

SUPPORTING INFORMATION

Organocatalytic vs Ru-based Electrochemical Hydrogenation of Nitrobenzene in Competition with Hydrogen Evolution Reaction

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1. Experimental Results

1.1. Electrochemical Data

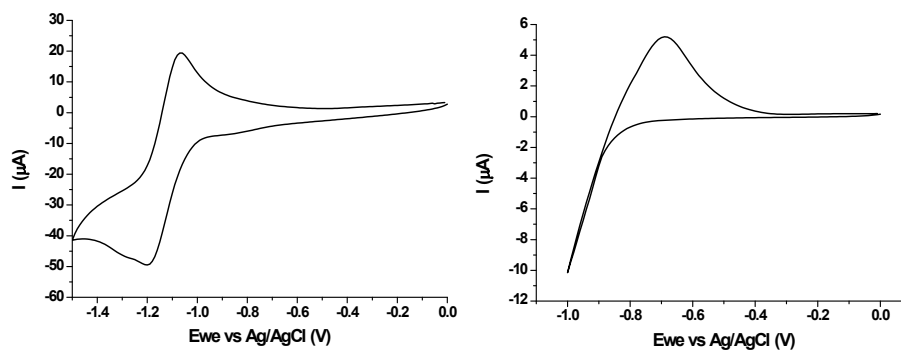


Fig. S1 Cyclic voltammetry of 10 mM of nitrobenzene at a scan rate of 50 mV/s and potential windows of -1.5 – 0 V (left) and -1 V – 0 V (right).

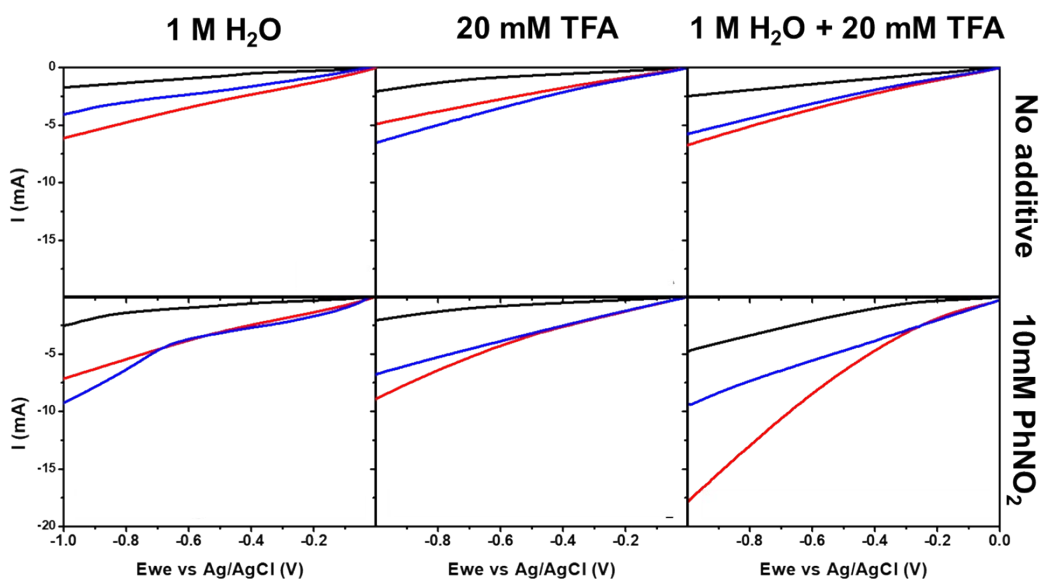


Fig. S2 Linear voltammetry measured using pristine (black), oxidised (red) and Ru-based (blue) carbon fibre electrodes in the absence (top) and in the presence (bottom) of 10 mM of nitrobenzene using as electrolyte: 0.2 M of NaClO_4 in CH_3CN with different proton sources: 1 M of H_2O (left), 20 mM of TFA (middle) and their mixture (right).

Table S1. Current intensities at -1 V vs Ag/AgCl corresponding to the linear sweep voltammetries of Fig. S2.

[PhNO ₂] (mM)	Proton Source	I of CF (mA)	I of ox-CF (mA)	I of Ru-CF (mA)
0	1 M H ₂ O	-1.72	-6.13	-4.08
	20 mM TFA	-2.08	-4.92	-6.53
	1 M H ₂ O + 20 mM TFA	-2.48	-6.76	-5.77
10	1 M H ₂ O	-2.53	-7.14	-9.24
	20 mM TFA	-2.05	-8.93	-6.78
	1 M H ₂ O + 20 mM TFA	-4.85	-17.89	-9.31

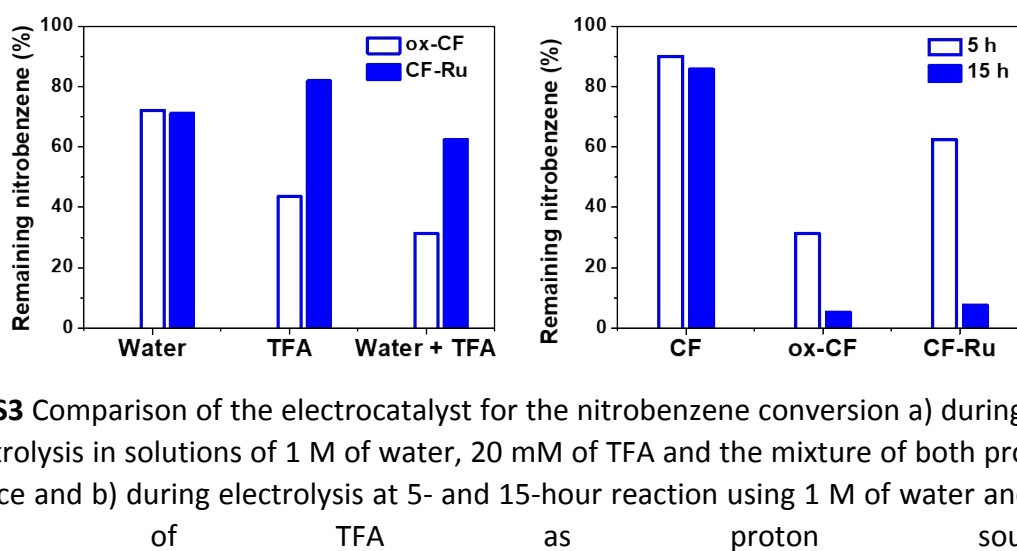


Fig. S3 Comparison of the electrocatalyst for the nitrobenzene conversion a) during 5 h electrolysis in solutions of 1 M of water, 20 mM of TFA and the mixture of both proton source and b) during electrolysis at 5- and 15-hour reaction using 1 M of water and 20 mM of TFA as proton source.

1.2. Chromatography Data

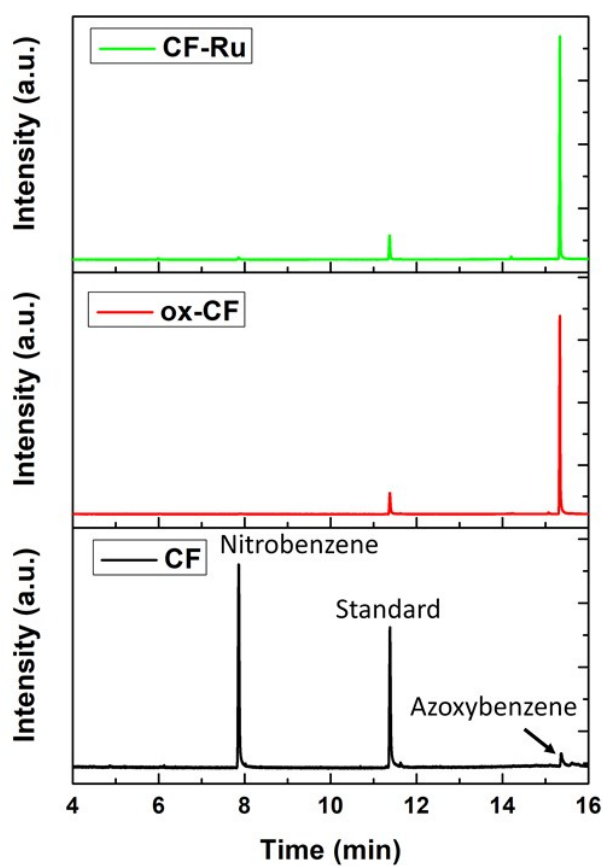


Fig. S4 Gas chromatograms of electrocatalytic nitrobenzene reduction using pristine carbon fibre (black curve), oxidised carbon fibre (red curve) and Ru-modified carbon fibre (green curve).

2. Computational Details

2.1. Adsorption Energies of Reagents on $H_{88}Ru_{57}$ NPs

Table S2. Adsorption energies (in kcal·mol⁻¹) of the different reagents on the $H_{88}Ru_{57}$ nanoparticle model.

Species	E_{ads}
PhNO ₂ (perpendicular)	-10.5
PhNO ₂ (parallel)	-10.6
CH ₃ COOH	-9.0
(H ₃ O)(H ₂ O) ₃ Cl	-3.3
PhNO	-18.0
PhNHOH	-8.4
PhNONPh	-10.8
PhNNPh	-11.1
PhNHNHPh	-8.8

2.2. Comparative Energy Data of ox-CF and Ru-CF catalyst models

Table S3 Electronic energies (in kcal·mol⁻¹) of the hydride transfer to PhNO₂ using ox-CF as catalyst.

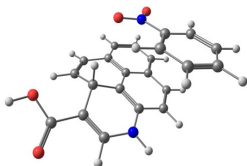
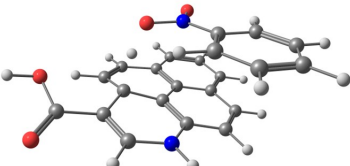
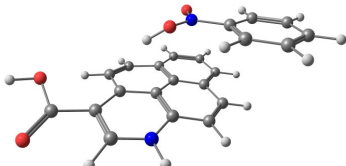
				
M062X	ΔG	0.0	$E_a = +23.5$	+3.6
	ΔE	0.0	$E_a = +25.5$	+5.7
PBE-D2	ΔG	0.0	$E_a = +7.0$	+0.6
	ΔE	0.0	$E_a = +8.7$	+1.0

Table S4 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to PhNO₂ using Ru-CF catalyst model.

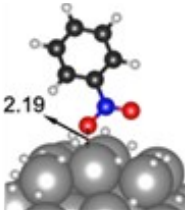
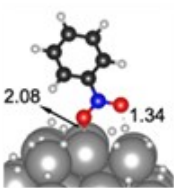
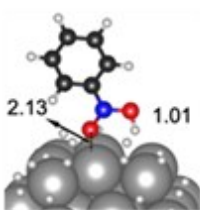
			
		TS1 b	
ΔE	0.0	$E_a = +10.8$	+4.3

Table S5 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to TFA using ox-CF catalyst model.

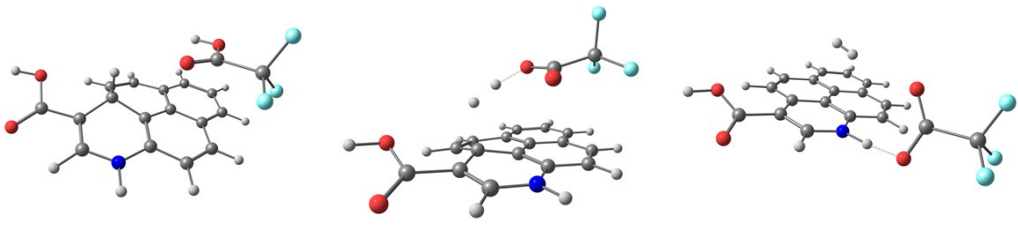
				
M062X	ΔG	0.0	$E_a = +31.2$	-12.4
	ΔE	0.0	$E_a = +38.7$	-3.9
PBE-D2	ΔG	0.0	$E_a = +19.2$	-18.3
	ΔE	0.0	$E_a = +23.7$	-10.7

Table S6 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to TFA using Ru-CF catalyst model.

			
ΔE	0.0	$E_a = +17.0$	+7.3

Table S7 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to [(H₃O)(H₂O)₃]⁺ using ox-CF catalyst model.

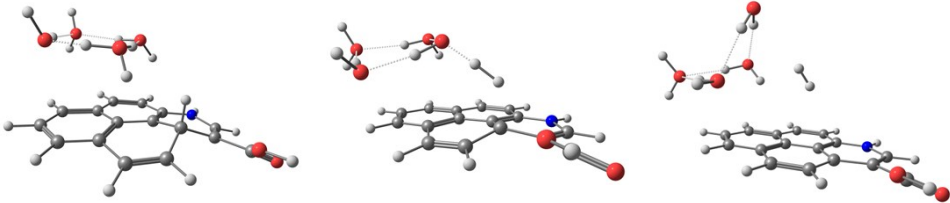
				
M062X	ΔG	0.0	E _a = +35.1	-6.2
	ΔE	0.0	E _a = +40.1	+0.7
PBE-D2	ΔG	0.0	E _a = +19.2	-6.0
	ΔE	0.0	E _a = +23.7	-0.3

Table S8 Electronic energies (in kcal·mol⁻¹) of the catalytic hydride transfer to [(H₃O)(H₂O)₃]⁺ using Ru-CF catalyst model.

				
ΔE	0.0	E _a = +24.9	+1.5	

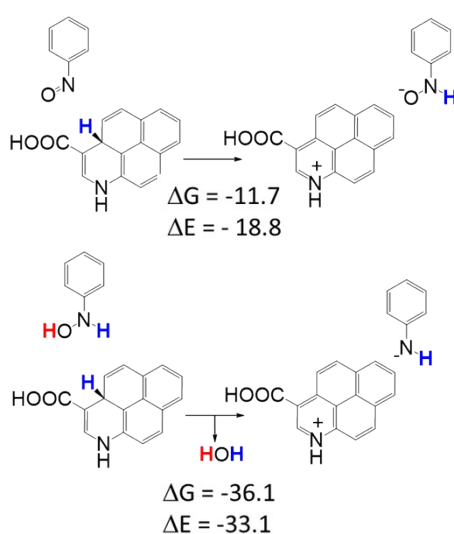


Fig. S5 Catalytic hydrogenation of PhNO using ox-CF (M062X). Energy values are in kcal·mol⁻¹.

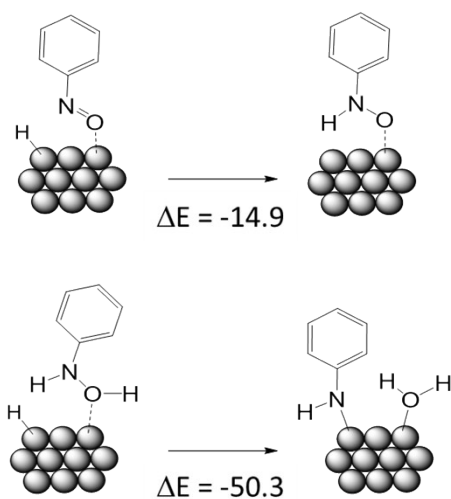


Fig. S6 Catalytic hydrogenation of PhNO using Ru-CF. Energy values are in kcal·mol⁻¹.

Table S9 Electronic energies (in kcal·mol⁻¹) of the catalytic hydrogenation of azoxynitrobenzene using ox-CF catalyst model.

M062X	ΔG	0.0	E _a = +22.1	+8.1
	ΔE	0.0	E _a = +23.2	+8.1
PBE-D2	ΔG	0.0	E _a = +6.7	+0.8
	ΔE	0.0	E _a = +8.2	+0.5

Table S10 Electronic energies (in kcal·mol⁻¹) of the catalytic hydrogenation of azoxynitrobenzene using Ru-CF catalyst model.

ΔE	0.0	E _a = +24.9	-31.9

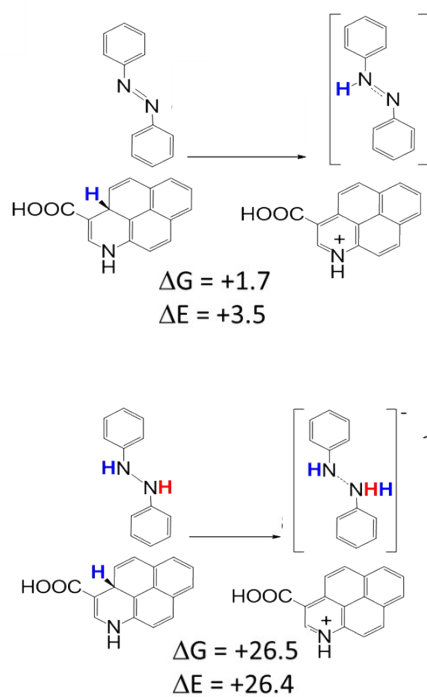


Fig. S7 Catalytic hydrogenation of PhNONPh using ox-CF (M062X). Energy values are in $\text{kcal}\cdot\text{mol}^{-1}$.

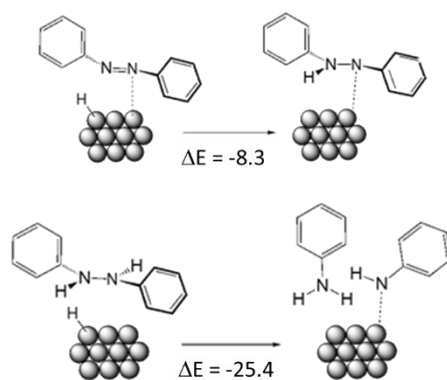
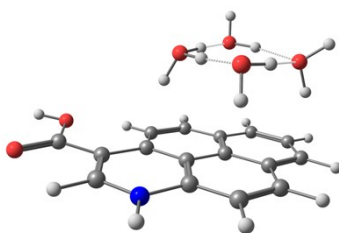


Fig. S8 Catalytic hydrogenation of PhNONPh using Ru-CF. Energy values are in $\text{kcal}\cdot\text{mol}^{-1}$.

