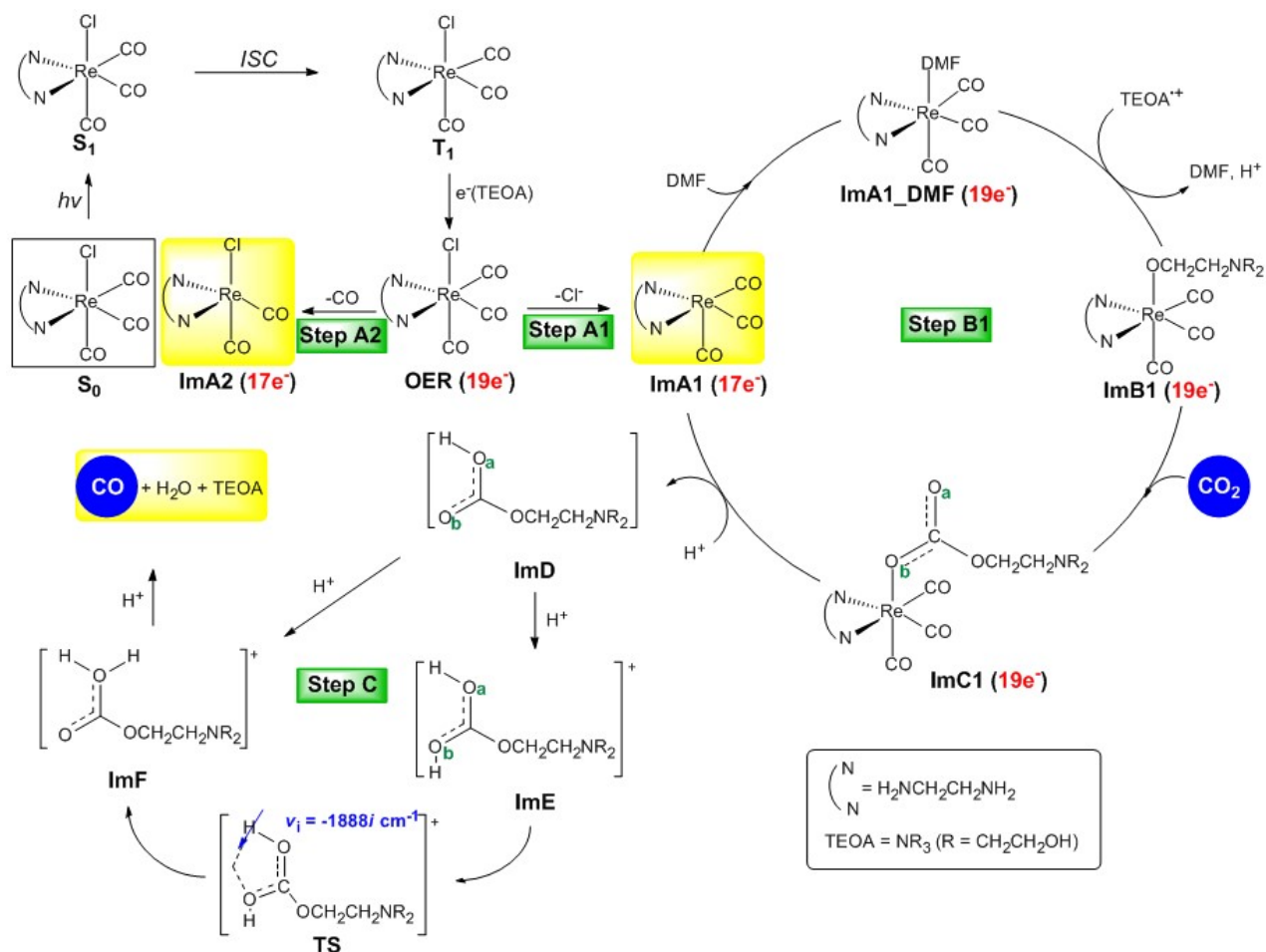
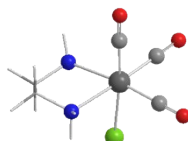


Fig S1. Reaction steps for the photocatalytic reduction of CO_2 to CO catalyzed by the $[(\text{en})(\text{CO})_3\text{ReCl}]$ catalyst starting with the $[(\text{en})(\text{CO})_3\text{Re}]$ intermediate resulted upon one electron reduction of the T_1 state by TEOA calculated at the wB97XD/Def2-TZVP level in DMF solution.

Table S1. Cartesian coordinates of reactants, intermediates and products involved in the proposed catalytic cycles

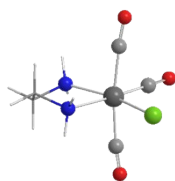
Reaction steps A1 and A2: Photophysics of [(en)(CO)₃ReCl] Catalyst



S₀ (*fac*-[(en)(CO)₃ReCl]

Re	0.208361000	0.016315000	-0.001900000
Cl	-0.609327000	-2.368473000	0.175484000
O	2.371441000	-0.286009000	2.146521000
O	0.997117000	2.956907000	-0.213332000
N	-1.559320000	0.189021000	-1.409133000
N	-1.535350000	0.396167000	1.374928000
C	1.557131000	-0.180577000	1.341016000
C	1.538803000	-0.378171000	-1.323282000
C	0.685594000	1.848264000	-0.133804000
O	2.341733000	-0.600876000	-2.115769000
C	-2.839124000	0.194467000	-0.664158000
C	-2.670473000	0.970647000	0.622245000
H	-1.556458000	-0.590140000	-2.058223000
H	-1.487964000	1.026907000	-1.974988000
H	-1.307365000	0.993292000	2.160735000
H	-1.806891000	-0.503088000	1.764104000
H	-3.089066000	-0.841521000	-0.437993000
H	-3.642818000	0.618661000	-1.265230000
H	-2.438760000	2.015297000	0.412298000
H	-3.590438000	0.936731000	1.206507000

Sum of electronic and zero-point Energies=	-1069.219211
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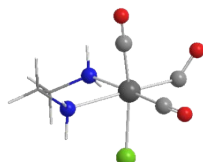


S₀ (*mer*-[(en)(CO)₃ReCl]

Re	-0.151356000	0.008487000	-0.052070000
O	-0.508319000	-3.052941000	-0.570046000
N	1.592158000	0.170490000	-1.417576000
N	1.632334000	-0.202266000	1.356649000
Cl	-1.529943000	-0.262435000	2.024448000
C	-1.509480000	0.192622000	-1.346184000
C	-0.314478000	-1.948091000	-0.354077000
O	-2.329956000	0.308729000	-2.161577000
C	2.832574000	0.437843000	-0.654074000
C	2.857188000	-0.448939000	0.570441000
O	-0.448893000	3.104740000	0.232177000
C	-0.276095000	1.977510000	0.156061000

H	1.458815000	0.901004000	-2.105979000
H	1.711040000	-0.682182000	-1.952533000
H	1.480629000	-0.952180000	2.021440000
H	1.747098000	0.636223000	1.915217000
H	2.820769000	1.487306000	-0.356775000
H	3.714628000	0.267453000	-1.271343000
H	2.858656000	-1.498113000	0.271584000
H	3.756734000	-0.262117000	1.157102000

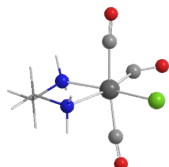
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T₁ (*fac*-[(en)(CO)₃ReCl])

Re	-0.211338000	-0.024177000	0.016385000
Cl	0.649747000	-2.281372000	-0.396881000
O	-2.572118000	-0.351126000	-1.900858000
O	-1.024800000	2.942717000	-0.148593000
N	1.532188000	0.151574000	1.425132000
N	1.594505000	0.506534000	-1.357600000
C	-1.675168000	-0.236056000	-1.187148000
C	-1.457732000	-0.722395000	1.503405000
C	-0.697295000	1.844435000	-0.057256000
O	-2.175058000	-0.194162000	2.279805000
C	2.825387000	0.201577000	0.708815000
C	2.688537000	1.044891000	-0.534707000
H	1.534119000	-0.644986000	2.054933000
H	1.436877000	0.972135000	2.015973000
H	1.367226000	1.148816000	-2.108190000
H	1.879198000	-0.366371000	-1.793513000
H	3.084383000	-0.821998000	0.435044000
H	3.615324000	0.592531000	1.352719000
H	2.438836000	2.075393000	-0.272605000
H	3.635293000	1.060157000	-1.080451000