2.3. M062X optimized geometries associated with the Organic Catalyst: ox-CF

2.3.1. Hydride generation

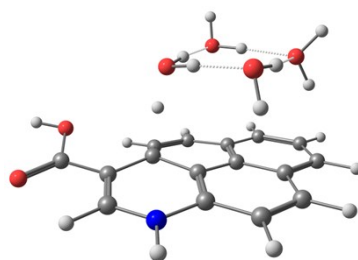


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1126.899548

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6	-3.338805000	0.947485000	-1.112017000
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6	1.118998000	-1.533745000	-1.088456000
6	2.807565000	0.190953000	-0.194265000
6	2.974853000	1.500925000	0.169501000
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6	-1.692267000	2.619636000	-0.285161000
1	-2.479405000	3.358399000	-0.184978000
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1	-4.610827000	-0.614058000	-1.832913000
1	-2.819883000	-2.307898000	-1.997698000
1	-4.130562000	1.686677000	-1.060340000
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6	-0.376194000	2.958818000	0.030075000



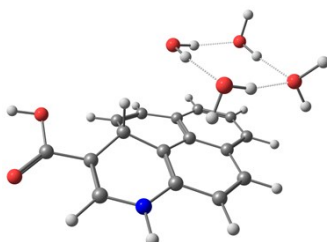
(Transition state)

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6	-2.140672000	1.335993000	-0.613762000
6	-3.473996000	0.932294000	-0.933476000
6	-0.234512000	-1.766340000	-1.638984000
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6	1.322268000	-0.262111000	-0.487551000
6	1.032629000	-1.430619000	-1.272673000
6	2.709565000	0.279465000	-0.277426000
6	2.875769000	1.587927000	0.051654000
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1	-2.878481000	-2.227454000	-2.047712000
1	-4.282350000	1.641142000	-0.789615000
1	1.840978000	-2.114843000	-1.498915000
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6	3.914647000	-0.527318000	-0.186732000
8	5.061317000	-0.105377000	-0.122635000
8	3.676513000	-1.853490000	-0.140928000
1	4.530901000	-2.304921000	-0.063424000
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6	-0.525791000	2.984439000	0.122465000

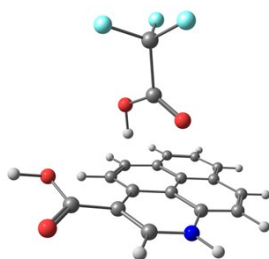


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Sum of electronic and thermal Free Energies= -1126.925658

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1	-2.251632000	-2.886542000	-1.850359000
1	-3.925384000	1.062487000	-1.616248000
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1	2.118423000	3.369993000	-0.168142000
1	-0.185590000	3.833683000	-0.515914000

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1	-1.968849000	1.163626000	1.993471000
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1	-3.664078000	-0.793611000	1.345153000
1	-3.893761000	-1.986057000	2.272658000
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1	-4.047063000	1.560040000	0.802358000
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6	-0.373788000	2.768522000	-0.600836000

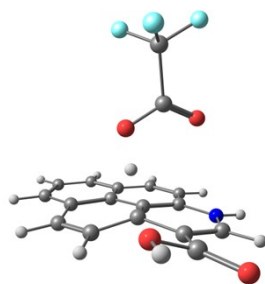


Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.558819

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6	-3.298852000	-0.645225000	0.785528000
6	-4.323169000	-1.502039000	0.285854000
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7	-0.249932000	1.956731000	2.155748000
1	-0.189148000	2.151731000	3.145598000
1	-2.047530000	0.729874000	3.654863000
6	-2.147756000	0.498724000	2.598088000
6	1.931286000	-1.200899000	0.274719000
8	1.515208000	-0.778521000	1.315317000
8	1.549476000	-0.893513000	-0.938781000
1	0.825690000	-0.218199000	-0.922956000
6	3.057188000	-2.248401000	0.217725000
9	3.471920000	-2.558439000	1.438811000
9	2.632140000	-3.363171000	-0.380019000
9	4.097806000	-1.784451000	-0.477091000



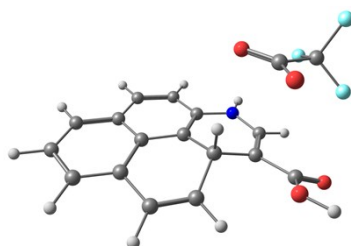
(Transition state)

Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.554150

6	-4.376217000	-1.584684000	-1.107139000
6	-3.490997000	-0.968302000	-2.014720000
6	-2.454590000	-0.161942000	-1.558902000
6	-2.275807000	0.010669000	-0.141849000
6	-3.210346000	-0.575812000	0.767589000
6	-4.256631000	-1.394051000	0.245655000
6	-1.572970000	0.558300000	-2.447733000
6	-1.192020000	0.798057000	0.343872000
6	-0.155631000	1.275164000	-0.578769000
6	-0.522363000	1.280039000	-1.967098000
6	0.833888000	2.229540000	0.032544000
6	0.784942000	2.480143000	1.369911000
6	-1.137412000	1.061760000	1.714240000
6	-3.068867000	-0.319859000	2.146912000
1	-3.771298000	-0.761542000	2.845153000
1	-1.763934000	0.508441000	-3.514123000
1	-5.174747000	-2.211290000	-1.491898000
1	-3.625719000	-1.106635000	-3.082292000
1	-4.953290000	-1.853931000	0.938709000
1	0.118166000	1.800419000	-2.668764000
1	1.520524000	3.121176000	1.840346000
6	2.013200000	2.743558000	-0.637269000
8	2.797626000	3.572157000	-0.190995000
8	2.227086000	2.199401000	-1.853767000
1	3.039358000	2.589056000	-2.210894000
7	-0.129373000	1.933147000	2.193122000
1	-0.103283000	2.150304000	3.178805000
1	-1.969103000	0.734868000	3.660468000
6	-2.059709000	0.506231000	2.602752000
6	1.819141000	-1.251221000	0.307914000
8	1.652401000	-0.771818000	1.408338000
8	1.314129000	-0.898307000	-0.814974000
1	0.645330000	0.059707000	-0.711833000
6	2.759628000	-2.463094000	0.141808000
9	3.310290000	-2.822204000	1.298762000

9	2.095552000	-3.518554000	-0.343395000
9	3.748628000	-2.183803000	-0.715664000

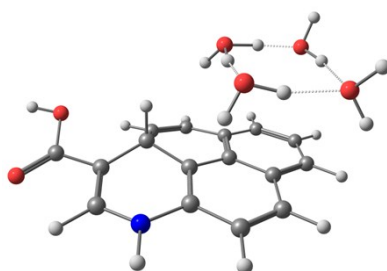


Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.592203

6	-5.309173000	0.050073000	-0.902684000
6	-4.507335000	1.213690000	-0.901333000
6	-3.201004000	1.173806000	-0.466227000
6	-2.647472000	-0.066409000	-0.017421000
6	-3.484709000	-1.209222000	0.074215000
6	-4.817013000	-1.130698000	-0.407159000
6	-2.391952000	2.382832000	-0.297522000
6	-1.295613000	-0.126483000	0.401097000
6	-0.348185000	1.012839000	0.047319000
6	-1.095441000	2.329744000	0.017635000
6	0.865978000	0.964709000	0.960075000
6	1.183471000	-0.168878000	1.634205000
6	-0.858316000	-1.261992000	1.051541000
6	-2.959516000	-2.387355000	0.666321000
1	-3.587225000	-3.269653000	0.731652000
1	-2.898451000	3.338484000	-0.394099000
1	-6.328791000	0.105745000	-1.266286000
1	-4.931244000	2.159320000	-1.224067000
1	-5.440632000	-2.017739000	-0.364173000
1	-0.534897000	3.242371000	0.176261000
1	2.100700000	-0.237397000	2.206704000
6	1.890231000	2.006990000	0.972333000
8	2.801393000	2.098940000	1.775872000
8	1.765426000	2.882826000	-0.038037000
1	2.491040000	3.523081000	0.024727000
7	0.414685000	-1.280625000	1.616834000
1	0.722063000	-2.106009000	2.111894000
1	-1.297221000	-3.284519000	1.669389000
6	-1.691832000	-2.401793000	1.177162000
6	2.157161000	-0.556463000	-1.472858000
8	1.222333000	-1.367550000	-1.530283000
8	2.291475000	0.563199000	-1.989958000
1	-0.004406000	0.839073000	-0.987217000
6	3.396438000	-1.020470000	-0.657291000
9	3.124355000	-2.005888000	0.210120000
9	4.356069000	-1.482761000	-1.482378000
9	3.947014000	-0.019931000	0.047832000

2.3.2. *Hydrogen Evolution Reaction*

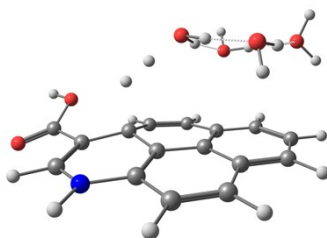


Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1127.359239

6	3.194606000	0.920883000	-1.783206000
6	2.096804000	1.801067000	-1.657893000
6	0.870030000	1.346433000	-1.226881000
6	0.707598000	-0.034422000	-0.893486000
6	1.789979000	-0.929198000	-1.092642000
6	3.042859000	-0.416726000	-1.520933000
6	-0.323256000	2.195454000	-1.217062000
6	-0.547455000	-0.511644000	-0.436994000
6	-1.605611000	0.472013000	0.045127000
6	-1.486654000	1.783733000	-0.704541000
6	-2.973044000	-0.190528000	0.002641000
6	-3.082544000	-1.540817000	-0.011751000
6	-0.743158000	-1.876102000	-0.358831000
6	1.571126000	-2.316393000	-0.885413000
1	2.395522000	-3.008131000	-1.022105000
1	-0.243316000	3.170599000	-1.687767000
1	4.151979000	1.306163000	-2.114333000
1	2.211782000	2.846003000	-1.926771000
1	3.869587000	-1.107663000	-1.654586000
1	-2.357005000	2.425098000	-0.752157000
1	-4.049433000	-2.023516000	0.059534000
6	-4.215050000	0.534054000	0.264631000
8	-5.340063000	0.089020000	0.128334000
8	-4.010399000	1.772805000	0.743475000
1	-4.874241000	2.179521000	0.913824000
7	-2.013406000	-2.370010000	-0.066318000
1	-2.165119000	-3.369094000	-0.099254000
1	0.136769000	-3.846761000	-0.459018000
1	-1.373531000	0.707854000	1.100130000
8	1.205379000	1.582739000	2.022991000
1	1.046153000	0.550126000	2.111264000
1	2.227981000	1.693071000	1.724844000
1	0.625610000	1.956284000	1.342106000

8	1.103781000	-0.882671000	2.298845000
1	0.465048000	-1.385525000	1.777830000
1	1.990626000	-1.142816000	1.973272000
8	3.570469000	1.656953000	1.372251000
1	3.803085000	0.703947000	1.368559000
1	4.120294000	2.068550000	2.051078000
8	3.731466000	-1.078408000	1.554265000
1	4.006183000	-1.594673000	0.785987000
1	4.286923000	-1.385059000	2.282241000
6	0.326083000	-2.784043000	-0.568057000



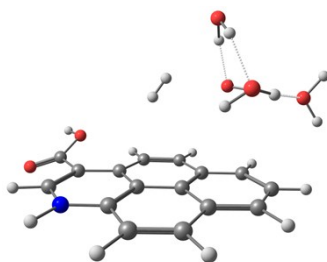
(Transition state)

Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1127.303289

6	-3.306205000	0.898714000	-1.264807000
6	-2.516572000	-0.240240000	-1.481535000
6	-1.170108000	-0.243214000	-1.149303000
6	-0.598118000	0.915252000	-0.560946000
6	-1.383359000	2.081374000	-0.387881000
6	-2.748380000	2.048100000	-0.743483000
6	-0.292860000	-1.351360000	-1.474004000
6	0.773668000	0.917254000	-0.194911000
6	1.541195000	-0.325016000	-0.228952000
6	0.993340000	-1.384127000	-1.087037000
6	2.971337000	-0.155562000	-0.040929000
6	3.466604000	1.050988000	0.371266000
6	1.338489000	2.097116000	0.276181000
6	-0.763925000	3.255614000	0.136305000
1	-1.367193000	4.146801000	0.271629000
1	-0.701521000	-2.159257000	-2.070565000
1	-4.356248000	0.881175000	-1.533110000
1	-2.951931000	-1.126617000	-1.931339000
1	-3.348305000	2.940720000	-0.601591000
1	1.630211000	-2.213872000	-1.355842000
1	4.521404000	1.190422000	0.569855000
6	3.955488000	-1.256287000	-0.078810000
8	5.151912000	-1.093831000	-0.169533000
8	3.399775000	-2.460440000	0.058969000
1	4.099633000	-3.133680000	0.042786000
7	2.679266000	2.117434000	0.570039000
1	3.096570000	2.985032000	0.892815000
1	1.042778000	4.168603000	0.823844000
1	1.168503000	-0.961399000	1.159693000
8	-0.831163000	-1.737605000	1.789056000
1	-1.446716000	-0.964472000	1.903826000
1	-1.245557000	-2.290163000	1.079220000
1	0.339345000	-1.297377000	1.450650000
8	-2.684866000	0.137087000	2.031812000

	1	-2.512178000	0.999643000	1.638169000
	1	-3.396711000	-0.261307000	1.496705000
	8	-2.334637000	-3.088181000	0.019694000
	1	-3.159367000	-2.598532000	0.200792000
	1	-2.501491000	-3.986231000	0.327953000
	8	-4.504713000	-1.460522000	0.670265000
	1	-5.050372000	-1.140789000	-0.058247000
	1	-5.122157000	-1.870122000	1.288915000
6		0.562069000	3.274280000	0.444090000

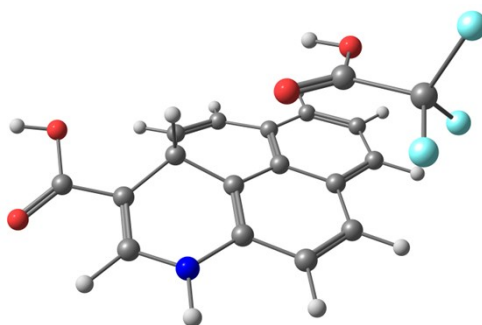


Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1127.369125

6	-2.934456000	1.372643000	-1.410944000
6	-2.249943000	0.201095000	-1.712355000
6	-0.918628000	0.033173000	-1.311457000
6	-0.280841000	1.064318000	-0.583662000
6	-0.982481000	2.256834000	-0.277820000
6	-2.310626000	2.390393000	-0.698228000
6	-0.172334000	-1.149053000	-1.612020000
6	1.065345000	0.896587000	-0.164112000
6	1.782552000	-0.300775000	-0.450167000
6	1.116979000	-1.314567000	-1.210350000
6	3.120482000	-0.385511000	0.023830000
6	3.669962000	0.682944000	0.695231000
6	1.674207000	1.948602000	0.551221000
6	-0.312491000	3.289078000	0.454697000
1	-0.858381000	4.197789000	0.683824000
1	-0.661702000	-1.931325000	-2.182105000
1	-3.964316000	1.491411000	-1.726082000
1	-2.737075000	-0.595045000	-2.265173000
1	-2.849746000	3.299689000	-0.456271000
1	1.645318000	-2.218931000	-1.466934000
1	4.687805000	0.670814000	1.060176000
6	4.047579000	-1.548653000	-0.123057000
8	5.246828000	-1.433389000	-0.054455000
8	3.433684000	-2.711741000	-0.288583000
1	4.100560000	-3.413694000	-0.371905000
7	2.960436000	1.789563000	0.942917000
1	3.407777000	2.549146000	1.454372000
1	1.493623000	3.926377000	1.408053000
1	-0.154364000	-1.198218000	1.484765000
8	-2.866499000	-2.484807000	2.759454000
1	-3.002174000	-1.531320000	2.639756000
1	-2.769648000	-2.777609000	1.838198000
1	-0.739737000	-1.523033000	1.807908000
8	-3.092628000	0.118656000	1.653903000
1	-2.248382000	-0.012217000	1.206079000
1	-3.753906000	-0.140538000	0.988744000

8	-2.690910000	-2.672358000	-0.038143000
1	-3.504147000	-2.159737000	-0.193746000
1	-2.818821000	-3.500588000	-0.512745000
8	-4.891704000	-0.979963000	-0.198967000
1	-5.153187000	-0.543880000	-1.018196000
1	-5.708396000	-1.321851000	0.184147000
6	0.977309000	3.148661000	0.857698000

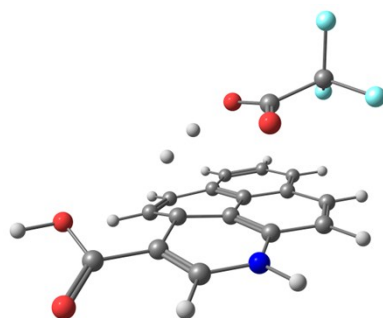


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1348.026567

6	2.168104000	-3.043656000	0.695892000
6	0.928822000	-3.325295000	0.077192000
6	-0.083694000	-2.390863000	0.060046000
6	0.130680000	-1.111087000	0.662805000
6	1.348388000	-0.859868000	1.348833000
6	2.367596000	-1.847049000	1.334645000
6	-1.428367000	-2.693376000	-0.434944000
6	-0.878513000	-0.120671000	0.598793000
6	-2.039695000	-0.283401000	-0.373443000
6	-2.363718000	-1.750077000	-0.569715000
6	-3.196631000	0.599369000	0.071144000
6	-2.971086000	1.667975000	0.871794000
6	-0.716043000	1.034703000	1.335957000
6	1.505957000	0.383707000	2.015726000
1	2.439303000	0.593674000	2.526927000
1	-1.656341000	-3.732339000	-0.653233000
1	2.951427000	-3.792665000	0.683988000
1	0.758818000	-4.300617000	-0.367702000
1	3.304876000	-1.634054000	1.837643000
1	-3.358317000	-2.012545000	-0.904536000
1	-3.768556000	2.360495000	1.110621000
6	-4.536382000	0.543714000	-0.520966000
8	-5.513926000	1.138653000	-0.123153000
8	-4.589835000	-0.220398000	-1.631366000
1	-5.501261000	-0.184239000	-1.962113000
7	-1.753464000	1.963273000	1.387924000
1	-1.656621000	2.764040000	1.997118000
1	0.585108000	2.232155000	2.574125000
1	-1.680270000	0.080612000	-1.352173000
6	0.485826000	1.294096000	2.037996000
6	3.236917000	1.344141000	-0.778048000
9	2.908926000	2.475450000	-0.168433000
9	3.904859000	0.575964000	0.081258000
9	4.061894000	1.635063000	-1.788957000
6	1.979885000	0.642234000	-1.324546000

8	0.931546000	1.201210000	-1.426963000
8	2.280650000	-0.589547000	-1.689400000
1	1.479225000	-1.042646000	-2.008855000



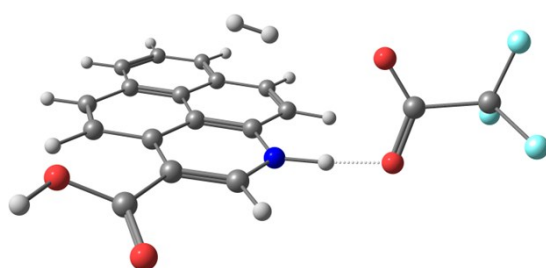
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.974330

6	-2.256312000	3.582511000	-0.066897000
6	-0.976696000	3.674389000	-0.629124000
6	-0.025099000	2.690714000	-0.392330000
6	-0.359230000	1.588539000	0.435558000
6	-1.636948000	1.519317000	1.038972000
6	-2.581753000	2.525063000	0.760284000
6	1.328948000	2.780501000	-0.900110000
6	0.598264000	0.565415000	0.669886000
6	1.824278000	0.518578000	-0.114509000
6	2.215920000	1.780314000	-0.755220000
6	2.798783000	-0.453146000	0.342635000
6	2.446826000	-1.377091000	1.288837000
6	0.288131000	-0.444955000	1.575691000
6	-1.927835000	0.426117000	1.911872000
1	-2.915007000	0.364052000	2.357008000
1	1.621350000	3.695563000	-1.404521000
1	-2.988202000	4.354695000	-0.271416000
1	-0.715652000	4.523487000	-1.251936000
1	-3.566305000	2.457852000	1.210526000
1	3.217943000	1.871690000	-1.146157000
1	3.140324000	-2.142128000	1.611997000
6	4.136975000	-0.660272000	-0.253743000
8	5.017302000	-1.303822000	0.261194000
8	4.265940000	-0.104379000	-1.465172000
1	5.158668000	-0.304772000	-1.791847000
7	1.234037000	-1.392160000	1.856577000
1	1.007845000	-2.126808000	2.519286000
1	-1.197804000	-1.342400000	2.867616000
1	1.319304000	-0.187638000	-1.491678000
6	-0.989412000	-0.517534000	2.195991000
6	-2.642572000	-1.854140000	-0.772407000
9	-2.928734000	-2.551789000	0.329316000
9	-3.275893000	-0.680040000	-0.683582000

9	-3.177647000	-2.513951000	-1.813885000
6	-1.114858000	-1.700826000	-0.978254000
8	-0.384138000	-2.521308000	-0.463744000
8	-0.831896000	-0.709077000	-1.727110000
1	0.417620000	-0.458724000	-1.675684000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1348.045083

6	-3.970466000	-3.572466000	-0.190061000
6	-4.541824000	-2.311593000	-0.314733000
6	-3.756858000	-1.160767000	-0.183448000
6	-2.374064000	-1.292184000	0.080364000
6	-1.795863000	-2.579215000	0.211022000
6	-2.611137000	-3.707499000	0.070221000
6	-4.303886000	0.157398000	-0.299015000
6	-1.569448000	-0.127980000	0.214399000
6	-2.126228000	1.174668000	0.063855000
6	-3.537331000	1.273122000	-0.183077000
6	-1.238880000	2.273051000	0.198472000
6	0.092010000	2.032135000	0.492194000
6	-0.195300000	-0.289217000	0.494976000
6	-0.392612000	-2.687116000	0.488697000
1	0.037572000	-3.677538000	0.590134000
1	-5.368680000	0.254338000	-0.483604000
1	-4.588081000	-4.456348000	-0.293438000
1	-5.602487000	-2.206026000	-0.515162000
1	-2.167300000	-4.692207000	0.169463000
1	-3.993867000	2.245284000	-0.275976000
1	0.795693000	2.847177000	0.605361000
6	-1.570140000	3.722091000	0.046552000
8	-0.859893000	4.602127000	0.457516000
8	-2.700897000	3.958498000	-0.620128000
1	-2.824778000	4.921606000	-0.672054000
7	0.581439000	0.803741000	0.634978000
1	1.687867000	0.656894000	0.779605000
1	1.443813000	-1.662235000	0.857078000
1	0.007992000	0.726076000	-2.442134000
6	0.387360000	-1.586097000	0.630443000
6	4.970150000	-0.461091000	-0.189842000
9	5.746134000	0.516401000	0.300740000
9	5.129357000	-1.526912000	0.613811000
9	5.455913000	-0.792492000	-1.387891000

6	3.482466000	-0.039299000	-0.243452000
8	3.071975000	0.394467000	0.871573000
8	2.883951000	-0.186695000	-1.296082000
1	0.670767000	0.589001000	-2.132482000

2.3.3. Hydride Transfer processes



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1257.874819

6	-2.466094000	3.215396000	0.753161000
6	-1.221471000	3.491054000	0.142834000
6	-0.209955000	2.556924000	0.141827000
6	-0.426466000	1.283975000	0.755337000
6	-1.649217000	1.038947000	1.433956000
6	-2.670551000	2.024032000	1.400304000
6	1.135499000	2.854661000	-0.350547000
6	0.589816000	0.295933000	0.719920000
6	1.787004000	0.454614000	-0.211082000
6	2.085165000	1.920692000	-0.445131000
6	2.941793000	-0.390148000	0.307323000
6	2.698161000	-1.456404000	1.106863000
6	0.421702000	-0.842903000	1.480603000
6	-1.804329000	-0.185743000	2.133829000
1	-2.740402000	-0.386223000	2.644642000
1	1.356075000	3.888460000	-0.599453000
1	-3.249780000	3.963868000	0.726849000
1	-1.049131000	4.460941000	-0.312830000
1	-3.610224000	1.817367000	1.902209000
1	3.078594000	2.191919000	-0.777045000
1	3.491991000	-2.135356000	1.392636000
6	4.301211000	-0.316491000	-0.224449000
8	5.277202000	-0.873261000	0.246103000
8	4.393283000	0.403144000	-1.355114000
1	5.317654000	0.388543000	-1.648669000
7	1.461648000	-1.768702000	1.564797000
1	1.355222000	-2.555568000	2.190799000
1	-0.878260000	-2.015708000	2.744900000
1	1.487704000	0.054114000	-1.195006000
6	-0.782342000	-1.091586000	2.183752000
8	-0.584979000	0.522384000	-2.384373000
8	-2.540600000	1.085216000	-1.724464000
6	-1.850636000	-1.073821000	-1.297857000
6	-0.805005000	-1.984873000	-1.364216000

6	-3.082972000	-1.380521000	-0.736970000
6	-1.006393000	-3.253294000	-0.836155000
6	-3.268279000	-2.656287000	-0.220425000
6	-2.233210000	-3.586829000	-0.266251000
1	0.139549000	-1.704748000	-1.812509000
1	-3.869646000	-0.638304000	-0.703770000
1	-0.203130000	-3.979283000	-0.870787000
1	-4.220890000	-2.919975000	0.222450000
1	-2.383495000	-4.579087000	0.143360000
7	-1.644742000	0.275162000	-1.842616000



(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1257.837384

6	2.668044000	3.443618000	-0.182413000
6	1.359469000	3.683194000	0.264410000
6	0.341309000	2.770104000	0.020515000
6	0.652295000	1.558723000	-0.657684000
6	1.971550000	1.326450000	-1.124551000
6	2.970024000	2.294122000	-0.879522000
6	-1.032553000	3.017037000	0.398691000
6	-0.348722000	0.567385000	-0.821298000
6	-1.649519000	0.712939000	-0.153964000
6	-1.983967000	2.066015000	0.276568000
6	-2.656971000	-0.286779000	-0.558088000
6	-2.273391000	-1.377042000	-1.272379000
6	-0.028368000	-0.591102000	-1.530610000
6	2.247710000	0.117329000	-1.824828000
1	3.254465000	-0.054903000	-2.190735000
1	-1.286488000	3.997348000	0.787072000
1	3.441665000	4.177051000	0.013293000
1	1.127822000	4.603590000	0.790099000
1	3.976972000	2.111459000	-1.239398000
1	-3.001985000	2.281494000	0.569206000
1	-2.969007000	-2.168419000	-1.517953000
6	-4.048944000	-0.326026000	-0.076182000
8	-4.922306000	-1.018579000	-0.556218000
8	-4.266171000	0.448296000	0.991249000
1	-5.193574000	0.349582000	1.260287000
7	-0.995659000	-1.559077000	-1.686382000
1	-0.760398000	-2.400649000	-2.199263000
1	1.469319000	-1.723461000	-2.593795000
1	-1.224859000	0.215412000	1.095074000
6	1.266504000	-0.805544000	-2.052402000
8	-0.675471000	-0.304424000	2.003261000
8	1.262431000	0.731431000	2.137679000
6	1.209581000	-1.433389000	1.268827000

6	0.437028000	-2.555212000	0.931071000
6	2.596488000	-1.424372000	1.075546000
6	1.067486000	-3.654567000	0.372685000
6	3.204195000	-2.544576000	0.524807000
6	2.448150000	-3.655778000	0.160826000
1	-0.631288000	-2.551471000	1.102612000
1	3.171006000	-0.553061000	1.358839000
1	0.476323000	-4.522331000	0.102442000
1	4.277172000	-2.543293000	0.371064000
1	2.929041000	-4.522819000	-0.276144000
7	0.603024000	-0.292997000	1.829149000

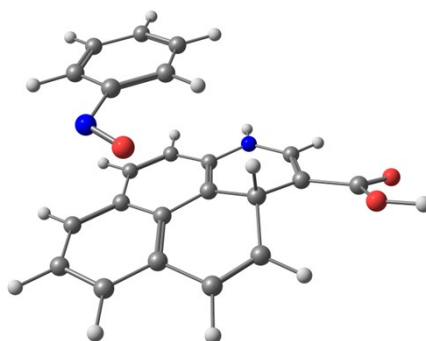


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1257.756958

6	-1.785793000	3.249003000	0.886830000
6	-0.506934000	3.461835000	0.323669000
6	0.416813000	2.441648000	0.256167000
6	0.068227000	1.144151000	0.748192000
6	-1.188558000	0.954253000	1.381429000
6	-2.113185000	2.029867000	1.421801000
6	1.798508000	2.655755000	-0.179439000
6	0.985096000	0.072362000	0.629391000
6	2.334576000	0.336070000	0.109495000
6	2.648408000	1.643117000	-0.366766000
6	3.244162000	-0.816349000	0.102750000
6	2.897250000	-1.918655000	0.808727000
6	0.695140000	-1.116967000	1.266664000
6	-1.479375000	-0.317593000	1.941684000
1	-2.443782000	-0.479288000	2.411068000
1	2.126516000	3.682929000	-0.307466000
1	-2.497272000	4.066128000	0.916079000
1	-0.235140000	4.448917000	-0.036723000
1	-3.081520000	1.866172000	1.882670000
1	3.672895000	1.837464000	-0.654651000
1	3.620665000	-2.698744000	1.010500000
6	4.601707000	-0.839235000	-0.449675000
8	5.508114000	-1.551598000	-0.077161000
8	4.759656000	0.000993000	-1.493122000
1	5.674177000	-0.093679000	-1.803102000
7	1.641996000	-2.139045000	1.269117000
1	1.453577000	-2.972485000	1.809117000
1	-0.748076000	-2.281485000	2.371641000
1	0.664489000	-0.327593000	-1.579010000
6	-0.547132000	-1.317700000	1.915586000
8	-0.284546000	-0.554556000	-1.797688000
8	-1.456817000	1.368712000	-1.947970000
6	-2.511315000	-0.662992000	-1.137207000
6	-2.438870000	-2.028599000	-0.814407000
6	-3.738489000	-0.003571000	-0.954064000
6	-3.552536000	-2.710053000	-0.326359000

6	-4.852505000	-0.684481000	-0.466053000
6	-4.764812000	-2.041143000	-0.149838000
1	-1.500832000	-2.558434000	-0.947917000
1	-3.817630000	1.051531000	-1.196879000
1	-3.472819000	-3.765841000	-0.083535000
1	-5.790923000	-0.153841000	-0.332638000
1	-5.632646000	-2.571877000	0.230403000
7	-1.279887000	0.090102000	-1.676758000

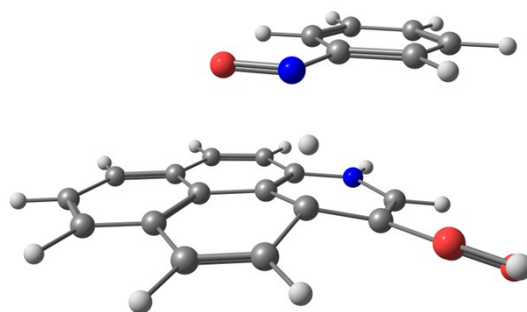


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= 1182.672835

6	-2.335260000	3.294362000	0.513606000
6	-1.034961000	3.549011000	0.025390000
6	-0.050144000	2.588628000	0.104007000
6	-0.357058000	1.316138000	0.678128000
6	-1.625847000	1.105783000	1.274312000
6	-2.619904000	2.109406000	1.146688000
6	1.343949000	2.851133000	-0.259221000
6	0.618096000	0.289573000	0.679629000
6	1.835839000	0.419487000	-0.224713000
6	2.249624000	1.872790000	-0.337815000
6	2.914031000	-0.548815000	0.231332000
6	2.602035000	-1.611050000	1.013925000
6	0.371888000	-0.851703000	1.411035000
6	-1.860187000	-0.117208000	1.957864000
1	-2.830632000	-0.289698000	2.411774000
1	1.631132000	3.885584000	-0.421725000
1	-3.099745000	4.056781000	0.416414000
1	-0.801214000	4.518842000	-0.401885000
1	-3.604056000	1.927313000	1.566686000
1	3.283359000	2.099809000	-0.564977000
1	3.345142000	-2.360040000	1.258865000
6	4.256160000	-0.570170000	-0.343254000
8	5.188741000	-1.249488000	0.048802000
8	4.382395000	0.222024000	-1.421723000
1	5.291663000	0.143911000	-1.749852000
7	1.359303000	-1.832296000	1.502501000
1	1.196887000	-2.632549000	2.098354000
1	-1.034962000	-1.984465000	2.597337000
1	1.513391000	0.127185000	-1.240879000
6	-0.873969000	-1.057822000	2.055743000
8	-1.254203000	0.970677000	-2.224752000
6	-2.294352000	-0.809553000	-1.361613000
6	-1.159073000	-1.621205000	-1.393734000
6	-3.501442000	-1.263974000	-0.836594000

6	-1.244110000	-2.906884000	-0.883736000
6	-3.576379000	-2.551107000	-0.320108000
6	-2.448172000	-3.367503000	-0.345301000
1	-0.237157000	-1.240636000	-1.817650000
1	-4.356989000	-0.597146000	-0.835476000
1	-0.374875000	-3.554326000	-0.899492000
1	-4.506555000	-2.918694000	0.096187000
1	-2.505704000	-4.374301000	0.053024000
7	-2.317837000	0.536699000	-1.859463000



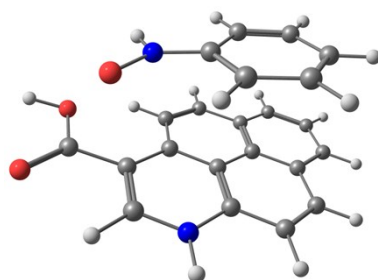
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1182.652759

6	4.844068000	0.140425000	0.350808000
6	4.051351000	1.275301000	0.617626000
6	2.709015000	1.293134000	0.297896000
6	2.118204000	0.148579000	-0.313113000
6	2.927407000	-0.971200000	-0.629908000
6	4.297165000	-0.958318000	-0.265319000
6	1.874781000	2.466357000	0.507963000
6	0.737065000	0.155268000	-0.648840000
6	-0.147120000	1.250710000	-0.201194000
6	0.563357000	2.480507000	0.218630000
6	-1.434952000	1.305854000	-0.924506000
6	-1.833173000	0.245859000	-1.683511000
6	0.230498000	-0.912587000	-1.386693000
6	2.340624000	-2.068527000	-1.315241000
1	2.956022000	-2.930738000	-1.548871000
1	2.357645000	3.367562000	0.872069000
1	5.893275000	0.146412000	0.622461000
1	4.498660000	2.150843000	1.076553000
1	4.904498000	-1.827916000	-0.493433000
1	-0.016312000	3.381002000	0.365898000
1	-2.808093000	0.226421000	-2.153955000
6	-2.472593000	2.319285000	-0.687037000
8	-3.446670000	2.492366000	-1.390087000
8	-2.277564000	3.018553000	0.437487000
1	-3.009109000	3.647892000	0.540620000
7	-1.064554000	-0.843007000	-1.867676000
1	-1.421629000	-1.613937000	-2.419361000
1	0.586712000	-2.853436000	-2.260195000
1	-0.500180000	0.891927000	1.011087000
6	1.031666000	-2.035543000	-1.703645000
8	0.670823000	-0.286718000	2.294892000
6	-1.365706000	-0.935699000	1.528867000
6	-2.689274000	-0.572101000	1.264559000
6	-0.906068000	-2.225622000	1.253689000

6	-3.553125000	-1.499558000	0.699018000
6	-1.777697000	-3.144900000	0.687793000
6	-3.093554000	-2.780465000	0.396691000
1	-3.018988000	0.433247000	1.508192000
1	0.120910000	-2.481864000	1.481682000
1	-4.579773000	-1.224554000	0.486090000
1	-1.432447000	-4.147913000	0.463302000
1	-3.767186000	-3.503156000	-0.049936000
7	-0.513780000	0.083586000	2.063714000

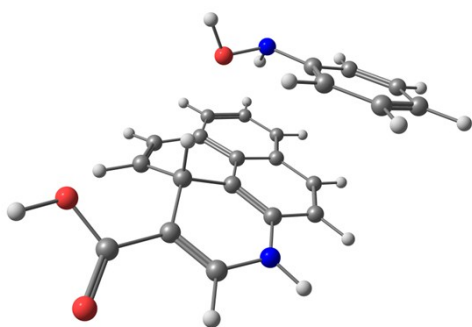


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1182.697115

6	-4.031507000	0.696633000	1.445388000
6	-2.914705000	1.455196000	1.798109000
6	-1.626980000	0.967350000	1.577333000
6	-1.461238000	-0.310221000	0.988772000
6	-2.598694000	-1.079935000	0.638461000
6	-3.880340000	-0.557030000	0.876285000
6	-0.449518000	1.717944000	1.910731000
6	-0.148793000	-0.808782000	0.743789000
6	1.012334000	-0.028485000	1.048750000
6	0.802187000	1.246557000	1.673894000
6	2.275179000	-0.600295000	0.728091000
6	2.326725000	-1.876712000	0.211610000
6	-0.029449000	-2.089718000	0.177310000
6	-2.409848000	-2.369277000	0.046241000
1	-3.285827000	-2.949429000	-0.223142000
1	-0.579393000	2.690567000	2.374354000
1	-5.025198000	1.092640000	1.619958000
1	-3.039025000	2.436124000	2.244550000
1	-4.748093000	-1.146833000	0.601147000
1	1.655986000	1.844321000	1.949315000
1	3.265620000	-2.350286000	-0.038315000
6	3.607756000	0.063377000	0.792600000
8	4.648401000	-0.523896000	0.589758000
8	3.579088000	1.346146000	1.149606000
1	4.490371000	1.679963000	1.141808000
7	1.221511000	-2.583338000	-0.029881000
1	1.314944000	-3.514540000	-0.428310000
1	-1.011928000	-3.848644000	-0.609497000
6	-1.164925000	-2.869511000	-0.169641000
8	2.741549000	0.650573000	-1.557109000
6	0.438173000	1.182521000	-1.713236000
6	0.126947000	-0.003276000	-2.418800000
6	-0.608611000	2.096468000	-1.428556000
6	-1.185911000	-0.263038000	-2.790587000
6	-1.907093000	1.805830000	-1.802806000
6	-2.219182000	0.620751000	-2.480510000

1	0.925183000	-0.693944000	-2.658678000
1	-0.375154000	3.019078000	-0.906419000
1	-1.406160000	-1.180931000	-3.327324000
1	-2.695156000	2.513804000	-1.565205000
1	-3.240930000	0.400879000	-2.766563000
7	1.693884000	1.432354000	-1.282926000
1	1.879652000	2.303432000	-0.795430000

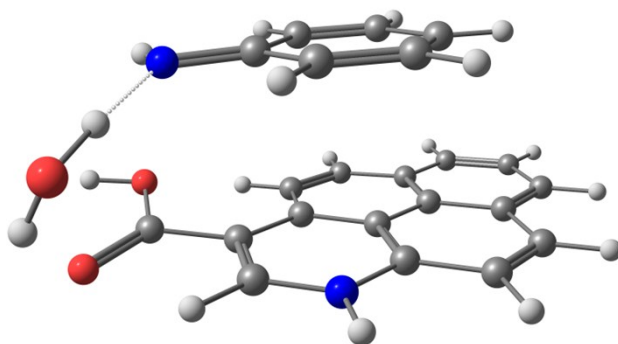


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1183.888552

6	2.315717000	3.100579000	-0.856386000
6	1.054008000	3.391939000	-0.286697000
6	0.056235000	2.443391000	-0.257115000
6	0.304256000	1.142658000	-0.796913000
6	1.534018000	0.886198000	-1.454783000
6	2.544378000	1.882969000	-1.446461000
6	-1.299249000	2.739763000	0.207224000
6	-0.691139000	0.137087000	-0.710475000
6	-1.883639000	0.320161000	0.220411000
6	-2.224554000	1.788958000	0.359019000
6	-3.017941000	-0.590290000	-0.226540000
6	-2.755783000	-1.688293000	-0.976984000
6	-0.499135000	-1.036781000	-1.408660000
6	1.717438000	-0.370735000	-2.087758000
1	2.660345000	-0.579810000	-2.582051000
1	-1.546617000	3.781600000	0.387834000
1	3.090667000	3.858664000	-0.851984000
1	0.861016000	4.381375000	0.115410000
1	3.495342000	1.665678000	-1.922226000
1	-3.226920000	2.053716000	0.668837000
1	-3.533550000	-2.405629000	-1.208098000
6	-4.364296000	-0.534685000	0.336922000
8	-5.329119000	-1.162626000	-0.063036000
8	-4.457799000	0.261312000	1.415807000
1	-5.372488000	0.228993000	1.736274000
7	-1.521486000	-1.986259000	-1.445432000
1	-1.400143000	-2.804315000	-2.026887000
1	0.830604000	-2.247381000	-2.606208000
1	-1.557778000	-0.004441000	1.223960000
6	0.712389000	-1.296617000	-2.096298000