Sum of electronic and zero-point Energies= -1068.492190
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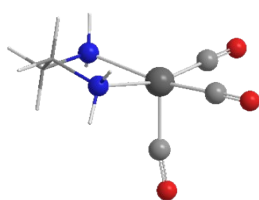


T₁ (*mer*-[(en)(CO)₃ReCl])

Re	0.138210000	0.000956000	0.017909000
Cl	1.821030000	-0.094887000	-1.716178000
O	0.325935000	3.102745000	-0.215850000
O	0.447798000	-3.094095000	0.231159000
N	-1.606976000	0.056326000	1.383267000
N	-1.666472000	-0.128097000	-1.387458000

C	0.211132000	1.966757000	-0.129575000
C	1.238672000	0.160996000	1.790735000
C	0.290039000	-1.963405000	0.149816000
O	2.390014000	0.182073000	2.058323000
C	-2.853008000	0.380675000	0.663370000
C	-2.888626000	-0.417516000	-0.616873000
H	-1.432247000	0.738536000	2.115094000
H	-1.713312000	-0.832703000	1.862062000
H	-1.521350000	-0.842410000	-2.093023000
H	-1.779084000	0.743145000	-1.895352000
H	-2.843311000	1.450102000	0.442662000
H	-3.731083000	0.168094000	1.276492000
H	-2.897938000	-1.486258000	-0.392191000
H	-3.790064000	-0.185539000	-1.188444000

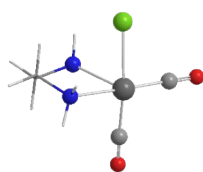
Sum of electronic and zero-point Energies= -1068.481290
Sum of electronic and thermal Energies= -1068.466484
Sum of electronic and thermal Enthalpies= -1068.465540
Sum of electronic and thermal Free Energies= -1068.525919



ImA₁

Re	0.158956000	0.011932000	-0.135398000
O	2.299230000	-2.027320000	-0.952396000
O	0.976139000	-0.294440000	2.784028000
N	-1.645520000	1.413721000	-0.037053000
N	-1.638139000	-1.380275000	-0.289993000
C	1.481820000	-1.255648000	-0.653447000
C	1.466058000	1.375745000	-0.371148000
C	0.544161000	-0.178943000	1.706216000
O	2.267334000	2.208907000	-0.497280000
C	-2.888485000	0.699124000	-0.397270000
C	-2.852811000	-0.693133000	0.191401000
H	-1.532283000	2.220250000	-0.639046000
H	-1.727025000	1.781256000	0.903918000
H	-1.492241000	-2.232007000	0.238005000
H	-1.774840000	-1.671510000	-1.252428000
H	-2.933064000	0.638537000	-1.485592000
H	-3.771589000	1.236757000	-0.050769000
H	-2.794851000	-0.640871000	1.279406000
H	-3.756248000	-1.241455000	-0.078663000

Sum of electronic and zero-point Energies= -608.895072
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Sum of electronic and thermal Free Energies= -608.936450



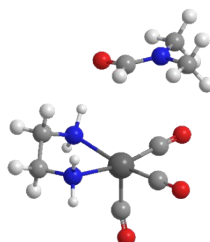
ImA₂

Re	0.332364000	-0.030136000	-0.167910000
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Cl	-0.831092000	-2.325647000	-0.386872000
O	3.000458000	-0.995445000	0.935816000
O	1.670709000	2.675225000	-0.494420000
N	-1.685343000	0.663686000	-1.081291000
N	-1.096843000	0.250316000	1.635628000
C	1.957207000	-0.634354000	0.506231000
C	1.140375000	1.620732000	-0.361164000
C	-2.770574000	0.633181000	-0.082294000
C	-2.240691000	1.095158000	1.258426000
H	-1.928108000	0.066769000	-1.863116000
H	-1.585548000	1.599926000	-1.454186000
H	-0.619759000	0.642252000	2.435817000
H	-1.425288000	-0.670857000	1.908852000
H	-3.110326000	-0.399804000	-0.001014000
H	-3.618965000	1.248342000	-0.386946000
H	-1.884736000	2.124047000	1.187345000
H	-3.037972000	1.060964000	2.004590000

Sum of electronic and zero-point Energies= -955.914303
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Sum of electronic and thermal Enthalpies= -955.901167
Sum of electronic and thermal Free Energies= -955.955586

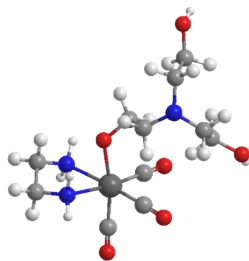
Reaction step B1



ImA₁_DMF

Re	0.748054000	-0.234865000	-0.013510000
C	2.078341000	-0.872818000	1.169574000
O	2.812881000	-1.447216000	1.871414000
C	-0.631736000	-1.151068000	0.921854000
O	-1.462932000	-1.724161000	1.498978000
C	0.854715000	-1.744748000	-1.167477000
O	0.923868000	-2.679283000	-1.858195000
N	0.328422000	1.842602000	0.834707000
N	2.044453000	1.151970000	-1.268947000
C	2.225022000	2.444904000	-0.579289000
C	0.886133000	2.892889000	-0.039090000
C	-2.674970000	1.164543000	-0.412059000
O	-2.569152000	2.059565000	0.424907000
N	-3.512138000	0.129113000	-0.341968000
C	-4.383008000	-0.063404000	0.797194000
C	-3.489138000	-0.919778000	-1.336885000
H	0.725136000	1.923119000	1.763009000
H	-0.677680000	1.995533000	0.924472000
H	1.614328000	1.311638000	-2.173923000
H	2.946976000	0.735459000	-1.462896000
H	2.640038000	3.199804000	-1.248464000
H	2.927186000	2.287688000	0.240560000
H	0.986947000	3.841383000	0.489864000
H	0.185296000	3.040735000	-0.863212000
H	-5.416116000	-0.169840000	0.461606000

H	-4.302336000	0.796100000	1.456445000
H	-4.091812000	-0.964578000	1.340378000
H	-4.481561000	-1.052420000	-1.771520000
H	-3.173398000	-1.861074000	-0.881332000
H	-2.786972000	-0.663019000	-2.128144000
H	-2.054757000	1.154181000	-1.319921000
Sum of electronic and zero-point Energies=			-857.343294
Sum of electronic and thermal Energies=			-857.323375
Sum of electronic and thermal Enthalpies=			-857.322431
Sum of electronic and thermal Free Energies=			-857.394906