8	0.619632000	0.840866000	2.333863000
6	2.310750000	-0.541881000	1.469048000
6	1.468102000	-1.648408000	1.561747000
6	3.562537000	-0.672061000	0.852843000
6	1.874204000	-2.869974000	1.025988000
6	3.953824000	-1.893095000	0.326470000
6	3.110198000	-3.002383000	0.404699000
1	0.502962000	-1.549799000	2.041570000
1	4.217199000	0.192125000	0.793141000
1	1.207103000	-3.722682000	1.094794000
1	4.923795000	-1.980672000	-0.150843000
1	3.418529000	-3.955067000	-0.009431000
7	1.987537000	0.708097000	2.037320000
1	2.229188000	1.472700000	1.408582000
1	0.582776000	0.914666000	3.295238000

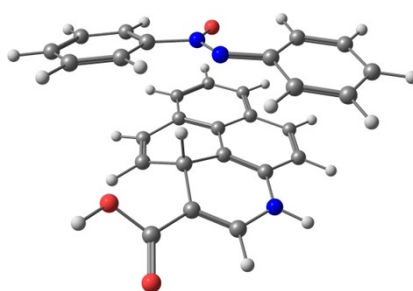


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1183.943104

6	4.755883000	-0.858804000	-0.286716000
6	3.781809000	-1.832717000	-0.481953000
6	2.459940000	-1.604070000	-0.088092000
6	2.120099000	-0.370020000	0.512685000
6	3.118128000	0.612817000	0.727044000
6	4.430756000	0.350416000	0.313920000
6	1.427499000	-2.581552000	-0.264978000
6	0.773203000	-0.120342000	0.889717000
6	-0.252658000	-1.080580000	0.648875000
6	0.137640000	-2.342849000	0.084702000
6	-1.576395000	-0.729750000	1.026587000
6	-1.805451000	0.493536000	1.618407000
6	0.473978000	1.118586000	1.487217000
6	2.755015000	1.851079000	1.347652000
1	3.527359000	2.594996000	1.509732000
1	1.699663000	-3.540216000	-0.694302000
1	5.775305000	-1.046142000	-0.601978000
1	4.038042000	-2.779778000	-0.944666000
1	5.191846000	1.107507000	0.469207000
1	-0.605631000	-3.109664000	-0.063059000
1	-2.795796000	0.818988000	1.901310000
6	-2.817672000	-1.523175000	0.794324000
8	-3.858260000	-1.289002000	1.367358000
8	-2.687572000	-2.517472000	-0.075634000
1	-3.545363000	-2.964411000	-0.163394000
7	-0.811019000	1.358396000	1.838903000
1	-1.035914000	2.256068000	2.264256000
1	1.187603000	3.039502000	2.185611000
1	-3.978344000	0.904539000	-0.522702000
6	1.473890000	2.103441000	1.720052000
8	-4.551765000	1.359373000	0.191674000
6	-1.737619000	0.674210000	-1.769867000
6	-1.387972000	1.983959000	-1.313704000
6	-0.671809000	-0.066118000	-2.371235000

6	-0.102106000	2.481593000	-1.433028000
6	0.609519000	0.452620000	-2.489062000
6	0.923759000	1.729061000	-2.017784000
1	-2.165051000	2.582268000	-0.845402000
1	-0.884507000	-1.070275000	-2.731028000
1	0.112065000	3.479718000	-1.059291000
1	1.383906000	-0.157063000	-2.948077000
1	1.928621000	2.126041000	-2.104433000
7	-2.983819000	0.210261000	-1.592983000
1	-3.063907000	-0.733002000	-1.964476000
1	-4.761861000	0.639106000	0.7954740000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1468.945955

6	2.588979	-0.012305	2.552357
6	2.092191	-1.224196	2.022234
6	0.826276	-1.295303	1.484139
6	0.000316	-0.128777	1.464639
6	0.472209	1.065542	2.070332
6	1.793549	1.105219	2.587142
6	0.237496	-2.556369	1.031569
6	-1.299177	-0.185406	0.899447
6	-1.717187	-1.370360	0.034801
6	-0.955584	-2.616075	0.432793
6	-3.236428	-1.479802	0.031909
6	-3.991631	-0.385096	0.283672
6	-2.141518	0.890810	1.088461
6	-0.406330	2.177016	2.159487
1	-0.047779	3.097063	2.609134
1	0.794474	-3.466279	1.235551
1	3.596627	0.022496	2.950585
1	2.711837	-2.115798	2.042689
1	2.155101	2.031442	3.021913
1	-1.363842	-3.573059	0.136694
1	-5.068344	-0.413522	0.172285
6	-3.978526	-2.626815	-0.501986
8	-5.173833	-2.802148	-0.410454
8	-3.198960	-3.491456	-1.182971
1	-3.773574	-4.202232	-1.508633
7	-3.462507	0.810463	0.649769
1	-4.087011	1.573456	0.872999
1	-2.386690	2.910404	1.812142
1	-1.388083	-1.142297	-0.992621
6	-1.694152	2.081044	1.712898
8	0.460633	-0.179958	-1.965526
6	0.217732	2.034478	-1.339646
6	-1.112553	1.969784	-1.730917
6	0.789820	3.210149	-0.865828

6	-1.893121	3.116448	-1.639781
6	-0.001507	4.349358	-0.789039
6	-1.340068	4.305052	-1.172536
1	-1.523338	1.035161	-2.089565
1	1.828553	3.228536	-0.566500
1	-2.935057	3.076105	-1.934550
1	0.430594	5.273482	-0.424292
1	-1.950567	5.198297	-1.108628
6	3.042131	-0.243553	-1.015865
6	4.294886	0.043000	-0.446977
6	2.780820	-1.548470	-1.468441
6	5.259920	-0.940004	-0.313693
6	3.761327	-2.527822	-1.325577
6	4.992557	-2.237673	-0.749896
1	4.477098	1.053079	-0.098238
1	1.834321	-1.801467	-1.913770
1	6.216872	-0.699613	0.134491
1	3.549827	-3.533478	-1.670832
1	5.741431	-3.013985	-0.642911
7	2.189707	0.873691	-0.995940



(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1468.910784

6	-3.807437	0.212198	2.001011
6	-3.364923	1.353889	1.320416
6	-2.017235	1.510184	1.005830
6	-1.080205	0.521626	1.432652
6	-1.539832	-0.637460	2.115084
6	-2.923320	-0.778595	2.374715
6	-1.527248	2.634019	0.248876
6	0.308465	0.697051	1.171115
6	0.769206	1.768502	0.279136
6	-0.211835	2.774636	-0.057526
6	2.237343	2.028889	0.348378
6	3.042526	1.111718	0.947574
6	1.205212	-0.244119	1.677372
6	-0.588563	-1.616481	2.510716
1	-0.937898	-2.517950	3.002120
1	-2.241525	3.385068	-0.071778
1	-4.863609	0.099725	2.220927
1	-4.071396	2.117686	1.013567
1	-3.271823	-1.668745	2.887446
1	0.107917	3.635014	-0.627518
1	4.116671	1.242738	0.965804
6	2.961338	3.128774	-0.303355
8	4.129530	3.395378	-0.125279
8	2.215749	3.827788	-1.179016
1	2.786410	4.516061	-1.556982
7	2.570713	-0.020926	1.513215
1	3.221801	-0.681797	1.916762
1	1.484655	-2.132180	2.671484
1	0.635610	0.945694	-0.878652
6	0.754097	-1.405940	2.330181
8	0.570902	0.121603	-1.732768
6	1.445387	-1.912303	-0.995327
6	2.728235	-1.406532	-1.191267
6	1.248231	-3.229357	-0.569489

6	3.824655	-2.227156	-0.948028
6	2.354450	-4.029550	-0.328146
6	3.645995	-3.534944	-0.512626
1	2.864851	-0.388422	-1.529173
1	0.245430	-3.607746	-0.432286
1	4.822556	-1.832390	-1.098845
1	2.205951	-5.050025	0.004873
1	4.503680	-4.168250	-0.319780
7	0.317013	-1.066674	-1.247458
6	-2.013895	-0.881816	-1.374041
6	-3.174210	-1.564759	-0.931919
6	-2.180445	0.316958	-2.111166
6	-4.436571	-1.066004	-1.181062
6	-3.460705	0.798923	-2.352057
6	-4.589614	0.134448	-1.879568
1	-3.037371	-2.490936	-0.385381
1	-1.331526	0.856381	-2.496035
1	-5.307230	-1.602794	-0.821397
1	-3.573435	1.720389	-2.912707
1	-5.578554	0.535582	-2.068392
7	-0.854186	-1.542692	-1.030390

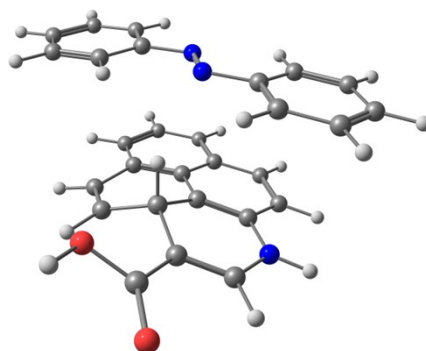


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1468.933017

6	2.972041000	-2.176068000	1.833236000
6	2.105995000	-3.069778000	1.216028000
6	0.795305000	-2.686859000	0.903511000
6	0.352987000	-1.388197000	1.244306000
6	1.233753000	-0.483396000	1.885441000
6	2.546081000	-0.892418000	2.156818000
6	-0.103127000	-3.545275000	0.201551000
6	-0.963374000	-0.983833000	0.903142000
6	-1.851445000	-1.860389000	0.217394000
6	-1.365220000	-3.157579000	-0.136180000
6	-3.147272000	-1.356997000	-0.100490000
6	-3.469008000	-0.061535000	0.234906000
6	-1.363313000	0.326770000	1.249148000
6	0.765196000	0.822348000	2.226863000
1	1.447801000	1.504017000	2.723004000
1	0.246036000	-4.533156000	-0.080865000
1	3.989895000	-2.475541000	2.053056000
1	2.441984000	-4.066708000	0.951003000
1	3.226650000	-0.193911000	2.632165000
1	-2.001825000	-3.834682000	-0.682885000
1	-4.431164000	0.371424000	-0.003101000
6	-4.251838000	-2.092352000	-0.783761000
8	-5.180856000	-1.527805000	-1.310382000
8	-4.146195000	-3.413858000	-0.729065000
1	-4.901122000	-3.806912000	-1.197591000
7	-2.607428000	0.726357000	0.887357000
1	-2.888976000	1.680822000	1.107443000
1	-0.873633000	2.203642000	2.195860000
1	0.107180000	0.889701000	-2.734781000
6	-0.506421000	1.215715000	1.941085000
8	0.464446000	1.764745000	-2.548652000
6	0.020903000	2.895482000	-0.590554000

6	-1.325294000	3.080306000	-0.930622000
6	0.621556000	3.777664000	0.309698000
6	-2.058414000	4.112957000	-0.362346000
6	-0.122077000	4.812105000	0.873821000
6	-1.463484000	4.984292000	0.551383000
1	-1.790419000	2.400361000	-1.634775000
1	1.661035000	3.633688000	0.564166000
1	-3.101717000	4.236929000	-0.632332000
1	0.357497000	5.488262000	1.573614000
1	-2.038297000	5.787183000	0.998320000
7	0.701858000	1.755337000	-1.102429000
6	2.667917000	0.595358000	-1.062013000
6	4.074059000	0.506874000	-0.823593000
6	2.051507000	-0.601426000	-1.536386000
6	4.793728000	-0.646368000	-1.073259000
6	2.792898000	-1.749024000	-1.783001000
6	4.170036000	-1.798609000	-1.568624000
1	4.573984000	1.395788000	-0.450597000
1	0.978552000	-0.633066000	-1.685989000
1	5.862838000	-0.651277000	-0.881127000
1	2.274946000	-2.634029000	-2.144478000
1	4.737294000	-2.697880000	-1.776966000
7	2.074178000	1.785746000	-0.838266000

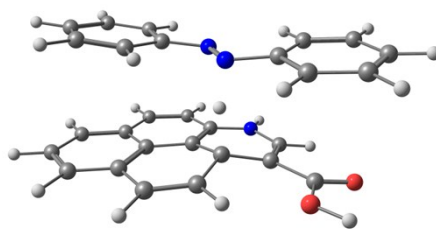


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1393.770166

6	2.995561000	0.566055000	2.326964000
6	2.631740000	-0.740066000	1.929012000
6	1.343934000	-1.023917000	1.532517000
6	0.363491000	0.017466000	1.535816000
6	0.701020000	1.295740000	2.049306000
6	2.050485000	1.558672000	2.403066000
6	0.890344000	-2.385666000	1.237435000
6	-0.952368000	-0.252053000	1.089041000
6	-1.207536000	-1.497455000	0.254416000
6	-0.316755000	-2.631790000	0.720571000
6	-2.696398000	-1.791333000	0.209287000
6	-3.605712000	-0.848538000	0.563074000
6	-1.939945000	0.675513000	1.348016000
6	-0.333184000	2.255464000	2.210010000
1	-0.085598000	3.237934000	2.598146000
1	1.558311000	-3.201771000	1.496820000
1	4.023797000	0.771640000	2.603197000
1	3.372495000	-1.534101000	1.943813000
1	2.315007000	2.550814000	2.754158000
1	-0.645885000	-3.649540000	0.551774000
1	-4.667600000	-1.030051000	0.448172000
6	-3.240108000	-2.975903000	-0.445854000
8	-4.407160000	-3.327548000	-0.437214000
8	-2.313664000	-3.666377000	-1.134248000
1	-2.748559000	-4.428613000	-1.546671000
7	-3.265209000	0.369364000	1.039194000
1	-3.989681000	1.031829000	1.279547000
1	-2.432432000	2.650097000	2.074238000
1	-0.868536000	-1.260235000	-0.769464000
6	-1.629995000	1.937446000	1.912816000
6	-0.399460000	1.824080000	-1.564812000

6	-1.694716000	1.413305000	-1.875806000
6	-0.148243000	3.146059000	-1.184425000
6	-2.747511000	2.317924000	-1.796975000
6	-1.202137000	4.044678000	-1.113786000
6	-2.502027000	3.632943000	-1.413038000
1	-1.860420000	0.381490000	-2.168404000
1	0.861571000	3.450133000	-0.939758000
1	-3.755800000	1.996269000	-2.031029000
1	-1.014742000	5.070506000	-0.817279000
1	-3.320729000	4.340774000	-1.348502000
7	0.596127000	0.807816000	-1.631931000
6	2.727432000	0.147646000	-1.349754000
6	4.010802000	0.546181000	-0.984034000
6	2.459249000	-1.193089000	-1.641357000
6	5.031032000	-0.394212000	-0.891283000
6	3.479663000	-2.126796000	-1.545620000
6	4.764356000	-1.731920000	-1.166061000
1	4.186788000	1.591906000	-0.756952000
1	1.456683000	-1.492331000	-1.920881000
1	6.027727000	-0.085013000	-0.598867000
1	3.275513000	-3.169655000	-1.760795000
1	5.554769000	-2.469680000	-1.085978000
7	1.744202000	1.177163000	-1.339385000



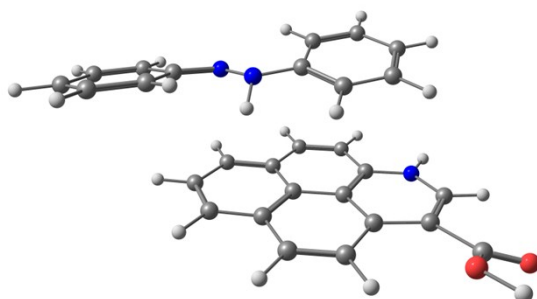
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1393.745642

6	4.385954000	-1.762067000	-0.464063000
6	3.286974000	-2.296001000	-1.146262000
6	1.988590000	-2.031485000	-0.724566000
6	1.781930000	-1.214287000	0.422227000
6	2.900828000	-0.692046000	1.123853000
6	4.200039000	-0.968677000	0.651108000
6	0.833847000	-2.568028000	-1.405743000
6	0.461520000	-0.917102000	0.854869000
6	-0.697350000	-1.283312000	0.027609000
6	-0.425063000	-2.249984000	-1.039611000
6	-1.995081000	-1.231733000	0.761759000
6	-2.056158000	-0.546295000	1.938920000
6	0.298235000	-0.164270000	2.016705000
6	2.673540000	0.112576000	2.277121000
1	3.528636000	0.521324000	2.805008000
1	1.002463000	-3.243718000	-2.237852000
1	5.389290000	-1.971881000	-0.816999000
1	3.441153000	-2.923173000	-2.018241000
1	5.050107000	-0.552010000	1.181335000
1	-1.259038000	-2.665508000	-1.583983000
1	-2.993838000	-0.427358000	2.465283000
6	-3.297115000	-1.739884000	0.307047000
8	-4.342746000	-1.591161000	0.914440000
8	-3.272045000	-2.406074000	-0.854305000
1	-4.179561000	-2.681187000	-1.059134000
7	-0.978741000	0.014440000	2.520119000
1	-1.092695000	0.515284000	3.392313000
1	1.228088000	0.930301000	3.626174000
1	-0.679031000	-0.132806000	-0.750353000
6	1.407770000	0.347109000	2.729378000
6	-2.134950000	1.366942000	-0.833277000
6	-2.986250000	0.644782000	-1.670570000
6	-2.667908000	2.230834000	0.125282000
6	-4.363893000	0.769164000	-1.541588000

6	-4.046841000	2.349247000	0.248542000
6	-4.899836000	1.616575000	-0.575595000
1	-2.554104000	-0.024387000	-2.408426000
1	-2.001623000	2.791157000	0.767825000
1	-5.018088000	0.195353000	-2.188647000
1	-4.459705000	3.017094000	0.996497000
1	-5.974254000	1.709573000	-0.467008000
7	-0.739660000	1.136938000	-1.012884000
6	1.376634000	1.813400000	-0.575465000
6	2.243095000	2.552056000	0.249462000
6	1.915566000	1.143393000	-1.693270000
6	3.599815000	2.625757000	-0.030337000
6	3.272209000	1.224478000	-1.963067000
6	4.125656000	1.955878000	-1.133708000
1	1.819553000	3.066531000	1.105298000
1	1.260731000	0.574912000	-2.342837000
1	4.250485000	3.204480000	0.616425000
1	3.675274000	0.706273000	-2.826859000
1	5.185773000	2.009923000	-1.353721000
7	0.033855000	1.825134000	-0.222053000