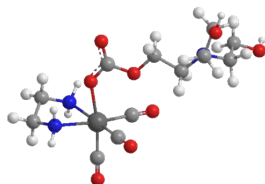


ImB₁

Re	-1.424005000	0.133732000	0.080212000
N	-2.420572000	-1.543479000	1.252262000
N	-2.258725000	-1.219430000	-1.512414000
C	-3.273663000	-2.135361000	-0.957504000
C	-2.763115000	-2.672500000	0.360986000
C	-2.947124000	1.290998000	0.174579000
O	-3.856112000	2.003844000	0.231390000
C	-0.691006000	1.091398000	1.561529000
O	-0.262300000	1.686370000	2.452543000
C	-0.650694000	1.442174000	-1.066648000
O	-0.220586000	2.263245000	-1.757122000
N	3.393452000	-0.323988000	-1.142982000
C	1.362315000	-1.200752000	0.126451000
C	2.038714000	-0.819545000	-1.201503000
O	-0.001281000	-1.396035000	-0.028396000
C	4.721592000	-1.165161000	0.834024000
C	4.431651000	-1.198070000	-0.664896000
O	5.720108000	-2.139368000	1.092974000
C	3.002665000	1.793701000	0.175872000
C	3.587395000	1.100362000	-1.052761000
O	3.338036000	3.168738000	0.085115000
H	-3.247083000	-1.226571000	1.745600000
H	-1.766291000	-1.863054000	1.956956000
H	-1.433532000	-1.748065000	-1.787566000
H	-2.617413000	-0.756497000	-2.338064000
H	-3.485357000	-2.957851000	-1.642088000
H	-4.193988000	-1.568832000	-0.810602000
H	-3.502103000	-3.329891000	0.818819000
H	-1.848790000	-3.239451000	0.193419000
H	1.590823000	-0.426694000	0.875490000
H	1.825959000	-2.128651000	0.497222000
H	1.999846000	-1.697428000	-1.858879000
H	1.426610000	-0.049178000	-1.677827000
H	3.809685000	-1.377787000	1.401975000
H	5.075574000	-0.168507000	1.121495000
H	5.370358000	-0.969552000	-1.184212000
H	4.162113000	-2.223415000	-0.935350000
H	5.960518000	-2.093584000	2.019553000
H	3.405225000	1.351789000	1.094424000
H	1.915472000	1.664643000	0.190694000

H	3.148038000	1.584828000	-1.933761000
H	4.661732000	1.304231000	-1.082278000
H	2.888610000	3.640051000	0.788207000

Sum of electronic and zero-point Energies= -1126.264287
Sum of electronic and thermal Energies= -1126.238910
Sum of electronic and thermal Enthalpies= -1126.237965
Sum of electronic and thermal Free Energies= -1126.322045



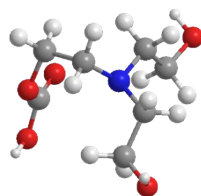
ImC₁

Re	2.129407000	0.232448000	0.201639000
N	3.345725000	0.095916000	-1.702551000
N	3.515200000	-1.499091000	0.582754000
C	4.646266000	-1.480421000	-0.368702000
C	4.111384000	-1.170551000	-1.748339000
C	3.225998000	1.539921000	1.036130000
O	3.880283000	2.340850000	1.550675000
C	0.958504000	1.645166000	-0.345490000
O	0.262242000	2.505880000	-0.658681000
C	1.120985000	0.131920000	1.822364000
O	0.512460000	0.086706000	2.798378000
N	-4.450867000	0.030567000	0.031626000
C	-2.309111000	-0.937538000	-0.648769000
C	-3.006235000	0.171164000	0.115936000
O	-0.913030000	-0.750564000	-0.463719000
C	-6.192613000	-1.648493000	0.443553000
C	-4.985837000	-0.915955000	0.998622000
O	-6.707721000	-2.482006000	1.467264000
C	-5.184367000	1.935522000	-1.334098000
C	-5.144124000	1.309536000	0.047135000
O	-5.798821000	3.207289000	-1.218714000
C	-0.081330000	-1.653064000	-1.036339000
O	1.154204000	-1.391657000	-0.839480000
O	-0.516613000	-2.604585000	-1.666608000
H	3.977893000	0.883409000	-1.790675000
H	2.727936000	0.140953000	-2.505210000
H	2.959962000	-2.336872000	0.430302000
H	3.863956000	-1.549515000	1.532211000
H	5.175062000	-2.433987000	-0.373982000
H	5.342547000	-0.705809000	-0.045675000
H	4.925227000	-1.113541000	-2.470724000
H	3.424513000	-1.955169000	-2.062214000
H	-2.561521000	-0.879438000	-1.709429000
H	-2.604043000	-1.923601000	-0.284014000
H	-2.655148000	0.180057000	1.158751000
H	-2.711928000	1.125740000	-0.322148000
H	-5.882126000	-2.236019000	-0.427373000
H	-6.950670000	-0.930252000	0.110295000
H	-5.257657000	-0.422269000	1.943831000
H	-4.220047000	-1.655025000	1.239574000
H	-7.460562000	-2.962615000	1.119826000
H	-5.751307000	1.281009000	-2.005115000
H	-4.169688000	2.031026000	-1.737429000
H	-4.683147000	2.013949000	0.756183000

H	-6.171602000	1.154997000	0.380368000
H	-5.834731000	3.609050000	-2.088040000

Sum of electronic and zero-point Energies= -1314.879498
Sum of electronic and thermal Energies= -1314.851139
Sum of electronic and thermal Enthalpies= -1314.850194
Sum of electronic and thermal Free Energies= -1314.944089

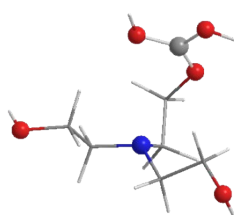
Reaction step C



ImD

N	0.672418000	0.197032000	0.609081000
C	-1.442328000	-0.502905000	1.674639000
C	0.068829000	-0.444756000	1.763702000
O	-1.819164000	-1.281917000	0.530913000
C	0.599317000	2.275431000	-0.713695000
C	0.629665000	1.647918000	0.673464000
O	0.609190000	3.691261000	-0.653896000
C	1.889558000	-1.578905000	-0.574761000
C	1.990307000	-0.335088000	0.298078000
O	3.158302000	-2.141577000	-0.854712000
C	-2.197880000	-0.632157000	-0.564470000
O	-2.462916000	0.534502000	-0.656387000
O	-2.292602000	-1.463308000	-1.599432000
H	-1.894284000	0.484026000	1.595852000
H	-1.854501000	-1.016740000	2.541098000
H	0.340093000	0.053840000	2.707181000
H	0.440612000	-1.468048000	1.830617000
H	-0.278695000	1.903419000	-1.249747000
H	1.485523000	1.993447000	-1.284221000
H	1.474535000	2.059467000	1.247502000
H	-0.282740000	1.946526000	1.194756000
H	-0.221574000	3.983785000	-0.273231000
H	1.449863000	-1.305962000	-1.534966000
H	1.228200000	-2.318376000	-0.108983000
H	2.559196000	-0.567046000	1.212619000
H	2.567515000	0.415356000	-0.242901000
H	3.526671000	-2.483881000	-0.037490000
H	-2.014629000	-2.347952000	-1.335271000

Sum of electronic and zero-point Energies= -706.489917
Sum of electronic and thermal Energies= -706.475021
Sum of electronic and thermal Enthalpies= -706.474077
Sum of electronic and thermal Free Energies= -706.533973

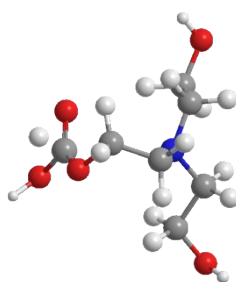


S10

ImE

N	-0.615605000	0.267098000	0.615805000
C	1.277420000	-0.839188000	1.725561000
C	0.196561000	0.212206000	1.819183000
O	2.162758000	-0.455160000	0.616203000
C	-2.190400000	-1.070100000	-0.756801000
C	-1.703699000	-0.703852000	0.639344000
O	-3.282320000	-1.964698000	-0.711098000
C	-0.014325000	2.382244000	-0.492401000
C	-1.061415000	1.625207000	0.313450000
O	-0.409839000	3.707523000	-0.774295000
C	2.008170000	-0.921224000	-0.547000000
O	1.287282000	-1.955046000	-0.767398000
O	2.634342000	-0.389248000	-1.531796000
H	0.902418000	-1.841821000	1.539403000
H	1.926952000	-0.839035000	2.594866000
H	-0.393803000	0.000306000	2.721299000
H	0.677831000	1.177400000	1.978004000
H	-1.358583000	-1.483953000	-1.335950000
H	-2.549493000	-0.187345000	-1.286255000
H	-2.552859000	-0.344261000	1.238461000
H	-1.342913000	-1.617219000	1.119879000
H	-2.984295000	-2.799822000	-0.344530000
H	0.117065000	1.886609000	-1.455508000
H	0.953329000	2.362924000	0.024479000
H	-1.304232000	2.179195000	1.232159000
H	-1.977786000	1.583820000	-0.273803000
H	-0.434331000	4.205414000	0.045482000
H	1.281122000	-2.206654000	-1.703538000
H	3.137153000	0.396018000	-1.266029000

Sum of electronic and zero-point Energies= -706.872675
Sum of electronic and thermal Energies= -706.858013
Sum of electronic and thermal Enthalpies= -706.857069
Sum of electronic and thermal Free Energies= -706.914885

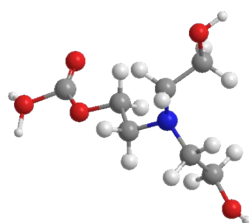


TS

N	0.706667000	-0.100109000	0.613245000
C	-1.393917000	0.293110000	1.824175000
C	-0.032900000	-0.359868000	1.835482000
O	-2.150060000	-0.286978000	0.692929000
C	1.664974000	1.729330000	-0.754025000
C	1.405975000	1.178587000	0.642555000
O	2.387947000	2.944596000	-0.708232000
C	0.796445000	-2.267683000	-0.553729000
C	1.565268000	-1.220362000	0.240253000
O	1.607533000	-3.372898000	-0.899339000
C	-2.167287000	0.338009000	-0.389628000
O	-1.838505000	1.455622000	-0.779046000
O	-2.693547000	-0.274496000	-1.520856000

H	-1.366466000	1.371313000	1.685127000
H	-1.984822000	0.038266000	2.697544000
H	0.491049000	-0.008297000	2.735455000
H	-0.174283000	-1.434101000	1.953524000
H	0.712335000	1.850929000	-1.277816000
H	2.276850000	1.039272000	-1.335747000
H	2.356469000	1.107581000	1.191549000
H	0.785908000	1.902385000	1.177677000
H	1.828481000	3.619405000	-0.317935000
H	0.455198000	-1.824823000	-1.490501000
H	-0.092006000	-2.593656000	-0.000444000
H	2.025609000	-1.683551000	1.125712000
H	2.383714000	-0.856880000	-0.379953000
H	1.828411000	-3.853452000	-0.098660000
H	-2.450390000	0.867745000	-1.848658000
H	-3.561014000	-0.714883000	-1.463719000

Sum of electronic and zero-point Energies= -706.806207
Sum of electronic and thermal Energies= -706.791254
Sum of electronic and thermal Enthalpies= -706.790309
Sum of electronic and thermal Free Energies= -706.849348

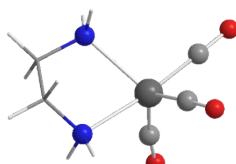


ImF

N	-1.179152000	-0.019394000	-0.244691000
C	1.173200000	0.015479000	0.229274000
C	0.110935000	-0.452052000	-0.741465000
O	2.480615000	-0.349208000	-0.350504000
C	-2.315104000	2.045565000	0.443712000
C	-1.528803000	1.336675000	-0.643044000
O	-2.658152000	3.329094000	-0.042229000
C	-2.261827000	-2.055945000	0.602398000
C	-2.241504000	-0.988143000	-0.475102000
O	-3.251217000	-3.003519000	0.250699000
C	3.511832000	0.064142000	0.269806000
O	4.672547000	-0.412169000	-0.552331000
O	3.758264000	0.692081000	1.223686000
H	1.090709000	-0.485434000	1.191197000
H	1.170665000	1.095423000	0.365902000
H	0.326720000	-0.071142000	-1.748663000
H	0.138923000	-1.540521000	-0.793902000
H	-1.695314000	2.112070000	1.345064000
H	-3.213095000	1.469965000	0.696436000
H	-2.101714000	1.348794000	-1.580822000
H	-0.615845000	1.906426000	-0.826857000
H	-3.172936000	3.784111000	0.625744000
H	-2.483173000	-1.584562000	1.566195000
H	-1.276953000	-2.533063000	0.682105000
H	-2.152001000	-1.463144000	-1.462480000
H	-3.200592000	-0.469540000	-0.461593000
H	-3.317304000	-3.655331000	0.949926000
H	4.530860000	-1.193434000	-1.115506000
H	5.516282000	-0.429422000	-0.067957000

Sum of electronic and zero-point Energies= -706.831578
 Sum of electronic and thermal Energies= -706.815558
 Sum of electronic and thermal Enthalpies= -706.814613
 Sum of electronic and thermal Free Energies= -706.876913

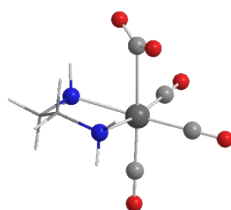
Reaction step B1'



ImA₁'

Re	0.224533000	0.006393000	0.028052000
O	2.722831000	-0.212222000	-1.721922000
O	1.139057000	-2.515907000	1.563485000
N	-1.802806000	0.159109000	1.146279000
N	-1.425748000	-0.236076000	-1.606263000
C	1.764185000	-0.127052000	-1.043174000
C	0.713357000	1.783634000	0.525496000
C	0.706762000	-1.602667000	0.937090000
O	1.141963000	2.822359000	0.915794000
C	-2.912740000	0.396424000	0.208391000
C	-2.738857000	-0.499786000	-0.997278000
H	-1.774128000	0.899253000	1.835104000
H	-1.971972000	-0.696062000	1.661500000
H	-1.185291000	-0.983386000	-2.243321000
H	-1.472868000	0.606916000	-2.164547000
H	-2.867227000	1.442111000	-0.101159000
H	-3.884570000	0.220882000	0.674472000
H	-2.755072000	-1.545286000	-0.683580000
H	-3.556024000	-0.342310000	-1.704471000

Sum of electronic and zero-point Energies= -608.990349
 Sum of electronic and thermal Energies= -608.977868
 Sum of electronic and thermal Enthalpies= -608.976924
 Sum of electronic and thermal Free Energies= -609.031379

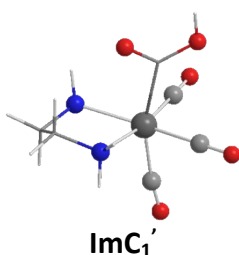


ImB₁'

Re	-0.268650000	-0.071464000	-0.005398000
O	-2.140131000	0.881746000	2.226946000
O	-1.923356000	-2.635948000	-0.185056000
N	1.357613000	-0.660727000	-1.456615000
N	1.343957000	-0.904473000	1.321414000
C	-1.438759000	0.523937000	1.388729000
C	-1.451845000	0.732349000	-1.282985000
C	-1.283448000	-1.680074000	-0.119227000
O	-2.163273000	1.211705000	-2.048076000

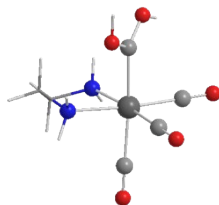
C	2.625262000	-0.945123000	-0.745437000
C	2.322253000	-1.687019000	0.536547000
C	1.154526000	1.944104000	0.145303000
O	1.259176000	2.450758000	-0.953281000
O	1.564828000	2.088111000	1.281692000
H	1.506683000	0.090856000	-2.121877000
H	1.083222000	-1.469268000	-2.003413000
H	0.978090000	-1.472977000	2.075573000
H	1.803039000	-0.108605000	1.759770000
H	3.101461000	0.009885000	-0.520655000
H	3.306443000	-1.521717000	-1.370330000
H	1.874225000	-2.655875000	0.314751000
H	3.238743000	-1.856128000	1.102031000

Sum of electronic and zero-point Energies= -797.502319
Sum of electronic and thermal Energies= -797.486529
Sum of electronic and thermal Enthalpies= -797.485584
Sum of electronic and thermal Free Energies= -797.548340