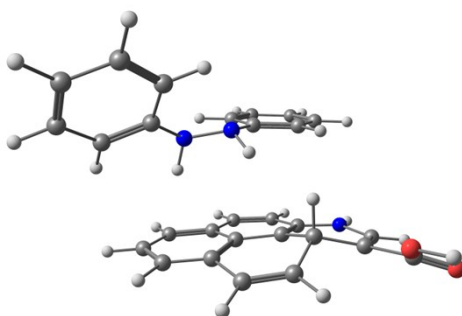


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1393.764744

6	2.361581000	-1.592842000	1.444879000
6	1.479262000	-2.418603000	0.765262000
6	0.129569000	-2.054282000	0.608922000
6	-0.314050000	-0.820990000	1.143453000
6	0.592310000	0.021481000	1.833325000
6	1.930514000	-0.374908000	1.966538000
6	-0.807895000	-2.867595000	-0.085524000
6	-1.661104000	-0.420144000	0.950927000
6	-2.571570000	-1.227464000	0.206820000
6	-2.104784000	-2.481845000	-0.280316000
6	-3.888206000	-0.709018000	0.015044000
6	-4.229646000	0.498230000	0.576404000
6	-2.061524000	0.830148000	1.470522000
6	0.130010000	1.276612000	2.331133000
1	0.837396000	1.921809000	2.841333000
1	-0.470109000	-3.823049000	-0.473761000
1	3.399510000	-1.886252000	1.551160000
1	1.821027000	-3.360415000	0.348429000
1	2.621949000	0.269205000	2.496893000
1	-2.779349000	-3.132342000	-0.814197000
1	-5.218650000	0.922442000	0.467996000
6	-4.984823000	-1.335976000	-0.778821000
8	-6.149585000	-1.061974000	-0.614441000
8	-4.563805000	-2.182204000	-1.710815000
1	-5.335056000	-2.533242000	-2.185660000
7	-3.344584000	1.221298000	1.274347000
1	-3.640187000	2.120034000	1.650673000
1	-1.517138000	2.631849000	2.531810000
6	-1.160815000	1.676436000	2.164463000
6	0.655986000	1.658249000	-1.095912000
6	-0.597444000	1.187843000	-1.541653000
6	0.767613000	3.012765000	-0.729566000
6	-1.690201000	2.036524000	-1.605954000
6	-0.342563000	3.848096000	-0.795365000

6	-1.581387000	3.377396000	-1.225414000
1	-0.695027000	0.144054000	-1.829586000
1	1.723627000	3.383654000	-0.386221000
1	-2.643167000	1.645415000	-1.950488000
1	-0.233840000	4.887131000	-0.500714000
1	-2.439595000	4.037221000	-1.272796000
7	1.731821000	0.804079000	-1.075454000
6	3.903056000	0.355147000	-0.541270000
6	5.093842000	0.593782000	0.221137000
6	3.943730000	-0.778608000	-1.413974000
6	6.189788000	-0.236716000	0.143669000
6	5.066153000	-1.600907000	-1.473288000
6	6.199199000	-1.361251000	-0.701631000
1	5.100616000	1.454816000	0.883274000
1	3.100368000	-0.998090000	-2.057738000
1	7.063516000	-0.012011000	0.749124000
1	5.049552000	-2.452766000	-2.148153000
1	7.063035000	-2.012759000	-0.754167000
7	2.861937000	1.171685000	-0.335894000
1	1.474830000	-0.182087000	-1.029013000

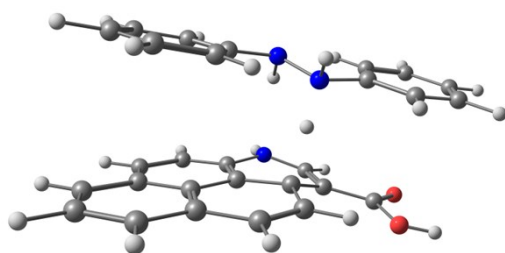


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1394.968254

6	2.119253000	0.013673000	3.087834000
6	1.652160000	-1.210678000	2.556648000
6	0.461070000	-1.274582000	1.865342000
6	-0.303159000	-0.081049000	1.668431000
6	0.125411000	1.128849000	2.275914000
6	1.365374000	1.154891000	2.967054000
6	-0.143547000	-2.545343000	1.459842000
6	-1.512102000	-0.128726000	0.931237000
6	-1.826949000	-1.351235000	0.078092000
6	-1.247122000	-2.599559000	0.710249000
6	-3.313630000	-1.387051000	-0.233191000
6	-4.067564000	-0.265539000	-0.128014000
6	-2.334120000	0.978921000	0.944575000
6	-0.716507000	2.268454000	2.187147000
1	-0.391302000	3.200182000	2.637727000
1	0.308818000	-3.455105000	1.842525000
1	3.062816000	0.038263000	3.620667000
1	2.221261000	-2.120080000	2.720877000
1	1.698688000	2.089471000	3.406223000
1	-1.700121000	-3.553502000	0.473180000
1	-5.103081000	-0.257760000	-0.445666000
6	-3.952199000	-2.508174000	-0.917332000
8	-5.149795000	-2.647985000	-1.091299000
8	-3.071588000	-3.397395000	-1.407549000
1	-3.567446000	-4.101516000	-1.853727000
7	-3.584830000	0.910696000	0.335284000
1	-4.203992000	1.706698000	0.406063000
1	-2.599408000	3.042067000	1.530200000
1	-1.288469000	-1.234001000	-0.879787000
6	-1.931779000	2.187335000	1.567218000
6	0.395306000	1.635179000	-1.404266000
6	-0.872453000	1.501952000	-1.990403000
6	0.828063000	2.899842000	-0.994833000
6	-1.690110000	2.610300000	-2.147450000

6	-0.002510000	4.004795000	-1.163978000
6	-1.264507000	3.872883000	-1.732562000
1	-1.207695000	0.522051000	-2.317049000
1	1.805147000	3.011680000	-0.542677000
1	-2.670075000	2.486000000	-2.596006000
1	0.345973000	4.978603000	-0.837107000
1	-1.907132000	4.736707000	-1.854670000
7	1.197977000	0.493160000	-1.286750000
6	3.406021000	-0.223536000	-0.784697000
6	4.403019000	-0.411430000	0.184162000
6	3.550171000	-0.824862000	-2.038641000
6	5.520927000	-1.180369000	-0.103546000
6	4.679474000	-1.591771000	-2.312459000
6	5.670257000	-1.778465000	-1.354712000
1	4.291948000	0.057307000	1.156898000
1	2.783359000	-0.687449000	-2.789899000
1	6.281864000	-1.314434000	0.657635000
1	4.779250000	-2.050007000	-3.290610000
1	6.544211000	-2.379069000	-1.576957000
7	2.319615000	0.599549000	-0.468426000
1	2.103541000	0.615190000	0.526750000
1	0.664099000	-0.360303000	-1.130536000



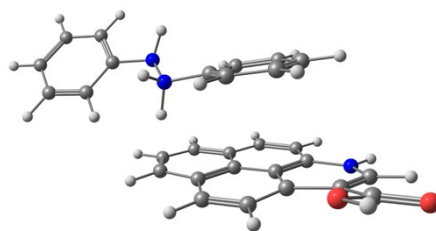
(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1394.919678

6	4.612936000	-1.579765000	-0.959367000
6	3.457702000	-1.945916000	-1.678308000
6	2.193141000	-1.783744000	-1.121520000
6	2.076421000	-1.220674000	0.195532000
6	3.255134000	-0.866180000	0.922593000
6	4.528859000	-1.058886000	0.306728000
6	0.982824000	-2.157170000	-1.810531000
6	0.786571000	-0.992509000	0.758641000
6	-0.434996000	-1.289441000	-0.002683000
6	-0.246229000	-1.968957000	-1.248663000
6	-1.676005000	-1.354728000	0.850141000
6	-1.662990000	-0.733741000	2.057286000
6	0.722165000	-0.419529000	2.030688000
6	3.123057000	-0.323724000	2.217849000
1	4.013986000	-0.062017000	2.778137000
1	1.069270000	-2.601074000	-2.796527000
1	5.586648000	-1.715365000	-1.420166000
1	3.548344000	-2.363274000	-2.675651000
1	5.420919000	-0.775686000	0.855569000
1	-1.120414000	-2.283189000	-1.802866000
1	-2.555417000	-0.684382000	2.668354000
6	-2.984157000	-1.883907000	0.472810000
8	-4.018126000	-1.729635000	1.107003000
8	-2.998203000	-2.582253000	-0.675732000
1	-3.911426000	-2.867052000	-0.834973000
7	-0.561595000	-0.116586000	2.561035000
1	-0.597454000	0.184134000	3.526155000
1	1.761467000	0.319944000	3.751037000
1	-0.759088000	0.054263000	-0.671705000
6	1.870171000	-0.108840000	2.759065000
6	-2.570919000	1.248603000	-0.762420000
6	-3.323623000	0.531041000	-1.686930000

6	-3.164551000	1.904209000	0.307361000
6	-4.701822000	0.462414000	-1.529765000
6	-4.546889000	1.820752000	0.453331000
6	-5.315854000	1.102835000	-0.456368000
1	-2.828917000	0.026377000	-2.510744000
1	-2.576576000	2.470621000	1.017730000
1	-5.293067000	-0.097651000	-2.244656000
1	-5.021425000	2.324803000	1.287024000
1	-6.390018000	1.041051000	-0.329048000
7	-1.129478000	1.187058000	-0.931719000
6	1.004572000	2.115313000	-0.399932000
6	1.820916000	2.755872000	0.537472000
6	1.567451000	1.591205000	-1.562334000
6	3.182870000	2.873022000	0.309638000
6	2.937876000	1.727708000	-1.785530000
6	3.750928000	2.364820000	-0.858867000
1	1.374753000	3.155743000	1.442507000
1	0.981173000	1.052804000	-2.297776000
1	3.804333000	3.365618000	1.048919000
1	3.363713000	1.313427000	-2.692494000
1	4.815514000	2.459490000	-1.037078000
7	-0.391262000	2.089382000	-0.109005000
1	-0.538593000	1.798293000	0.860090000
1	-0.914097000	1.398755000	-1.909700000



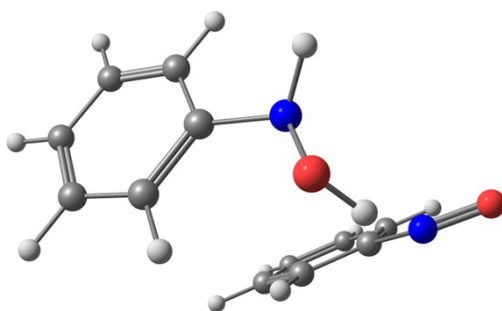
Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1394.926031

6	2.061248000	1.419208000	1.824985000
6	1.400035000	0.226077000	2.163082000
6	0.008724000	0.071067000	1.857863000
6	-0.645322000	1.098453000	1.092436000
6	0.067420000	2.294111000	0.727416000
6	1.440724000	2.429203000	1.126391000
6	-0.744068000	-1.052168000	2.231542000
6	-1.997388000	0.910051000	0.677401000
6	-2.697509000	-0.304100000	0.979462000
6	-2.059914000	-1.229706000	1.792945000
6	-4.052649000	-0.449801000	0.387448000
6	-4.610577000	0.622907000	-0.253834000
6	-2.619374000	1.959340000	-0.051965000
6	-0.598745000	3.273562000	-0.018707000
1	-0.069298000	4.177354000	-0.300298000
1	-0.279669000	-1.815213000	2.848054000
1	3.104922000	1.533704000	2.107951000
1	1.887028000	-0.518968000	2.783547000
1	1.976886000	3.332056000	0.855974000
1	-2.581013000	-2.130580000	2.085764000
1	-5.605591000	0.560051000	-0.676799000
6	-4.845702000	-1.664303000	0.310107000
8	-6.009531000	-1.733435000	-0.066275000
8	-4.189105000	-2.787785000	0.663705000
1	-4.803543000	-3.529859000	0.556087000
7	-3.973039000	1.785548000	-0.423503000
1	-4.427640000	2.527644000	-0.938091000
1	-2.451761000	3.882574000	-0.949954000
6	-1.937409000	3.108133000	-0.388392000
6	0.723194000	-0.720237000	-1.312809000
6	-0.199266000	-1.751775000	-1.240901000
6	0.479391000	0.450404000	-2.018497000
6	-1.420516000	-1.601310000	-1.889303000
6	-0.740576000	0.576595000	-2.675498000
6	-1.689865000	-0.439980000	-2.608672000

1	0.026155000	-2.649012000	-0.674434000
1	1.213560000	1.245710000	-2.045214000
1	-2.158560000	-2.392604000	-1.824511000
1	-0.951405000	1.483066000	-3.230747000
1	-2.641414000	-0.326024000	-3.115587000
7	1.971766000	-0.876518000	-0.548394000
6	4.342904000	-0.474552000	-0.580159000
6	5.464444000	-0.171839000	-1.358160000
6	4.503399000	-0.948860000	0.719816000
6	6.735670000	-0.338648000	-0.832088000
6	5.789242000	-1.111032000	1.234717000
6	6.906905000	-0.807608000	0.470092000
1	5.327934000	0.196494000	-2.369513000
1	3.652889000	-1.191150000	1.345688000
1	7.598273000	-0.099974000	-1.443686000
1	5.904931000	-1.481387000	2.246774000
1	7.901817000	-0.935495000	0.879356000
7	3.075425000	-0.214803000	-1.168090000
1	3.066286000	-0.459217000	-2.157992000
1	1.835098000	-0.454934000	0.430067000
1	2.157605000	-1.883236000	-0.412269000

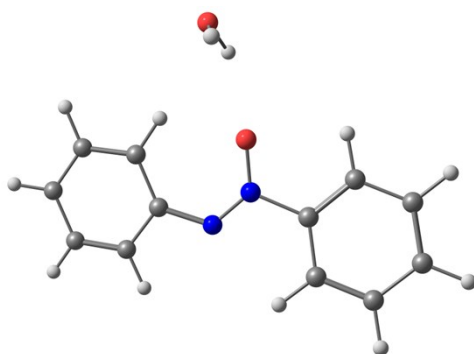
2.3.4. Thermodynamic assesment of dimerization processes



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -724.043376

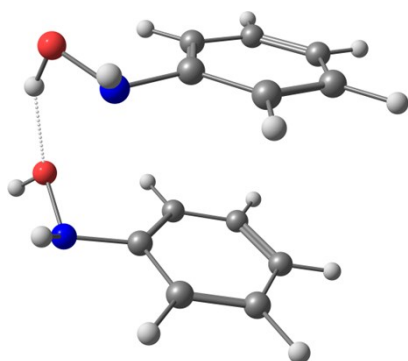
8	-0.540165000	2.520777000	0.735278000
6	-1.767549000	0.791663000	-0.272082000
6	-2.161593000	0.322778000	0.982671000
6	-2.317723000	0.220018000	-1.427219000
6	-3.088675000	-0.713382000	1.072606000
6	-3.239363000	-0.810947000	-1.321734000
6	-3.631691000	-1.288395000	-0.070742000
1	-1.750685000	0.776262000	1.874474000
1	-2.009298000	0.587680000	-2.400646000
1	-3.390099000	-1.066646000	2.052581000
1	-3.656648000	-1.243630000	-2.224175000
1	-4.352681000	-2.093095000	0.008209000
7	-0.777094000	1.776215000	-0.430919000
6	2.134013000	0.126789000	0.161038000
6	2.994955000	-0.593144000	-0.669102000
6	1.198129000	-0.506380000	0.972997000
6	2.904427000	-1.974942000	-0.677727000
6	1.115774000	-1.893302000	0.959538000
6	1.967426000	-2.621560000	0.133517000
1	3.707700000	-0.065826000	-1.290920000
1	0.551312000	0.095309000	1.601635000
1	3.558114000	-2.557191000	-1.316033000
1	0.391297000	-2.401607000	1.584210000
1	1.903075000	-3.703446000	0.116838000
7	2.130979000	1.559195000	0.231180000
1	-1.009638000	2.424349000	-1.178686000
8	2.979792000	2.122281000	-0.405521000
1	0.414563000	2.400322000	0.870066000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -724.097352

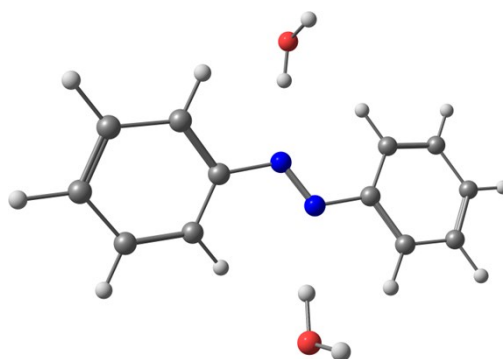
7	0.497953000	0.192350000	0.027318000
7	-0.279720000	-0.790430000	-0.060311000
6	1.930368000	-0.120899000	0.010200000
6	2.816811000	0.931258000	-0.172490000
6	2.362793000	-1.430869000	0.179959000
6	4.179551000	0.657452000	-0.193729000
6	3.727527000	-1.685413000	0.160372000
6	4.635558000	-0.646087000	-0.027614000
1	2.443776000	1.938259000	-0.296917000
1	1.646738000	-2.226867000	0.327841000
1	4.883802000	1.467385000	-0.340363000
1	4.081353000	-2.700374000	0.295444000
1	5.699124000	-0.853563000	-0.042351000
6	-1.677344000	-0.631823000	-0.038112000
6	-2.341872000	-1.869863000	-0.071329000
6	-2.435257000	0.551784000	-0.001282000
6	-3.723613000	-1.937292000	-0.060936000
6	-3.824898000	0.466063000	0.003874000
6	-4.473455000	-0.762469000	-0.023383000
1	-1.741328000	-2.771535000	-0.103057000
1	-1.968064000	1.521768000	0.020085000
1	-4.216858000	-2.901863000	-0.084566000
1	-4.403771000	1.382281000	0.030047000
1	-5.556391000	-0.806907000	-0.016934000
8	0.183812000	1.399860000	0.125286000
8	-1.170515000	3.872226000	0.074013000
1	-0.712565000	3.385611000	-0.620377000
1	-0.846837000	3.444635000	0.874528000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -725.257059

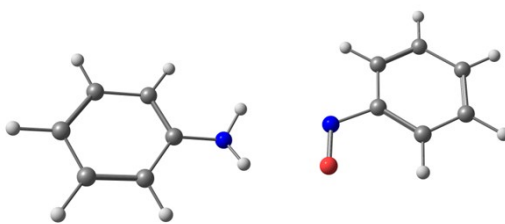
8	0.234400000	3.041247000	-0.418306000
6	-1.076271000	1.088899000	-0.561518000
6	-1.596388000	1.325884000	0.712064000
6	-1.578717000	0.030555000	-1.328665000
6	-2.605878000	0.504747000	1.208180000
6	-2.584140000	-0.779465000	-0.821290000
6	-3.104461000	-0.551700000	0.453298000
1	-1.204807000	2.143326000	1.302224000
1	-1.165617000	-0.152885000	-2.315799000
1	-3.002874000	0.696823000	2.199122000
1	-2.961406000	-1.597818000	-1.424680000
1	-3.886986000	-1.188700000	0.847599000
7	0.015031000	1.816372000	-1.070513000
6	1.832843000	-0.529061000	0.112332000
6	1.098037000	-0.852836000	1.251354000
6	1.804801000	-1.378010000	-0.998169000
6	0.336612000	-2.018945000	1.270938000
6	1.051600000	-2.544101000	-0.961871000
6	0.309796000	-2.872374000	0.172601000
1	1.109723000	-0.187205000	2.104242000
1	2.373455000	-1.115709000	-1.884839000
1	-0.240640000	-2.257909000	2.157583000
1	1.036158000	-3.194016000	-1.829682000
1	-0.286129000	-3.777121000	0.194711000
7	2.665373000	0.612832000	0.053979000
1	-0.085777000	2.012636000	-2.061850000
8	2.216847000	1.633386000	0.922070000
1	1.005642000	2.842782000	0.134455000
1	2.636138000	1.009028000	-0.882635000
1	2.973306000	1.823718000	1.489657000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -725.333415