Re	-0.076258000	-0.174709000	-0.008232000
O	-2.135446000	-0.273238000	2.295364000
O	-0.566507000	-3.262785000	-0.087293000
N	1.655645000	0.058799000	-1.400146000
N	1.656451000	-0.004008000	1.381299000
C	-1.390985000	-0.246880000	1.436040000
C	-1.397423000	-0.156267000	-1.448814000
C	-0.297546000	-2.160053000	-0.061349000
O	-2.146297000	-0.129400000	-2.304356000
C	2.878460000	0.471762000	-0.663813000
C	2.926746000	-0.257596000	0.657034000
C	-0.526799000	1.927003000	0.072693000
O	-1.744414000	2.446667000	0.067692000
O	0.482161000	2.598246000	0.124456000
H	1.463631000	0.735381000	-2.131856000
H	1.834273000	-0.814066000	-1.887714000
H	1.597147000	-0.614657000	2.188852000
H	1.670875000	0.943388000	1.751404000
H	2.812314000	1.545665000	-0.497062000
H	3.770476000	0.264535000	-1.252347000
H	3.015431000	-1.332988000	0.503351000
H	3.779994000	0.074993000	1.246471000
H	-1.680146000	3.413682000	0.110601000

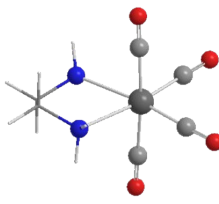
Sum of electronic and zero-point Energies= -797.918245
Sum of electronic and thermal Energies= -797.902235
Sum of electronic and thermal Enthalpies= -797.901291
Sum of electronic and thermal Free Energies= -797.963659



ImD₁'

Re	0.166841000	0.148064000	0.037253000
O	2.543799000	-0.225990000	2.024185000
O	0.389121000	3.324657000	-0.145185000
N	-1.586870000	0.230993000	-1.314239000
N	-1.525166000	0.250331000	1.471935000
C	1.674401000	-0.079302000	1.318050000
C	1.623047000	0.167931000	-1.318491000
C	0.289737000	2.209756000	-0.056619000
O	2.460516000	0.194339000	-2.075716000
C	-2.845521000	-0.012525000	-0.558427000
C	-2.763501000	0.691856000	0.773716000
C	-0.049821000	-1.994390000	-0.099707000
O	-0.357749000	-2.459627000	-1.262996000
O	0.088089000	-2.924102000	0.783830000
H	-1.504859000	-0.466644000	-2.050698000
H	-1.654968000	1.115457000	-1.809206000
H	-1.331367000	0.888285000	2.240005000
H	-1.704735000	-0.639979000	1.927208000
H	-2.948432000	-1.088000000	-0.417015000
H	-3.703355000	0.336961000	-1.128855000
H	-2.707189000	1.771125000	0.638404000
H	-3.639665000	0.470668000	1.380100000
H	-0.423456000	-3.430707000	-1.284517000
H	0.328911000	-2.605440000	1.662649000

Sum of electronic and zero-point Energies= -798.304534
 Sum of electronic and thermal Energies= -798.288571
 Sum of electronic and thermal Enthalpies= -798.287627
 Sum of electronic and thermal Free Energies= -798.349428



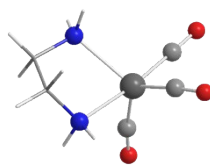
ImE₁'

Re	0.167825000	0.003798000	0.005492000
C	0.066428000	2.036080000	-0.103437000
O	2.286468000	-0.036076000	-2.349674000
N	-1.532656000	0.011592000	1.404827000
N	-1.534875000	-0.140479000	-1.386954000
C	1.542763000	-0.021799000	-1.511065000
C	1.614976000	0.142485000	1.445072000
O	2.406996000	0.207911000	2.235870000
C	-2.796637000	0.299939000	0.662513000
C	-2.787223000	-0.464251000	-0.638203000
C	0.263716000	-2.027208000	0.132696000
O	0.342386000	-3.144775000	0.207510000
O	0.033216000	3.156790000	-0.162188000
H	-1.431169000	0.703454000	2.144262000

H	-1.634104000	-0.874464000	1.893611000
H	-1.397116000	-0.845512000	-2.107238000
H	-1.672059000	0.726385000	-1.899269000
H	-2.844759000	1.373993000	0.487854000
H	-3.654595000	0.016976000	1.268802000
H	-2.800791000	-1.538641000	-0.462315000
H	-3.656232000	-0.207119000	-1.240328000

Sum of electronic and zero-point Energies= -721.864828
 Sum of electronic and thermal Energies= -721.850165
 Sum of electronic and thermal Enthalpies= -721.849221
 Sum of electronic and thermal Free Energies= -721.908120

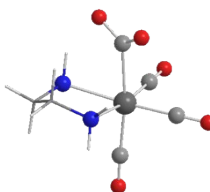
Reaction step B1''



ImA₁''

Re	0.224533000	0.006393000	0.028052000
O	2.722831000	-0.212222000	-1.721922000
O	1.139057000	-2.515907000	1.563485000
N	-1.802806000	0.159109000	1.146279000
N	-1.425748000	-0.236076000	-1.606263000
C	1.764185000	-0.127052000	-1.043174000
C	0.713357000	1.783634000	0.525496000
C	0.706762000	-1.602667000	0.937090000
O	1.141963000	2.822359000	0.915794000
C	-2.912740000	0.396424000	0.208391000
C	-2.738857000	-0.499786000	-0.997278000
H	-1.774128000	0.899253000	1.835104000
H	-1.971972000	-0.696062000	1.661500000
H	-1.185291000	-0.983386000	-2.243321000
H	-1.472868000	0.606916000	-2.164547000
H	-2.867227000	1.442111000	-0.101159000
H	-3.884570000	0.220882000	0.674472000
H	-2.755072000	-1.545286000	-0.683580000
H	-3.556024000	-0.342310000	-1.704471000

Sum of electronic and zero-point Energies= -608.990349
 Sum of electronic and thermal Energies= -608.977868
 Sum of electronic and thermal Enthalpies= -608.976924
 Sum of electronic and thermal Free Energies= -609.031379

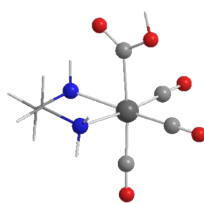


ImB₁''

Re	-0.283645000	-0.067616000	-0.001865000
O	-2.143278000	0.862189000	2.243709000
O	-1.787153000	-2.784363000	-0.176320000
N	1.352405000	-0.593937000	-1.490494000

N	1.396697000	-0.813569000	1.288528000
C	-1.439363000	0.502914000	1.395007000
C	-1.499501000	0.723162000	-1.239752000
C	-1.200594000	-1.789020000	-0.124192000
O	-2.238242000	1.212925000	-1.985660000
C	2.638756000	-0.828547000	-0.799627000
C	2.392113000	-1.559289000	0.503466000
C	1.018064000	1.760040000	0.139758000
O	1.103378000	2.556612000	-0.835332000
O	1.738301000	1.899670000	1.185891000
H	1.447237000	0.202389000	-2.110927000
H	1.115258000	-1.392713000	-2.065786000
H	1.121219000	-1.346811000	2.102265000
H	1.768198000	0.102626000	1.591029000
H	3.079416000	0.146031000	-0.592490000
H	3.328744000	-1.391932000	-1.428603000
H	1.995729000	-2.556907000	0.305271000
H	3.332963000	-1.670738000	1.046641000

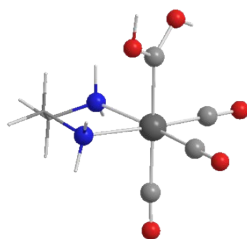
Sum of electronic and zero-point Energies= -797.642158
Sum of electronic and thermal Energies= -797.626943
Sum of electronic and thermal Enthalpies= -797.625999
Sum of electronic and thermal Free Energies= -797.686314