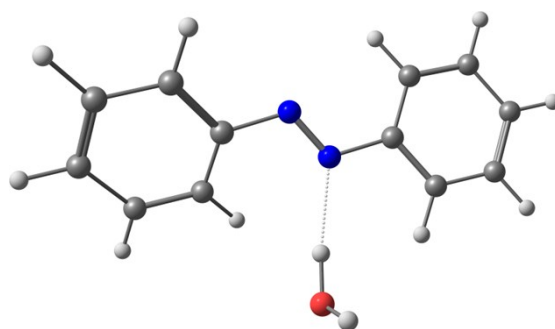
8	0.034584000	3.318129000	0.575084000
6	1.765280000	-0.197600000	-0.087988000
6	2.651124000	-1.160905000	0.394182000
6	2.240753000	1.013891000	-0.598659000
6	4.015195000	-0.895071000	0.408777000
6	3.605474000	1.263234000	-0.593529000
6	4.492939000	0.316079000	-0.082652000
1	2.264382000	-2.104141000	0.762424000
1	1.549586000	1.734591000	-1.017091000
1	4.703653000	-1.635939000	0.797260000
1	3.981036000	2.196763000	-0.995876000
1	5.557426000	0.519320000	-0.081144000
7	0.382000000	-0.539229000	-0.062709000
6	-1.785987000	0.152665000	-0.051897000
6	-2.603665000	1.283474000	-0.027119000
6	-2.347171000	-1.128197000	-0.088211000
6	-3.985913000	1.139852000	-0.040069000
6	-3.727198000	-1.260291000	-0.099380000
6	-4.548354000	-0.131352000	-0.076020000
1	-2.140221000	2.263224000	0.002890000
1	-1.718334000	-2.008436000	-0.108924000
1	-4.619197000	2.018656000	-0.022902000
1	-4.168396000	-2.249561000	-0.128572000
1	-5.625691000	-0.248452000	-0.086699000
7	-0.390801000	0.431246000	-0.041113000
1	-0.259009000	3.426791000	1.484858000
1	0.018024000	2.359823000	0.434066000
8	0.173307000	-3.531907000	-0.006096000
1	0.247713000	-2.576506000	-0.143059000
1	-0.027349000	-3.604693000	0.933010000



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -648.883699

6	-2.893022000	-0.005087000	-0.296965000
6	-3.469674000	1.268970000	-0.178275000
6	-3.692776000	-1.127964000	-0.034598000
6	-4.802264000	1.408499000	0.188899000
6	-5.024190000	-0.975860000	0.331395000
6	-5.593416000	0.290839000	0.446574000
1	-2.860573000	2.144662000	-0.379098000
1	-3.256936000	-2.118038000	-0.123401000
1	-5.225173000	2.403540000	0.276980000
1	-5.621358000	-1.858940000	0.532026000
1	-6.631633000	0.404598000	0.733685000
7	-1.580432000	-0.153209000	-0.719945000
6	2.796229000	-0.111780000	-0.017698000
6	3.749735000	-1.124134000	0.118042000
6	3.154554000	1.232895000	-0.040547000
6	5.082713000	-0.769305000	0.231982000
6	4.495127000	1.579910000	0.076109000
6	5.452750000	0.579163000	0.211220000
1	3.433842000	-2.160053000	0.130811000
1	2.377605000	1.981548000	-0.148516000
1	5.840834000	-1.535992000	0.337976000
1	4.792147000	2.621384000	0.062018000
1	6.499387000	0.846394000	0.301733000
7	1.392032000	-0.364958000	-0.142782000
1	-1.131535000	-1.020163000	-0.452488000
8	1.068105000	-1.524705000	-0.113362000
1	-0.977235000	0.638995000	-0.542575000



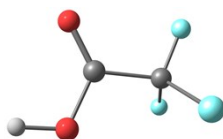
Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -648.926788

8	0.156242000	3.013141000	0.505492000
6	1.756557000	-0.518634000	-0.058728000
6	2.607716000	-1.478876000	0.485934000
6	2.274010000	0.640463000	-0.643748000
6	3.980115000	-1.261468000	0.489721000
6	3.647018000	0.840908000	-0.651595000
6	4.499899000	-0.101728000	-0.077706000
1	2.177890000	-2.378883000	0.910716000
1	1.608740000	1.356257000	-1.110822000
1	4.643287000	-1.999415000	0.925539000
1	4.056291000	1.732622000	-1.111888000
1	5.570994000	0.063987000	-0.086483000
7	0.367913000	-0.820365000	-0.010439000
6	-1.779001000	-0.117771000	-0.051434000
6	-2.616015000	0.994648000	0.015574000
6	-2.312681000	-1.407570000	-0.123763000
6	-3.995417000	0.820909000	0.019966000
6	-3.689258000	-1.570922000	-0.120798000
6	-4.532154000	-0.460252000	-0.047870000
1	-2.173195000	1.983280000	0.065456000
1	-1.648702000	-2.260309000	-0.184484000
1	-4.647461000	1.684720000	0.072319000
1	-4.111355000	-2.567476000	-0.180080000
1	-5.607191000	-0.598747000	-0.048367000
7	-0.382297000	0.166511000	-0.056232000
1	-0.121463000	3.116040000	1.421552000
1	0.058183000	2.061537000	0.335982000

2.3.5. Thermodynamic assessment of protonation steps

Reactants in order to make this evaluation: addition of the Free energies of the products of hydride transfer processes to the free energy of Trifluoroacetic acid molecule .

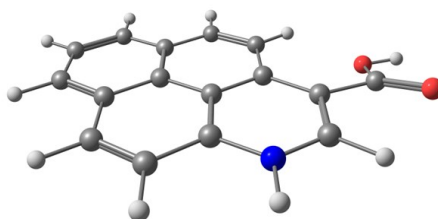


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -526.775920

8	-1.473787000	1.221330000	-0.001979000
6	-0.941748000	0.151928000	-0.004002000
8	-1.509495000	-1.033177000	-0.002052000
6	0.589057000	-0.002565000	-0.001437000
9	0.992615000	-0.630301000	1.104548000
9	0.996086000	-0.718092000	-1.050180000
9	1.173546000	1.186117000	-0.047782000
1	-2.477824000	-0.940924000	0.005597000

Product in order to make this evaluation: addition of the Free energies of the products of protonation (including carboxylate) to the free energy of model organic fragment shown below generated as a result of hydride transfer.

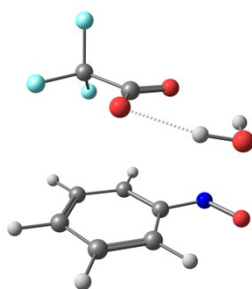


Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -820.546340

6	-4.074661000	-1.199152000	-0.009765000
6	-2.976234000	-2.049425000	-0.040520000
6	-1.675928000	-1.530983000	-0.038412000
6	-1.489313000	-0.130361000	-0.004697000
6	-2.611754000	0.733748000	0.021759000
6	-3.896966000	0.179058000	0.020343000
6	-0.519158000	-2.369107000	-0.080233000
6	-0.172333000	0.401524000	-0.001955000
6	0.969835000	-0.452304000	-0.020956000
6	0.744753000	-1.864818000	-0.075446000
6	2.248310000	0.173130000	-0.012191000
6	2.327672000	1.547826000	-0.008865000
6	-0.025434000	1.804027000	0.018846000
6	-2.398990000	2.149211000	0.047157000

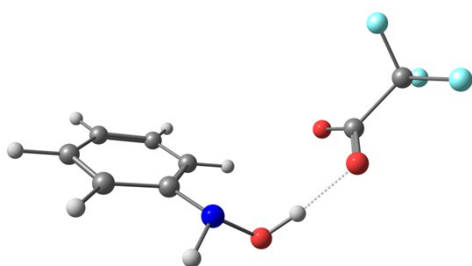
1	-3.264058000	2.802979000	0.066156000
1	-0.667628000	-3.443015000	-0.122023000
1	-5.076146000	-1.611450000	-0.011009000
1	-3.115241000	-3.124647000	-0.067437000
1	-4.755713000	0.841274000	0.042051000
1	1.586190000	-2.537153000	-0.116425000
1	3.275772000	2.067713000	-0.013300000
6	3.583386000	-0.501283000	-0.006624000
8	4.601437000	0.082339000	-0.289529000
8	3.555577000	-1.772610000	0.366428000
1	4.459841000	-2.127741000	0.342349000
7	1.230236000	2.311624000	0.009527000
1	1.344698000	3.324274000	0.022579000
1	-0.974496000	3.745801000	0.059763000
6	-1.146681000	2.676036000	0.044129000



Charge = -1 Multiplicity = 1

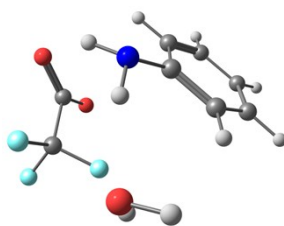
Sum of electronic and thermal Free Energies= -964.165898

1	-1.193708000	-2.550054000	0.553844000
8	-1.586369000	-2.265276000	1.388768000
8	-3.320831000	-1.240662000	-0.869041000
6	-1.820363000	0.398224000	-0.648754000
6	-0.748088000	1.034607000	-1.266873000
6	-2.284734000	0.798155000	0.605803000
6	-0.118615000	2.089981000	-0.618377000
6	-1.653489000	1.852700000	1.244246000
6	-0.573392000	2.494718000	0.633472000
1	-0.416428000	0.679394000	-2.236011000
1	-3.113879000	0.272754000	1.062325000
1	0.723410000	2.589922000	-1.081478000
1	-1.992381000	2.175447000	2.221374000
1	-0.078664000	3.312578000	1.145060000
7	-2.383335000	-0.689919000	-1.389492000
8	0.670432000	-1.775472000	-0.413958000
1	-0.932100000	-1.602739000	1.668791000
6	1.072474000	-0.902073000	0.368782000
8	0.637364000	-0.540957000	1.474582000
6	2.358484000	-0.177257000	-0.114758000
9	3.418587000	-1.000497000	-0.018601000
9	2.274422000	0.191097000	-1.403142000
9	2.650176000	0.920149000	0.591575000



Charge = -1 Multiplicity = 1
Sum of electronic and thermal Free Energies= -888.967034

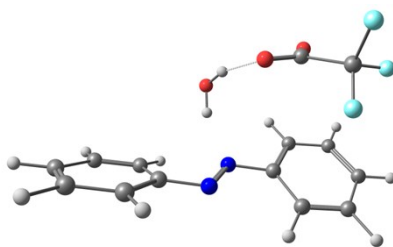
1	0.149739000	-1.705490000	-0.722451000
8	-0.773209000	-1.887240000	-1.022094000
6	-2.427971000	-0.635158000	0.077879000
6	-2.130729000	0.498482000	-0.681886000
6	-3.593600000	-0.660969000	0.853247000
6	-2.994151000	1.589293000	-0.660014000
6	-4.442056000	0.437518000	0.870582000
6	-4.151184000	1.571133000	0.112936000
1	-1.228069000	0.516840000	-1.278142000
1	-3.826164000	-1.545824000	1.437815000
1	-2.753544000	2.463726000	-1.255044000
1	-5.342502000	0.403819000	1.474290000
1	-4.817767000	2.425263000	0.125311000
7	-1.541476000	-1.724237000	0.144817000
8	1.633765000	-1.317783000	-0.054155000
1	-2.038530000	-2.595267000	0.307014000
6	1.960818000	-0.154929000	-0.363469000
8	1.395183000	0.672593000	-1.082867000
6	3.276755000	0.352287000	0.280327000
9	4.025022000	-0.626713000	0.798000000
9	4.038485000	1.010851000	-0.604699000
9	3.004711000	1.213649000	1.277011000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -890.218175

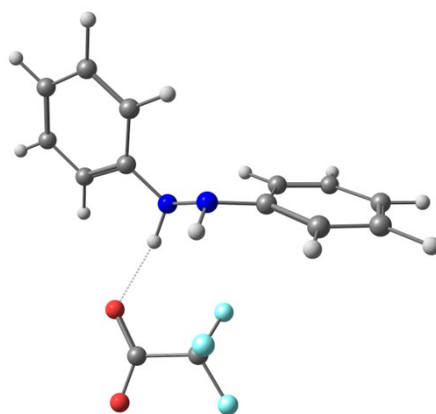
6	-1.381901000	0.362572000	0.795121000
6	-2.007794000	1.220018000	-0.123288000
6	-1.825922000	-0.966200000	0.876976000
6	-3.043021000	0.760982000	-0.927112000
6	-2.859753000	-1.414994000	0.064694000
6	-3.481827000	-0.558905000	-0.841454000
1	-1.660316000	2.244660000	-0.204267000
1	-1.335649000	-1.643933000	1.568565000
1	-3.507497000	1.442532000	-1.632154000
1	-3.179318000	-2.448975000	0.140071000
1	-4.287233000	-0.914407000	-1.472924000
7	-0.380893000	0.836316000	1.632600000
1	0.256213000	0.120608000	1.962553000
1	0.103744000	1.654171000	1.274526000
8	1.422880000	-1.644339000	1.392547000
8	0.823632000	3.221946000	0.149989000
1	0.110473000	3.864768000	0.070836000
1	0.786460000	2.724111000	-0.674324000
6	1.335668000	-1.494670000	0.163575000
8	0.830516000	-2.216034000	-0.705923000
6	1.968182000	-0.194405000	-0.412521000
9	2.482819000	0.615750000	0.519328000
9	2.958765000	-0.485266000	-1.273002000
9	1.063011000	0.527658000	-1.105207000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1175.262559

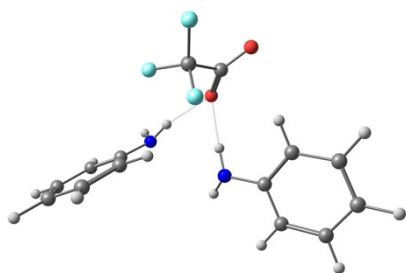
8	0.887934000	-1.650436000	-2.109452000
6	-0.280883000	1.448783000	-0.453526000
6	-1.205521000	0.992621000	-1.390645000
6	-0.635923000	2.423496000	0.481399000
6	-2.507028000	1.479653000	-1.370691000
6	-1.930908000	2.919746000	0.480825000
6	-2.869116000	2.445026000	-0.437256000
1	-0.901663000	0.231536000	-2.100768000
1	0.099173000	2.780140000	1.191847000
1	-3.232926000	1.102087000	-2.081381000
1	-2.215442000	3.679395000	1.199885000
1	-3.882174000	2.830411000	-0.421646000
7	1.011920000	0.859505000	-0.537865000
6	3.041640000	0.456595000	0.328013000
6	3.715120000	0.227890000	1.526372000
6	3.642967000	0.144291000	-0.894291000
6	4.977855000	-0.352025000	1.509664000
6	4.910228000	-0.419775000	-0.903392000
6	5.575214000	-0.676987000	0.295562000
1	3.230078000	0.497285000	2.457629000
1	3.131474000	0.370791000	-1.821724000
1	5.496787000	-0.543540000	2.441501000
1	5.386731000	-0.654580000	-1.848141000
1	6.564882000	-1.118761000	0.279513000
7	1.748591000	1.039559000	0.444111000
8	-0.783239000	-1.910317000	0.119071000
1	0.301789000	-1.937591000	-1.385773000
1	1.138582000	-0.763243000	-1.813719000
6	-1.952171000	-1.708026000	-0.264166000
8	-2.484817000	-1.917579000	-1.357554000
6	-2.864147000	-1.120417000	0.845780000
9	-2.289428000	-0.085189000	1.473295000
9	-4.048085000	-0.698232000	0.387158000
9	-3.118472000	-2.050573000	1.786287000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1100.044317

6	2.355092000	-0.084085000	-0.036143000
6	3.074543000	0.957873000	-0.639372000
6	3.051245000	-1.084042000	0.651461000
6	4.459718000	0.988903000	-0.559383000
6	4.439712000	-1.038215000	0.724011000
6	5.156506000	-0.008404000	0.121416000
1	2.534426000	1.740890000	-1.162092000
1	2.500294000	-1.887578000	1.124164000
1	4.998184000	1.803689000	-1.031402000
1	4.965137000	-1.822358000	1.258844000
1	6.237925000	0.019151000	0.181973000
7	0.968236000	-0.121186000	-0.202146000
6	-0.698887000	-1.758709000	0.268289000
6	-1.781738000	-2.117201000	1.081585000
6	-0.545291000	-2.376577000	-0.977079000
6	-2.683280000	-3.084518000	0.657844000
6	-1.458448000	-3.340265000	-1.389829000
6	-2.530720000	-3.705747000	-0.580390000
1	-1.909735000	-1.627177000	2.041684000
1	0.286058000	-2.094274000	-1.610769000
1	-3.517805000	-3.348171000	1.298645000
1	-1.326788000	-3.811049000	-2.358377000
1	-3.238480000	-4.456825000	-0.910382000
7	0.236680000	-0.836874000	0.746337000
1	-0.107426000	-0.259628000	1.507229000
8	0.031413000	2.673613000	-0.334767000
1	0.558719000	0.789843000	-0.416440000
6	-1.158191000	3.012207000	-0.184892000
8	-1.684302000	4.127218000	-0.204327000
6	-2.106131000	1.813010000	0.092242000
9	-3.400985000	2.128539000	0.021904000
9	-1.892419000	0.805173000	-0.770571000
9	-1.888439000	1.311607000	1.326644000



Charge = -1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1101.264872

6	2.816497000	-0.760774000	0.760843000
6	4.099408000	-1.262461000	1.029210000
6	2.349941000	-0.796783000	-0.563975000
6	4.886147000	-1.778552000	0.006236000
6	3.146779000	-1.311744000	-1.577741000
6	4.421085000	-1.808132000	-1.306443000
1	4.471340000	-1.239670000	2.048771000
1	1.353720000	-0.426677000	-0.778142000
1	5.875376000	-2.157584000	0.240003000
1	2.765355000	-1.325565000	-2.593150000
1	5.038529000	-2.208064000	-2.101579000
7	2.002727000	-0.295072000	1.781240000
6	-2.285468000	-1.398046000	0.283754000
6	-3.075038000	-0.272865000	-0.008790000
6	-2.867091000	-2.670039000	0.164459000
6	-4.397495000	-0.425418000	-0.405149000
6	-4.190799000	-2.808589000	-0.234486000
6	-4.970099000	-1.690643000	-0.524033000
1	-2.646219000	0.720386000	0.079510000
1	-2.267704000	-3.546286000	0.390801000
1	-4.987128000	0.458535000	-0.624136000
1	-4.616843000	-3.802798000	-0.317627000
1	-6.001881000	-1.802212000	-0.834447000
7	-0.950500000	-1.251261000	0.625554000
1	-0.707340000	-0.357447000	1.044863000
1	2.492747000	-0.052074000	2.631949000
1	1.305902000	0.403546000	1.526706000
8	-0.331544000	1.482880000	1.596023000
6	0.143571000	2.412929000	-0.505905000
9	0.011879000	3.559166000	-1.183492000
9	1.455159000	2.254026000	-0.255433000
9	-0.205306000	1.419917000	-1.356433000
1	-0.540211000	-2.037019000	1.112554000
6	-0.730539000	2.340019000	0.778925000
8	-1.710733000	3.077855000	0.791871000