ImC₁

Re	-0.241495000	-0.115202000	0.003449000
O	-2.201033000	0.544905000	2.261648000
O	-1.360050000	-3.011817000	-0.059565000
N	1.406476000	-0.550112000	-1.508035000
N	1.546727000	-0.602271000	1.278598000
C	-1.461992000	0.294362000	1.411894000
C	-1.582550000	0.417762000	-1.251295000
C	-0.918538000	-1.950458000	-0.045361000
O	-2.391802000	0.739057000	-2.007575000
C	2.727343000	-0.607738000	-0.842795000
C	2.584015000	-1.299455000	0.494673000
C	0.672545000	1.896131000	0.145445000
O	0.130105000	2.898423000	-0.596748000
O	1.630276000	2.196286000	0.852001000
H	1.429107000	0.149728000	-2.240361000
H	1.225780000	-1.429895000	-1.977637000
H	1.335493000	-1.127156000	2.117720000
H	1.892589000	0.316836000	1.562740000
H	3.066108000	0.416694000	-0.691439000
H	3.459352000	-1.123341000	-1.464199000
H	2.267803000	-2.334231000	0.355838000
H	3.541524000	-1.303741000	1.017301000
H	0.637027000	3.703507000	-0.406020000

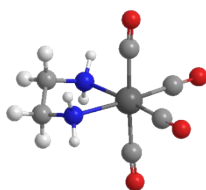
Sum of electronic and zero-point Energies= -798.122886
Sum of electronic and thermal Energies= -798.107366
Sum of electronic and thermal Enthalpies= -798.106422
Sum of electronic and thermal Free Energies= -798.167368



ImD₁

Re	0.221711000	0.109323000	-0.008291000
O	2.496044000	-0.293656000	2.007857000
O	1.257568000	3.027997000	-0.361523000
N	-1.609042000	0.440155000	-1.300258000
N	-1.371124000	0.745189000	1.475631000
C	1.641338000	-0.150582000	1.251657000
C	1.413722000	-0.427659000	-1.420308000
C	0.846906000	1.972585000	-0.223646000
O	2.122942000	-0.745811000	-2.263656000
C	-2.827780000	0.574545000	-0.469323000
C	-2.503552000	1.383155000	0.764942000
C	-0.487898000	-1.925102000	0.130889000
O	-1.229571000	-2.431499000	-0.808472000
O	-0.246885000	-2.809939000	1.056189000
H	-1.736930000	-0.322459000	-1.957068000
H	-1.494976000	1.272383000	-1.868158000
H	-0.997909000	1.392069000	2.160884000
H	-1.717256000	-0.040722000	2.016008000
H	-3.152271000	-0.427827000	-0.188673000
H	-3.634963000	1.043433000	-1.030948000
H	-2.197608000	2.392023000	0.487323000
H	-3.378108000	1.458955000	1.410376000
H	-1.455683000	-3.362086000	-0.642505000
H	0.301332000	-2.440825000	1.758521000

Sum of electronic and zero-point Energies= -798.540894
 Sum of electronic and thermal Energies= -798.525249
 Sum of electronic and thermal Enthalpies= -798.524305
 Sum of electronic and thermal Free Energies= -798.584925



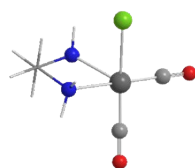
ImE₁

Re	0.167806000	-0.000005000	0.000000000
C	1.539626000	-0.075982000	1.369632000
C	1.539673000	0.075859000	-1.369590000
O	2.341395000	-0.118167000	2.180534000
O	2.341510000	0.117980000	-2.180430000
C	0.221752000	-2.011796000	-0.115574000
O	0.316931000	-3.137347000	-0.183255000
C	0.221921000	2.011774000	0.115509000
O	0.317328000	3.137308000	0.183160000
N	-1.607746000	-0.083421000	1.398590000
N	-1.607746000	0.083547000	-1.398590000
C	-2.847090000	-0.391775000	0.645526000
C	-2.847059000	0.392010000	-0.645519000

H	-1.726358000	0.798820000	1.885779000
H	-1.480623000	-0.772388000	2.131921000
H	-1.726432000	-0.798691000	-1.885767000
H	-1.480586000	0.772495000	-2.131933000
H	-3.731179000	-0.154430000	1.236190000
H	-2.855508000	-1.462423000	0.439361000
H	-3.731171000	0.154747000	-1.236182000
H	-2.855374000	1.462658000	-0.439351000

Sum of electronic and zero-point Energies= -722.132684
Sum of electronic and thermal Energies= -722.118461
Sum of electronic and thermal Enthalpies= -722.117517
Sum of electronic and thermal Free Energies= -722.174977

Reaction step A2

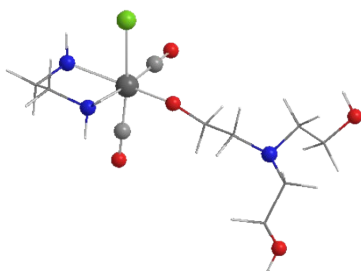


ImA₂

Re	0.332364000	-0.030136000	-0.167910000
Cl	-0.831092000	-2.325647000	-0.386872000
O	3.000458000	-0.995445000	0.935816000
O	1.670709000	2.675225000	-0.494420000
N	-1.685343000	0.663686000	-1.081291000
N	-1.096843000	0.250316000	1.635628000
C	1.957207000	-0.634354000	0.506231000
C	1.140375000	1.620732000	-0.361164000
C	-2.770574000	0.633181000	-0.082294000
C	-2.240691000	1.095158000	1.258426000
H	-1.928108000	0.066769000	-1.863116000
H	-1.585548000	1.599926000	-1.454186000
H	-0.619759000	0.642252000	2.435817000
H	-1.425288000	-0.670857000	1.908852000
H	-3.110326000	-0.399804000	-0.001014000
H	-3.618965000	1.248342000	-0.386946000
H	-1.884736000	2.124047000	1.187345000
H	-3.037972000	1.060964000	2.004590000

Sum of electronic and zero-point Energies= -955.914303
Sum of electronic and thermal Energies= -955.902111
Sum of electronic and thermal Enthalpies= -955.901167
Sum of electronic and thermal Free Energies= -955.955586

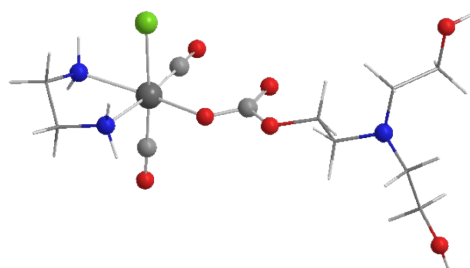
Reaction step B2'



ImB₂'

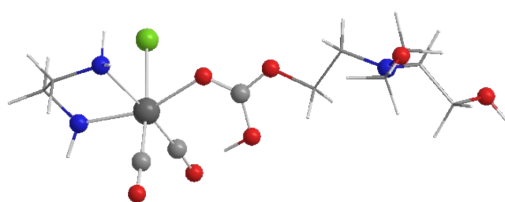
Re	1.621656000	-0.178439000	-0.141466000
O	1.088515000	0.580606000	-3.019059000
N	3.839216000	-0.133268000	-0.383457000
N	2.200348000	1.935205000	0.558032000
C	1.284848000	0.296284000	-1.887866000
C	1.347623000	-1.936807000	-0.675092000
Cl	2.348567000	-0.761970000	2.330848000
O	1.207197000	-3.048599000	-1.045464000
C	4.328731000	1.258769000	-0.424928000
C	3.664239000	2.049969000	0.683610000
N	-3.869680000	0.163393000	0.299530000
C	-5.075677000	-1.858293000	-0.420401000
C	-4.282365000	-1.175594000	0.685027000
O	-5.570857000	-3.125805000	-0.025232000
C	-4.842337000	2.266447000	-0.508431000
C	-4.907827000	1.155465000	0.522380000
O	-5.816636000	3.239616000	-0.169364000
C	-1.402696000	0.010543000	0.065504000
C	-2.583071000	0.543741000	0.871756000
O	-0.213924000	0.303813000	0.694711000
H	4.160198000	-0.633248000	-1.201804000
H	4.233520000	-0.606098000	0.425334000
H	1.750543000	2.119842000	1.447029000
H	1.846043000	2.622351000	-0.096077000
H	5.414581000	1.304568000	-0.319460000
H	4.061353000	1.674064000	-1.397424000
H	3.943348000	1.626581000	1.648457000
H	3.996314000	3.088890000	0.656991000
H	-4.446717000	-1.938523000	-1.313934000
H	-5.950657000	-1.262274000	-0.685833000
H	-4.876961000	-1.172273000	1.612378000
H	-3.389854000	-1.772968000	0.884183000
H	-4.823388000	-3.704572000	0.139362000
H	-5.035063000	1.843737000	-1.500574000
H	-3.840358000	2.710137000	-0.521777000
H	-4.846612000	1.590616000	1.532414000
H	-5.886810000	0.678342000	0.445137000
H	-5.788065000	3.939801000	-0.823020000
H	-1.464698000	0.451699000	-0.946448000
H	-1.530524000	-1.078614000	-0.081068000
H	-2.495113000	0.203362000	1.916307000
H	-2.513285000	1.633501000	0.892559000

Sum of electronic and zero-point Energies= -1473.281258
Sum of electronic and thermal Energies= -1473.255786
Sum of electronic and thermal Enthalpies= -1473.254842
Sum of electronic and thermal Free Energies= -1473.341829

**ImC₂'**

Re	2.516370000	0.051868000	-0.208083000
N	4.658783000	-0.358290000	0.161954000
N	2.803694000	0.802063000	1.927880000
C	4.242839000	1.023896000	2.149402000
C	5.008509000	-0.155629000	1.588015000
C	2.824107000	1.690736000	-1.002235000
O	3.041220000	2.723905000	-1.525617000
C	2.445353000	-0.660149000	-1.929592000
O	2.449287000	-1.092021000	-3.020291000
Cl	2.220631000	-2.215003000	1.026212000
N	-5.365971000	0.057060000	0.295414000
C	-2.972677000	0.004011000	-0.215327000
C	-4.043773000	0.441554000	0.765699000
O	-1.716342000	0.337912000	0.351864000
C	-6.575752000	-1.945376000	-0.449020000
C	-5.703819000	-1.319600000	0.622952000
O	-6.940537000	-3.243596000	-0.012979000
C	-6.469587000	2.174959000	-0.275353000
C	-6.401618000	1.001743000	0.683919000
O	-7.434270000	3.088280000	0.218929000
C	-0.606302000	0.010250000	-0.379710000
O	0.444830000	0.365725000	0.235121000
O	-0.725089000	-0.540612000	-1.465352000
H	5.240318000	0.231413000	-0.419637000
H	4.877153000	-1.314277000	-0.093788000
H	2.461552000	0.078787000	2.554197000
H	2.277263000	1.642274000	2.132627000
H	4.479474000	1.147512000	3.207959000
H	4.523580000	1.940448000	1.629366000
H	6.081827000	-0.009535000	1.711921000
H	4.721357000	-1.061349000	2.121817000
H	-3.112399000	0.516975000	-1.169493000
H	-3.025230000	-1.070992000	-0.404228000
H	-3.829578000	0.026301000	1.761893000
H	-4.000092000	1.527421000	0.861798000
H	-6.011842000	-1.986413000	-1.387224000
H	-7.466444000	-1.329461000	-0.619687000
H	-6.210273000	-1.393810000	1.597415000
H	-4.786501000	-1.905327000	0.700412000
H	-7.467846000	-3.658729000	-0.697095000
H	-6.745772000	1.806805000	-1.269475000
H	-5.487677000	2.655162000	-0.356793000
H	-6.249906000	1.374185000	1.708611000
H	-7.368925000	0.496745000	0.672930000
H	-7.490539000	3.829897000	-0.385507000

Sum of electronic and zero-point Energies= -1661.897252
Sum of electronic and thermal Energies= -1661.869061
Sum of electronic and thermal Enthalpies= -1661.868117
Sum of electronic and thermal Free Energies= -1661.961464

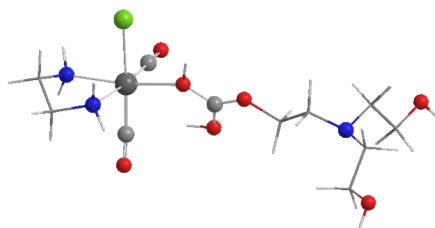


ImD₂'

Re	2.466537000	0.122746000	0.123418000
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N	4.651364000	0.130877000	0.264079000
N	3.000711000	-1.855453000	-0.838798000
C	4.375012000	-2.207560000	-0.430976000
C	5.243209000	-0.972884000	-0.533661000
C	2.266593000	-0.618493000	1.820299000
O	2.176442000	-1.079763000	2.892017000
C	2.287806000	1.837206000	0.867153000
O	2.248991000	2.903979000	1.340118000
Cl	2.875302000	0.976520000	-2.242791000
N	-5.381008000	-0.118463000	-0.305370000
C	-2.984104000	0.008728000	0.028728000
C	-4.096768000	-0.499198000	-0.865030000
O	-1.737068000	-0.323581000	-0.622350000
C	-6.576172000	1.897448000	0.424530000
C	-5.798530000	1.221752000	-0.689099000
O	-7.015271000	3.156259000	-0.053926000
C	-6.337740000	-2.211152000	0.549566000
C	-6.413647000	-1.123845000	-0.505673000
O	-7.311388000	-3.190782000	0.235689000
C	-0.610026000	0.007620000	-0.063664000
O	0.447338000	-0.277672000	-0.618859000
O	-0.685454000	0.636550000	1.079843000
H	4.956270000	0.055746000	1.226866000
H	5.019447000	1.011313000	-0.078962000
H	2.960705000	-1.731384000	-1.846973000
H	2.364374000	-2.610386000	-0.611694000
H	4.787863000	-3.004103000	-1.051372000
H	4.337201000	-2.562811000	0.598988000
H	6.258528000	-1.187707000	-0.201776000
H	5.282780000	-0.637342000	-1.569503000
H	-3.021888000	-0.476309000	1.003214000
H	-3.034516000	1.089150000	0.162381000
H	-3.958911000	-0.119022000	-1.886762000
H	-4.029956000	-1.586205000	-0.917568000
H	-5.923335000	2.009873000	1.297067000
H	-7.428703000	1.275700000	0.721387000
H	-6.403957000	1.211471000	-1.607380000
H	-4.915179000	1.826252000	-0.902737000
H	-7.496871000	3.598890000	0.646523000
H	-6.524246000	-1.766163000	1.533059000
H	-5.334593000	-2.653230000	0.566839000
H	-6.352825000	-1.577184000	-1.506159000
H	-7.392021000	-0.646551000	-0.435046000
H	-7.280271000	-3.877837000	0.903104000
H	0.239711000	0.814652000	1.354946000

Sum of electronic and zero-point Energies= -1662.336507
Sum of electronic and thermal Energies= -1662.308254
Sum of electronic and thermal Enthalpies= -1662.307310
Sum of electronic and thermal Free Energies= -1662.401090



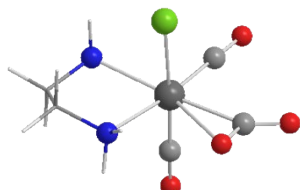
ImE₂'