+



Charge = 1 Multiplicity = 1

Sum of electronic and thermal Free Energies= -820.546340

6	-4.074661000	-1.199152000	-0.009765000
6	-2.976234000	-2.049425000	-0.040520000
6	-1.675928000	-1.530983000	-0.038412000
6	-1.489313000	-0.130361000	-0.004697000
6	-2.611754000	0.733748000	0.021759000
6	-3.896966000	0.179058000	0.020343000
6	-0.519158000	-2.369107000	-0.080233000
6	-0.172333000	0.401524000	-0.001955000
6	0.969835000	-0.452304000	-0.020956000
6	0.744753000	-1.864818000	-0.075446000
6	2.248310000	0.173130000	-0.012191000
6	2.327672000	1.547826000	-0.008865000
6	-0.025434000	1.804027000	0.018846000
6	-2.398990000	2.149211000	0.047157000
1	-3.264058000	2.802979000	0.066156000
1	-0.667628000	-3.443015000	-0.122023000
1	-5.076146000	-1.611450000	-0.011009000
1	-3.115241000	-3.124647000	-0.067437000
1	-4.755713000	0.841274000	0.042051000
1	1.586190000	-2.537153000	-0.116425000
1	3.275772000	2.067713000	-0.013300000
6	3.583386000	-0.501283000	-0.006624000
8	4.601437000	0.082339000	-0.289529000
8	3.555577000	-1.772610000	0.366428000
1	4.459841000	-2.127741000	0.342349000
7	1.230236000	2.311624000	0.009527000
1	1.344698000	3.324274000	0.022579000
1	-0.974496000	3.745801000	0.059763000
6	-1.146681000	2.676036000	0.044129000

2.4. PBE-D2 Optimized geometries associated with the Organic Catalyst: ox-CF

2.4.1. Hydrogen Evolution Reaction

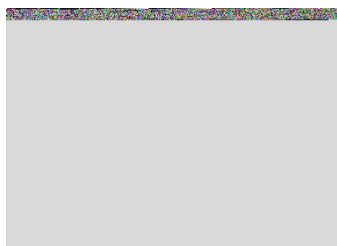


Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1126.527429

6	-3.383431	0.655284	-1.625123
6	-2.484535	-0.424027	-1.820431
6	-1.181563	-0.364185	-1.335097
6	-0.739142	0.798789	-0.615229
6	-1.629997	1.918812	-0.479423
6	-2.959988	1.809758	-0.977139
6	-0.199076	-1.405577	-1.618634
6	0.579173	0.857920	-0.089107
6	1.454636	-0.399441	-0.012522
6	1.038956	-1.407633	-1.068942
6	2.935110	-0.002833	-0.006757
6	3.285387	1.245353	0.429053
6	1.033659	2.076681	0.424062
6	-1.146105	3.105363	0.137783
1	-1.822645	3.955543	0.253660
1	-0.484347	-2.187522	-2.328976
1	-4.403307	0.586098	-2.010345
1	-2.805863	-1.309412	-2.374821
1	-3.636509	2.659548	-0.853544
1	1.751471	-2.190801	-1.325788
1	4.333685	1.522626	0.545603
6	4.056278	-0.932498	-0.196895
8	5.239523	-0.617420	-0.296937
8	3.671308	-2.247487	-0.200498
1	4.494949	-2.767632	-0.319977
7	2.376418	2.201962	0.770290
1	2.713691	3.113556	1.076180
1	0.562216	4.119393	0.980860
1	1.253681	-0.888782	0.971423
8	-0.892664	-2.635429	1.105210
1	-0.925372	-1.703485	1.629835
1	-1.930072	-2.847227	0.864736

1	-0.415541	-2.475771	0.248305
8	-1.212237	-0.464900	2.308808
1	-0.657538	0.285093	2.016138
1	-2.142478	-0.236946	2.031498
8	-3.300336	-2.920758	0.585957
1	-3.663619	-2.026021	0.836092
1	-3.769648	-3.575537	1.138439
8	-3.727964	-0.355378	1.323988
1	-3.789509	0.218973	0.526269
1	-4.471447	-0.093858	1.902033
6	0.166011	3.194802	0.552422



(Transition state)

Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1126.496841

6	-3.374540	-0.235356	-1.930788
6	-2.337542	-1.187500	-1.996591
6	-1.059775	-0.892950	-1.506643
6	-0.816024	0.385988	-0.911693
6	-1.865116	1.361049	-0.866552
6	-3.143991	1.024423	-1.380758
6	0.048650	-1.808457	-1.644779
6	0.478160	0.700800	-0.413929
6	1.518994	-0.338731	-0.322123
6	1.277686	-1.542975	-1.130090
6	2.872699	0.175224	-0.087296
6	3.037018	1.484938	0.314611
6	0.716783	2.002314	0.061091
6	-1.586226	2.648777	-0.316049
1	-2.390656	3.386528	-0.267275
1	-0.121296	-2.732524	-2.203622
1	-4.361711	-0.483444	-2.327472
1	-2.517298	-2.164949	-2.451076
1	-3.939292	1.773586	-1.346023
1	2.094615	-2.250546	-1.254184
1	4.022474	1.884147	0.553071
6	4.119440	-0.626681	-0.081955
8	5.245997	-0.150216	-0.118308
8	3.897274	-1.963464	0.026249
1	4.781049	-2.393217	0.034543
7	1.997683	2.336637	0.449973
1	2.176867	3.289792	0.772024
1	-0.092183	3.963181	0.524255
1	1.202432	-0.965343	1.043198
8	-0.373134	-1.346427	2.619239
1	-0.872608	-0.460818	2.630926
1	-1.007907	-1.969890	2.122309
1	0.593058	-1.150322	1.732596
8	-1.861377	0.831919	2.513570

	1	-1.542477	1.525775	1.907120
	1	-2.662844	0.454294	2.072208
	8	-2.119981	-2.763300	1.249096
	1	-2.845313	-2.091867	1.187046
	1	-2.505047	-3.497850	1.761539
	8	-3.862148	-0.629593	1.298922
	1	-4.082017	-0.307631	0.400998
	1	-4.716250	-0.728664	1.761819
6	-0.321286	2.971130	0.127887	



Charge = 1 Multiplicity =1

Sum of electronic and thermal Free Energies= -1126.537031

6	-2.960735	1.388398	-1.326475
6	-2.322706	0.161237	-1.536740
6	-0.974193	-0.018720	-1.162591
6	-0.264192	1.067477	-0.570416
6	-0.923248	2.318512	-0.351285
6	-2.274352	2.454714	-0.735199
6	-0.292167	-1.259464	-1.349278
6	1.094894	0.893829	-0.188557
6	1.768473	-0.363310	-0.386194
6	1.023947	-1.427948	-0.983924
6	3.141525	-0.442452	0.025226
6	3.746643	0.680055	0.578669
6	1.764481	1.997873	0.407125
6	-0.199455	3.390639	0.260071
1	-0.713655	4.339786	0.427863
1	-0.856560	-2.093840	-1.770286
1	-4.004582	1.518368	-1.621775
1	-2.855820	-0.681002	-1.981906
1	-2.777929	3.408618	-0.560836
1	1.505762	-2.389028	-1.143120
1	4.788586	0.673795	0.895051
6	4.063611	-1.619883	-0.077619
8	5.276741	-1.524013	0.020778
8	3.434673	-2.801486	-0.258708
1	4.134301	-3.490219	-0.313725
7	3.073734	1.830145	0.761546
1	3.565683	2.621418	1.188863
1	1.677688	4.052043	1.098622
1	-0.106430	-0.667223	1.790832
8	-2.499388	-2.512529	2.335547
1	-2.789292	-1.571413	2.379683
1	-2.575308	-2.697743	1.370985
1	-0.663814	-1.158200	1.934791
8	-3.239824	0.202266	1.990962
1	-2.446002	0.427965	1.471937
1	-3.899690	-0.039875	1.300462

8	-3.014322	-2.773784	-0.457083
1	-3.767547	-2.143816	-0.352172
1	-3.442969	-3.631618	-0.626769
8	-4.986371	-0.895091	0.101498
1	-5.331050	-0.345543	-0.628188
1	-5.775728	-1.274450	0.533537
6	1.115165	3.240386	0.632417

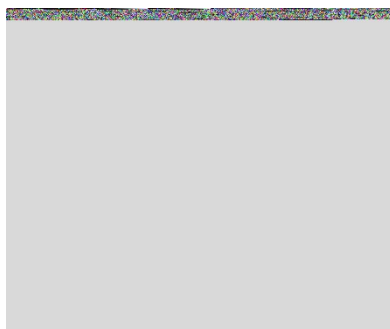


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.061464

6	-2.271086	3.048663	0.651999
6	-1.056668	3.312902	-0.027929
6	-0.010994	2.391043	-0.016498
6	-0.179085	1.145093	0.683638
6	-1.383160	0.916080	1.434951
6	-2.426704	1.881913	1.381832
6	1.302483	2.684096	-0.579916
6	0.849453	0.170255	0.654756
6	1.987157	0.288527	-0.361333
6	2.268201	1.746083	-0.678265
6	3.185760	-0.553010	0.086079
6	2.999246	-1.570418	0.984035
6	0.732642	-0.944764	1.485793
6	-1.493541	-0.284143	2.191056
1	-2.415366	-0.479068	2.744652
1	1.497552	3.714775	-0.892879
1	-3.078877	3.783698	0.614543
1	-0.918615	4.264376	-0.549612
1	-3.350823	1.683181	1.931140
1	3.250400	2.000953	-1.075936
1	3.819251	-2.240654	1.245057
6	4.503645	-0.526025	-0.554483
8	5.506180	-1.132190	-0.177514
8	4.528287	0.227289	-1.700792
1	5.445774	0.160403	-2.041631
7	1.803134	-1.837017	1.574557
1	1.738348	-2.607805	2.236957
1	-0.504912	-2.086035	2.852479
1	1.592277	-0.150641	-1.307104
6	-0.444597	-1.180108	2.243002
6	-3.120441	-1.483106	-0.839687
9	-2.666706	-2.555551	-0.160353
9	-3.941962	-0.780374	-0.025320
9	-3.859361	-1.929851	-1.890323
6	-1.928311	-0.640090	-1.368493

8	-0.826134	-1.113599	-1.524215
8	-2.335414	0.600238	-1.648063
1	-1.552027	1.136058	-1.914136



(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.030890

6	-2.258325	3.640170	-0.082933
6	-0.976887	3.714611	-0.660489
6	-0.023634	2.714169	-0.425052
6	-0.366031	1.610794	0.419400
6	-1.653152	1.563448	1.044623
6	-2.592443	2.585558	0.762016
6	1.322702	2.786311	-0.944928
6	0.583527	0.580571	0.657058
6	1.818340	0.513606	-0.140197
6	2.213055	1.770013	-0.790018
6	2.806872	-0.452937	0.344590
6	2.443970	-1.367187	1.313669
6	0.264674	-0.425830	1.585243
6	-1.948859	0.483184	1.930151
1	-2.939351	0.435904	2.388725
1	1.620946	3.698367	-1.469391
1	-2.989610	4.424788	-0.289915
1	-0.709071	4.561903	-1.297564
1	-3.581045	2.533993	1.225415
1	3.219334	1.847452	-1.196708
1	3.141698	-2.129671	1.658650
6	4.159107	-0.659849	-0.220925
8	5.052221	-1.294259	0.326220
8	4.310544	-0.112240	-1.457518
1	5.230697	-0.310865	-1.738011
7	1.218607	-1.377711	1.876066
1	0.988988	-2.108361	2.551593
1	-1.220754	-1.299423	2.903974
1	1.290859	-0.201608	-1.449137
6	-1.007222	-0.478521	2.215884
6	-2.639974	-1.896066	-0.758387
9	-2.893132	-2.539241	0.410383
9	-3.292076	-0.703671	-0.712015

9	-3.217344	-2.631112	-1.755729
6	-1.104243	-1.756767	-1.020018
8	-0.348554	-2.579444	-0.509622
8	-0.844404	-0.763040	-1.804829
1	0.432698	-0.502082	-1.715975



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1347.090569

6	3.969944	-3.657528	0.177401
6	4.571342	-2.398773	0.279382
6	3.799296	-1.223908	0.166070
6	2.393274	-1.331768	-0.057089
6	1.783957	-2.622042	-0.164401
6	2.592928	-3.771426	-0.042235
6	4.372605	0.082664	0.258968
6	1.604281	-0.153037	-0.172365
6	2.195866	1.153195	-0.056311
6	3.612160	1.223291	0.153367
6	1.319775	2.278572	-0.186811
6	-0.034927	2.050541	-0.435051
6	0.207560	-0.295776	-0.410489
6	0.373176	-2.708576	-0.396600
1	-0.081220	-3.698993	-0.478517
1	5.451144	0.163909	0.418051
1	4.579511	-4.558946	0.269348
1	5.647278	-2.309535	0.449674
1	2.124544	-4.755622	-0.122488
1	4.090730	2.196223	0.230151
1	-0.730971	2.882958	-0.544005
6	1.676552	3.728136	-0.093509
8	0.943213	4.624668	-0.482652
8	2.872309	3.969341	0.492884
1	2.995018	4.944757	0.493869
7	-0.557867	0.823507	-0.537192
1	-1.672942	0.694778	-0.664482
1	-1.474509	-1.637878	-0.709566
1	-0.414671	1.277456	2.632998
6	-0.400567	-1.580513	-0.520071
6	-5.033438	-0.491974	0.109472

9	-5.832586	0.245680	-0.715122
9	-4.918007	-1.733649	-0.457337
9	-5.707062	-0.652433	1.277252
6	-3.624358	0.157729	0.299352
8	-3.063595	0.397794	-0.826694
8	-3.215361	0.333284	1.452403
1	-1.059035	1.066423	2.300160

2.4.2. Hydride transfer processes

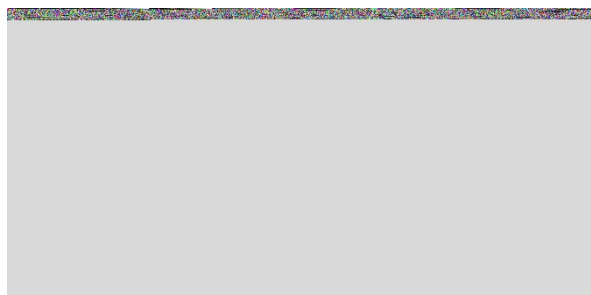


Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1256.946231

6	-2.945481	3.210722	0.459362
6	-1.685358	3.560679	-0.084360
6	-0.596760	2.695928	0.007878
6	-0.762595	1.422931	0.655720
6	-2.019798	1.107033	1.277116
6	-3.107098	2.015269	1.141083
6	0.748951	3.084374	-0.397754
6	0.327132	0.518097	0.736186
6	1.574060	0.739698	-0.121879
6	1.784424	2.217930	-0.387263
6	2.764470	-0.026736	0.456616
6	2.545010	-1.072988	1.312653
6	0.198656	-0.606453	1.554863
6	-2.124447	-0.098280	2.025418
1	-3.080860	-0.352028	2.489982
1	0.907381	4.130641	-0.678029
1	-3.784345	3.904711	0.363643
1	-1.548962	4.535389	-0.561747
1	-4.066002	1.755717	1.598490
1	2.784825	2.545731	-0.669478
1	3.371939	-1.694926	1.657769
6	4.144080	0.103928	-0.021316
8	5.136723	-0.423599	0.479225
8	4.247857	0.860833	-1.160508
1	5.202266	0.866716	-1.388262
7	1.309190	-1.427034	1.756622
1	1.217693	-2.218745	2.390418
1	-1.087449	-1.826023	2.801349
1	1.342823	0.300447	-1.122280
6	-1.028198	-0.920189	2.192178
8	-0.239971	0.034156	-2.672777
8	-2.324484	0.397857	-2.121721
6	-1.315723	-1.558656	-1.352616
6	-0.134723	-2.303579	-1.250136

6	-2.517200	-1.978017	-0.771016
6	-0.162596	-3.500299	-0.531337
6	-2.531150	-3.185787	-0.068190
6	-1.358188	-3.943470	0.055279
1	0.781203	-1.936376	-1.713538
1	-3.411469	-1.363895	-0.873520
1	0.752233	-4.087171	-0.427429
1	-3.459814	-3.531521	0.390523
1	-1.373962	-4.883293	0.612036
7	-1.293950	-0.286130	-2.098705



(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1256.935085

6	2.589867	3.639215	-0.191058
6	1.278887	3.822023	0.291767
6	0.290301	2.847729	0.086278
6	0.640166	1.639816	-0.602245
6	1.972639	1.464889	-1.105526
6	2.933498	2.487239	-0.888744
6	-1.078539	3.032411	0.503871
6	-0.330651	0.614087	-0.772465
6	-1.646277	0.705376	-0.091359
6	-2.008394	2.040197	0.381633
6	-2.646423	-0.301422	-0.547737
6	-2.213414	-1.379307	-1.282688
6	0.030521	-0.533441	-1.499796
6	2.289178	0.266257	-1.810566
1	3.304515	0.133409	-2.192209
1	-1.360248	3.998378	0.931578
1	3.338809	4.416882	-0.021666
1	1.012503	4.741113	0.820977
1	3.947368	2.345777	-1.272441
1	-3.030373	2.207607	0.717347
1	-2.896741	-2.178315	-1.568328
6	-4.066095	-0.371262	-0.149921
8	-4.898018	-1.133294	-0.634893
8	-4.390991	0.482431	0.864047
1	-5.346428	0.342351	1.041127
7	-0.919757	-1.531957	-1.669870
1	-0.656555	-2.365773	-2.194389
1	1.562693	-1.617806	-2.578456
1	-1.209345	0.170341	1.113943
6	1.330871	-0.702154	-2.028926
8	-0.682435	-0.420541	2.029599
8	1.306801	0.593379	2.222844
6	1.226334	-1.543699	1.258581

6	0.443391	-2.655611	0.883717
6	2.621391	-1.536842	1.052281
6	1.066903	-3.747407	0.279253
6	3.223916	-2.644367	0.452971
6	2.454538	-3.748881	0.056204
1	-0.631087	-2.644612	1.063534
1	3.197951	-0.664923	1.360192
1	0.463029	-4.607840	-0.019546
1	4.303935	-2.640919	0.286232
1	2.932526	-4.609550	-0.417191
7	0.629604	-0.406756	1.873210