S22

Re	2.529492000	0.171755000	0.070353000
N	4.675939000	0.213926000	0.285375000
N	3.041867000	-2.009830000	-0.253068000
C	4.417389000	-2.225854000	0.245397000
C	5.279716000	-1.061478000	-0.186444000
C	2.339628000	-0.068155000	1.921191000
O	2.286727000	-0.221578000	3.075402000
C	2.314943000	2.034972000	0.284931000
O	2.225281000	3.181277000	0.428912000
Cl	2.816406000	0.249084000	-2.418528000
N	-5.459252000	-0.118186000	-0.292185000
C	-3.090216000	0.002261000	0.040117000
C	-4.186470000	-0.464233000	-0.892436000
O	-1.805819000	-0.232230000	-0.660141000
C	-6.671838000	1.858833000	0.515648000
C	-5.915524000	1.221053000	-0.634543000
O	-7.142617000	3.119144000	0.074862000
C	-6.341479000	-2.230041000	0.596069000
C	-6.477541000	-1.145602000	-0.455950000
O	-7.310543000	-3.224509000	0.321137000
C	-0.720265000	-0.032304000	-0.062277000
O	0.395690000	-0.234317000	-0.704070000
O	-0.638668000	0.355072000	1.139656000
H	4.955388000	0.385990000	1.244429000
H	5.067203000	0.978359000	-0.255004000
H	3.007561000	-2.206648000	-1.250036000
H	2.409486000	-2.665112000	0.191628000
H	4.836535000	-3.158515000	-0.132553000
H	4.374766000	-2.287944000	1.332773000
H	6.293295000	-1.166399000	0.197542000
H	5.324483000	-1.015386000	-1.274071000
H	-3.071540000	-0.570238000	0.964039000
H	-3.140316000	1.068745000	0.249591000
H	-4.051941000	-0.018238000	-1.885963000
H	-4.111889000	-1.545277000	-1.009130000
H	-5.996577000	1.963479000	1.371990000
H	-7.505850000	1.217392000	0.822375000
H	-6.547507000	1.215777000	-1.534061000
H	-5.050996000	1.847686000	-0.861776000
H	-7.623147000	3.534906000	0.792322000
H	-6.494750000	-1.786521000	1.585868000
H	-5.331204000	-2.655921000	0.572558000
H	-6.443120000	-1.596746000	-1.457842000
H	-7.461059000	-0.686577000	-0.350269000
H	-7.249637000	-3.905714000	0.992561000
H	0.311526000	-0.407018000	-1.661170000
H	0.328168000	0.462893000	1.375550000

Sum of electronic and zero-point Energies= -1662.710293
Sum of electronic and thermal Energies= -1662.681620
Sum of electronic and thermal Enthalpies= -1662.680675
Sum of electronic and thermal Free Energies= -1662.775883

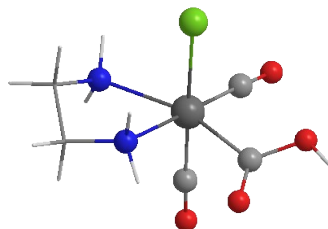
Reaction step B2''



ImB₂

Re	0.112895000	0.084819000	0.065703000
O	0.774773000	2.951637000	-0.660441000
N	-1.786004000	0.503923000	1.273603000
N	-1.587993000	-0.083370000	-1.458078000
C	0.509767000	1.846408000	-0.379452000
C	1.350030000	0.231732000	1.487229000
Cl	-0.559674000	-2.346677000	0.572313000
O	2.117877000	0.343249000	2.348408000
C	-2.890743000	0.874249000	0.370161000
C	-2.908101000	-0.085785000	-0.801072000
C	1.861110000	-0.553874000	-1.049604000
O	1.176343000	-0.942686000	-2.033597000
O	3.074193000	-0.565998000	-0.870583000
H	-1.657347000	1.220497000	1.976123000
H	-2.016595000	-0.355259000	1.764425000
H	-1.445781000	-0.942767000	-1.975675000
H	-1.532204000	0.669737000	-2.133142000
H	-3.854092000	0.856500000	0.883419000
H	-2.708773000	1.891871000	0.021980000
H	-3.092772000	-1.097418000	-0.439868000
H	-3.705007000	0.179025000	-1.496833000

Sum of electronic and zero-point Energies= -1144.533635
 Sum of electronic and thermal Energies= -1144.518334
 Sum of electronic and thermal Enthalpies= -1144.517390
 Sum of electronic and thermal Free Energies= -1144.578755

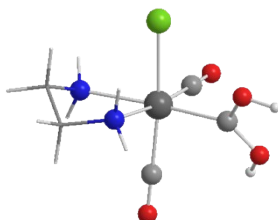


ImC₂

Re	0.082928000	0.041652000	0.162451000
O	0.903784000	2.954237000	-0.324950000
N	-1.886318000	0.612492000	1.128703000
N	-1.414064000	-0.209429000	-1.473104000
C	0.562974000	1.868253000	-0.166160000
C	1.351469000	0.270105000	1.595532000
Cl	-0.484642000	-2.293135000	0.672932000
O	2.118510000	0.452085000	2.429677000
C	-3.031331000	0.237807000	0.266716000
C	-2.667881000	0.508698000	-1.176777000
C	1.469829000	-0.424091000	-1.375713000
O	2.610936000	-1.041172000	-0.978952000
O	1.303871000	-0.219277000	-2.566351000
H	-1.923292000	1.602932000	1.340783000
H	-1.963190000	0.137272000	2.022454000
H	-1.601814000	-1.204035000	-1.568580000

H	-1.004321000	0.092840000	-2.352219000
H	-3.214189000	-0.827258000	0.407996000
H	-3.930778000	0.782641000	0.550878000
H	-3.474453000	0.194028000	-1.838914000
H	-2.493008000	1.573510000	-1.333698000
H	3.119847000	-1.245606000	-1.778556000

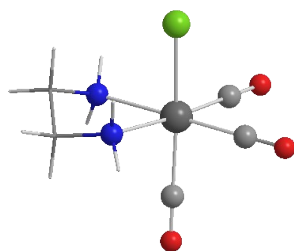
Sum of electronic and zero-point Energies= -1144.999286
Sum of electronic and thermal Energies= -1144.983754
Sum of electronic and thermal Enthalpies= -1144.982810
Sum of electronic and thermal Free Energies= -1145.044486



ImD₂''

Re	0.058038000	0.050952000	0.126706000
O	0.376613000	3.129018000	-0.242760000
N	-1.942908000	0.410890000	1.076756000
N	-1.356399000	-0.127900000	-1.607455000
C	0.264713000	2.004765000	-0.118688000
C	1.127906000	0.075343000	1.724518000
Cl	-0.403409000	-2.283416000	0.402514000
O	1.758287000	0.073039000	2.678755000
C	-3.035870000	0.018077000	0.151411000
C	-2.678631000	0.439451000	-1.255214000
C	1.787006000	-0.295939000	-0.999775000
O	1.908467000	-1.392839000	-1.680802000
O	2.829499000	0.474104000	-1.165898000
H	-2.065741000	1.379396000	1.355771000
H	-2.021561000	-0.124655000	1.935274000
H	-1.458189000	-1.119033000	-1.812822000
H	-1.021147000	0.301770000	-2.462330000
H	-3.133468000	-1.065534000	0.204722000
H	-3.980375000	0.464968000	0.457365000
H	-3.445409000	0.107141000	-1.954199000
H	-2.606033000	1.525069000	-1.322577000
H	2.762758000	-1.436220000	-2.141551000
H	2.795747000	1.266108000	-0.618349000

Sum of electronic and zero-point Energies= -1145.409429
Sum of electronic and thermal Energies= -1145.393972
Sum of electronic and thermal Enthalpies= -1145.393028
Sum of electronic and thermal Free Energies= -1145.454240



ImE₂''

Re	0.170667000	0.017992000	0.010786000
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S25

C	0.355410000	2.007234000	0.136258000
O	0.481945000	3.128967000	0.199347000
C	1.597240000	-0.262575000	1.329173000
O	2.434047000	-0.429316000	2.077341000
C	1.660175000	0.016518000	-1.292643000
O	2.531464000	0.015633000	-2.016143000
N	-1.568203000	0.013020000	1.401245000
N	-1.565959000	0.242846000	-1.372355000
C	-2.790137000	0.614565000	-0.622497000
C	-2.837659000	-0.187578000	0.655468000
Cl	-0.182159000	-2.315206000	-0.263509000
H	-1.627052000	0.872626000	1.939441000
H	-1.468783000	-0.724734000	2.092010000
H	-1.709474000	-0.655741000	-1.827231000
H	-1.416481000	0.907080000	-2.124393000
H	-3.680931000	0.431513000	-1.221543000
H	-2.739568000	1.681251000	-0.405716000
H	-3.690896000	0.105165000	1.264486000
H	-2.920795000	-1.250398000	0.432537000

Sum of electronic and zero-point Energies= -1069.005204
 Sum of electronic and thermal Energies= -1068.991075
 Sum of electronic and thermal Enthalpies= -1068.990131
 Sum of electronic and thermal Free Energies= -1069.048911