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1256.944633

6	-2.891221	-1.676066	1.502614
6	-2.209577	-0.484100	1.789413
6	-0.866897	-0.307239	1.392984
6	-0.202667	-1.368915	0.698574
6	-0.902568	-2.590559	0.419868
6	-2.255671	-2.717406	0.827673
6	-0.150047	0.904228	1.633689
6	1.153052	-1.203530	0.282878
6	1.864042	0.034390	0.544326
6	1.203670	1.028453	1.289165
6	3.216353	0.128451	0.012434
6	3.784988	-0.979065	-0.592169
6	1.784398	-2.283637	-0.378436
6	-0.216439	-3.637027	-0.264695
1	-0.753478	-4.564067	-0.480348
1	-0.633987	1.691167	2.214043
1	-3.933496	-1.788108	1.811571
1	-2.710102	0.323231	2.328326
1	-2.787420	-3.646269	0.605533
1	1.735610	1.938192	1.564264
1	4.801739	-0.953222	-0.982923
6	4.064882	1.341993	-0.035942
8	5.264071	1.349016	-0.285962
8	3.369275	2.497570	0.170726
1	4.014598	3.231500	0.073949
7	3.107205	-2.132261	-0.762733
1	3.569012	-2.913478	-1.231520
1	1.633780	-4.292768	-1.170693
1	0.851711	2.239735	-0.399047
6	1.101153	-3.492187	-0.651258
8	0.116900	2.399862	-1.038390
8	-1.226478	3.527631	0.477459
6	-2.095430	1.656050	-0.652625
6	-1.851644	0.547190	-1.494688
6	-3.402470	1.907831	-0.182421
6	-2.914213	-0.265586	-1.884513

6	-4.455988	1.083389	-0.590490
6	-4.224347	-0.005928	-1.441911
1	-0.834850	0.346797	-1.828966
1	-3.564558	2.760060	0.478656
1	-2.717907	-1.118807	-2.539056
1	-5.467435	1.295735	-0.234128
1	-5.049992	-0.649412	-1.754101
7	-1.041995	2.444077	-0.150560



Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1467.828706

6	-0.021320	-3.395865	2.492009
6	-1.144968	-2.557438	2.289795
6	-0.990048	-1.232930	1.886297
6	0.333015	-0.715976	1.662749
6	1.472044	-1.542296	1.956159
6	1.262958	-2.895723	2.345121
6	-2.111226	-0.304699	1.799953
6	0.508158	0.621540	1.223118
6	-0.681934	1.400996	0.662295
6	-1.975021	0.946063	1.309868
6	-0.396617	2.903446	0.681718
6	0.896029	3.347052	0.777960
6	1.794512	1.161065	1.229036
6	2.770382	-0.968523	1.860538
1	3.643020	-1.593317	2.068051
1	-3.078994	-0.647627	2.178957
1	-0.172643	-4.435350	2.793928
1	-2.152766	-2.942612	2.469667
1	2.135480	-3.525800	2.539514
1	-2.827205	1.624922	1.276154
1	1.128123	4.409964	0.698343
6	-1.384932	3.930419	0.345733
8	-1.228174	5.148179	0.432748
8	-2.553072	3.406250	-0.151658
1	-3.124443	4.178094	-0.351662
7	1.961800	2.517128	0.935690
1	2.896107	2.916299	0.999085
1	3.919624	0.823461	1.502392
1	-0.765748	1.088781	-0.404168
6	2.927916	0.364772	1.538960
8	0.078554	-2.717022	-1.370508
6	-1.829537	-1.375140	-1.516744
6	-2.583012	-2.402151	-0.939161
6	-2.429532	-0.198198	-1.983126
6	-3.964952	-2.235824	-0.806146
6	-3.812280	-0.047606	-1.846237

6	-4.581478	-1.059383	-1.253357
1	-2.078866	-3.301239	-0.586310
1	-1.819552	0.581845	-2.437465
1	-4.558960	-3.027222	-0.343662
1	-4.288065	0.868346	-2.203435
1	-5.660809	-0.931154	-1.142885
7	-0.372258	-1.558395	-1.582306
6	1.686566	-0.457477	-1.854160
6	2.201707	0.851665	-2.038380
6	2.598904	-1.535181	-1.705996
6	3.573940	1.086125	-2.062794
6	3.974405	-1.283019	-1.738754
6	4.470388	0.016106	-1.911044
1	1.490973	1.674408	-2.144686
1	2.227216	-2.545850	-1.566496
1	3.947438	2.104363	-2.195269
1	4.668673	-2.119066	-1.621946
1	5.548205	0.195115	-1.927900
7	0.290502	-0.476812	-1.827288



(Transition state)

Charge = 0 Multiplicity = 1

Sum of electronic and thermal Free Energies= -1467.818093

6	-3.781163	0.115700	2.044601
6	-3.351849	1.282318	1.386600
6	-1.998058	1.459739	1.060172
6	-1.043779	0.464166	1.457239
6	-1.489106	-0.719006	2.137259
6	-2.875691	-0.879265	2.399733
6	-1.525060	2.613169	0.337125
6	0.341169	0.653392	1.181642
6	0.789226	1.748404	0.285606
6	-0.207340	2.776080	0.009908
6	2.260002	2.033933	0.355358
6	3.083409	1.096874	0.933878
6	1.259037	-0.293872	1.668336
6	-0.521205	-1.692021	2.521500
1	-0.861205	-2.607468	3.012191
1	-2.254562	3.378142	0.057413
1	-4.843212	-0.015779	2.267535
1	-4.071561	2.052465	1.098146
1	-3.214421	-1.789691	2.901294
1	0.107810	3.660510	-0.541222
1	4.164769	1.231948	0.944535
6	2.973292	3.157056	-0.272900
8	4.161236	3.425686	-0.103488
8	2.200365	3.893794	-1.126438
1	2.787306	4.597714	-1.477827
7	2.620010	-0.051484	1.485858
1	3.286538	-0.729139	1.853242
1	1.576285	-2.196335	2.649694
1	0.665342	1.009130	-0.849409
6	0.828203	-1.469680	2.322643
8	0.584006	0.178373	-1.784603
6	1.410070	-1.903739	-1.065796

6	2.716678	-1.408996	-1.209424
6	1.191685	-3.241345	-0.680520
6	3.803502	-2.252635	-0.956641
6	2.288855	-4.067176	-0.429623
6	3.599550	-3.580858	-0.562463
1	2.871966	-0.374455	-1.513186
1	0.172287	-3.610970	-0.580780
1	4.817167	-1.859971	-1.066812
1	2.116498	-5.103511	-0.128936
1	4.452046	-4.234053	-0.362819
7	0.299009	-1.033085	-1.324462
6	-2.055167	-0.823577	-1.402903
6	-3.231909	-1.514165	-0.979118
6	-2.219935	0.425377	-2.078077
6	-4.497203	-0.980761	-1.190037
6	-3.501146	0.940438	-2.282395
6	-4.643905	0.262654	-1.831012
1	-3.105572	-2.473979	-0.473029
1	-1.352375	0.972323	-2.433835
1	-5.378237	-1.526712	-0.842681
1	-3.607020	1.899885	-2.796378
1	-5.637325	0.689186	-1.989608
7	-0.900498	-1.510473	-1.100744



Charge = 0 Multiplicity = 1

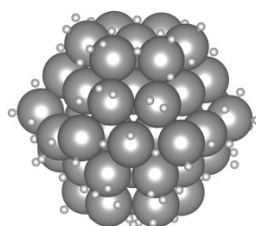
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6	3.415421	-1.659540	1.080365
6	2.029307	-1.795712	0.797546
6	1.114911	-0.805335	1.283408
6	1.614199	0.354529	1.965368
6	3.006981	0.470236	2.182866
6	1.505355	-2.864529	0.021426
6	-0.288592	-0.964812	1.063316
6	-0.802381	-2.091333	0.321533
6	0.144944	-3.008264	-0.208924
6	-2.260616	-2.202662	0.202192
6	-3.043630	-1.187630	0.722451
6	-1.159583	0.061477	1.537416
6	0.692873	1.369667	2.359263
1	1.080723	2.270785	2.840432
1	2.201563	-3.599343	-0.391791
1	4.952550	-0.442826	1.971452
1	4.103714	-2.432140	0.729332
1	3.387969	1.355646	2.697721
1	-0.208462	-3.849723	-0.799835
1	-4.129501	-1.216835	0.639359
6	-3.045507	-3.287026	-0.428238
8	-4.270670	-3.294037	-0.519499
8	-2.298262	-4.317327	-0.912759
1	-2.938437	-4.957378	-1.293298
7	-2.522750	-0.110708	1.341666
1	-3.153272	0.626923	1.658748
1	-1.378092	1.980121	2.498710
1	-0.542811	-0.581037	-1.127528
6	-0.670447	1.211067	2.181042
8	-0.663198	0.177222	-1.756323
6	-1.455550	2.183892	-0.768980

6	-2.772709	1.732787	-1.006176
6	-1.243111	3.488093	-0.260520
6	-3.853983	2.571154	-0.718623
6	-2.338781	4.305226	0.020091
6	-3.652183	3.857152	-0.198283
1	-2.937405	0.738030	-1.417351
1	-0.224237	3.833839	-0.091515
1	-4.867405	2.207762	-0.907677
1	-2.161591	5.309952	0.412844
1	-4.503006	4.504221	0.026255
7	-0.357954	1.333027	-0.992051
6	2.008404	1.146691	-1.182426
6	3.201166	1.756379	-0.667665
6	2.176663	0.012191	-2.047055
6	4.463557	1.273425	-0.990795
6	3.452957	-0.455493	-2.350403
6	4.607407	0.147903	-1.820227
1	3.087987	2.626734	-0.017616
1	1.312501	-0.472714	-2.491752
1	5.347302	1.764240	-0.573727
1	3.549667	-1.320266	-3.013399
1	5.598858	-0.239220	-2.066528
7	0.866512	1.767148	-0.771697

2.5. PBE-D2 Optimized geometries associated with the Inorganic Catalyst: Ru-CF

2.5.1. Adsorption energies of the different reagents



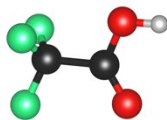
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H Ru
88 57
Direct
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0.4919664668746489 0.7545516563876662 0.4566448364547648
0.4143621078283493 0.7231358065397163 0.4823303392420863
0.3246353776829808 0.6701712400729040 0.4891105686804098
0.2441059146986728 0.6377349637674176 0.4758018934299579
0.2457786447590602 0.6376122308788509 0.5124561855028500
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0.2714116135462563 0.5311261759530692 0.6072668232337851
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0.5456987885156213 0.5809278623801658 0.7075031763690313
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0.5925226784541747 0.4943888176536463 0.7007448129099990
0.6272471891808843 0.5671575219658919 0.7022919670332651
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0.2766896344480308	0.4943705290297692	0.4244863018393003
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0.3268389937696998	0.5662294354537178	0.3396609375944530
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0.5361782359460141	0.2654097717724107	0.3843548684934747
0.5608797955157816	0.2858790338031942	0.3688025727347933
0.4910198464374878	0.3184187028337117	0.3332698923009137
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0.5460864037710320	0.4942335096433145	0.2693711814651129
0.3363921278252161	0.4624464654556060	0.6395261547386589
0.3961401462314986	0.4913768061210299	0.7075110253813405
0.4389391426865438	0.3973950552857021	0.7023218151983142
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0.4943619243609936	0.5062742510394265	0.7267072663602231
0.4890160224141581	0.4727289484292554	0.7262459768193053
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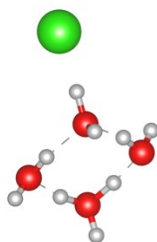
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0.7057922678495301	0.3677208266841435	0.5177009778548201
0.6116019603971853	0.2827986673047481	0.4432025922657100
0.6556711476563899	0.3306036413504502	0.4702632303753556
0.5622444980631350	0.2766867129873671	0.5872213909177716
0.5339198423455360	0.2732041405889814	0.6053519998988129
0.2787231944718289	0.4094753369970193	0.6037914997623224
0.2653478301230215	0.4380687555357127	0.5858165240229458
0.4620518570755392	0.3306006358705401	0.6107479043713490
0.3649392019528252	0.3834061472475416	0.6105544807716142
0.6293562300357056	0.3329418914133029	0.3575348602513587
0.6500446755155442	0.3603844318922066	0.3487481211588283
0.6601145906948288	0.4360125170791753	0.3998060312377487
0.6274855716404407	0.4923447622830400	0.3297132403636501
0.4241494237606716	0.4949684009319366	0.4033256240381024
0.4856261254842379	0.4922112171830769	0.3147829179144060
0.5188294472653271	0.4417199197536970	0.4004651242155092
0.5745089867113805	0.4352880887977146	0.3114633019586001
0.4235454283940441	0.6022692291562487	0.4073190638159837
0.4842731359446429	0.5970378819339065	0.3178903133043010
0.5172471727069251	0.5468551305554440	0.3995859036733314
0.5795846037441946	0.5449100448171661	0.3091848177319621
0.6119183461438445	0.4938171941711095	0.4009458519878123
0.5131950302622150	0.6580464724546221	0.4040426513534097
0.6039957148429459	0.6027562648763588	0.3979658119692590
0.4257431263061832	0.4919060881863814	0.5721534194528471
0.4890545272573271	0.4932334709213689	0.4877043447439321
0.5231107659314338	0.4355863584791411	0.5720206979395248
0.5788097671767348	0.4402344993361639	0.4835427913393750
0.4271509107084662	0.6010157640894691	0.5734583597073064
0.4890914443894241	0.5997055951160712	0.4886922118936043
0.5199619090320683	0.5480776078582139	0.5697921286951245
0.5778363109820187	0.5472180762998734	0.4841259036142738
0.6113667197248943	0.4938983658547701	0.5732074797503468
0.6760383431437336	0.4980602398196708	0.5008775908748145
0.4804639169553660	0.7039348110317051	0.4942215179024974
0.5201376924978061	0.6507117982903023	0.5734146400343382
0.5827878954659244	0.6572759037910978	0.4857884926759630
0.6165848702879354	0.6026924851126227	0.5706932564713830
0.6732600539979464	0.5941600908527420	0.4702649380121950
0.4916999784916741	0.4901964866872693	0.6574739595211548
0.5842491944471780	0.4363816200328258	0.6546975907365282
0.4885069601236747	0.5926533582595293	0.6582813513256467
0.5832467354862076	0.5493923794455671	0.6592576675310520
0.3342112091647244	0.4443803350935462	0.4035858418903364
0.3881741115694397	0.4392212789840704	0.3157339246716748

0.3343121969321828 0.5457829085783129 0.4069447887927198
0.3919109002696113 0.5449815619232667 0.3206824106650341
0.2986971057098973 0.4929037592706621 0.4918280284465255
0.3332294834139795 0.4388031082148705 0.5732595875770586
0.3962318777020799 0.4402797077385619 0.4877007925255878
0.3017561792386241 0.6046581195831664 0.4913234398753651
0.3340572700514442 0.5451175436217772 0.5767094210179181
0.3926475688924014 0.5457042311280148 0.4914864745337917
0.3944354926770676 0.6533876591690102 0.4861577768211073
0.4008387300977347 0.4355397597684436 0.6576961568031777
0.4009014029854843 0.5424699089120052 0.6606376107017891
0.4249794770748004 0.3872697727005329 0.4029582340164720
0.4794184835751416 0.3845738645448876 0.3138290853330069
0.5170549825832870 0.3308392444030502 0.3985529081835835
0.6059170948537770 0.3864641148743353 0.3958034134462969
0.4823203867411400 0.2823235712685128 0.4811513821168125
0.4279776213637102 0.3849856302372628 0.5711967896471325
0.4896907810408396 0.3868589367731674 0.4845612774043214
0.5218334205194434 0.3321416114912757 0.5649438874493179
0.5867891568311653 0.3277534059967582 0.4813112822728065
0.6142772674429705 0.3859772129171165 0.5640383694677654
0.6733859448635641 0.4016194773424500 0.4742172852486556
0.4929013338703559 0.3834142388765088 0.6550895450817197
0.3060563373945449 0.3841898895050570 0.4821893836864835
0.3986040166488615 0.3330535536054058 0.4873742346156350



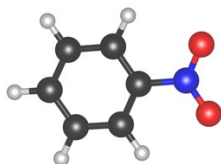
energy(sigma->0) = -48.00691281

H 1 C 2 O 2 F 3			
1.0000000000000000			
25.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	25.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	25.0000000000000000	
H C O F			
1	2	2	3
Direct			
0.5917318129753645	0.6454038775313128	0.2849535427366042	
0.6412560196093282	0.7621857248694578	0.3122700095831328	
0.6276842060866759	0.7020959774938634	0.3214630571504984	
0.6391393559477195	0.6791019043705844	0.3627110150834899	
0.6019569370789227	0.6829767510555350	0.2791610136900871	
0.6752557189292859	0.7802252921097891	0.3502312599670994	
0.5956447490775238	0.7920669660276860	0.3148489076400013	
0.6640492002951872	0.7708719065417790	0.2636279941490897	



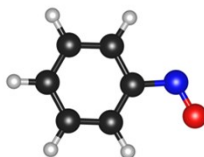
energy(sigma->0) = -65.56576519

H 9 O 4 Cl 1		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H O Cl		
9 4 1		
Direct		
0.9465747995529601	0.2792783683698929	0.1335062309989899
0.0100887688715582	0.3001698092476405	0.1498434773059441
0.9979316599933332	0.2356808309448935	0.1316618564474368
0.8720900175536600	0.2702896097940845	0.1636200468679650
0.9040829208840409	0.3230483336390697	0.1804084584770714
0.9964054090908305	0.3522472489041278	0.2028422514220474
0.0490511618980120	0.3662901994045042	0.1690920541077832
0.9305449351674787	0.3521972889501619	0.2608573361721861
0.9219829758793624	0.4023197524434374	0.2218266746187950
0.9880477974190167	0.2726825616314151	0.1236353477573833
0.8954642133822632	0.2982714366237035	0.1497659554046769
0.0297507989507820	0.3368527467168773	0.1859161416786206
0.9348479003032785	0.3633967533995514	0.2237756650052054
0.8969496710534167	0.4748335083306427	0.2174018717359116



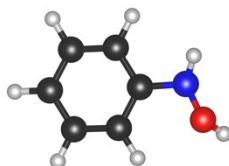
energy(sigma->0) = -91.77426776

	H 5	C 6	N 1	O 2
	1.0000000000000000			
25.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	25.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	25.0000000000000000	0.0000000000000000	
	H	C	N	O
	5	6	1	2
	Direct			
0.6776623837429930	0.7517324370619604	0.3970249818170600		
0.6979631255100849	0.8497244700412915	0.3975253307716620		
0.6683660606279220	0.9069400578059907	0.3216896763403396		
0.6169141907264790	0.8671482292930025	0.2462418149508693		
0.5965984399435774	0.7691587600129858	0.2459587309815022		
0.6368453610943338	0.7558299309230083	0.3211063814870356		
0.6190030047148243	0.7872918770023614	0.2785580653387039		
0.6649438817250560	0.7773796142550153	0.3642680646393538		
0.6305577188649231	0.8420366054057788	0.2791120025138468		
0.6760953378003510	0.8322071729860104	0.3641690640753480		
0.6592216752064920	0.8643329508312738	0.3216201185418595		
0.6261831993006763	0.6980716310858276	0.3202081401373779		
0.6411051956149946	0.6707845913256265	0.3590388531407674		
0.6030464251272906	0.6790048719698615	0.2804823752642808		



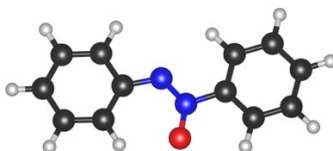
energy(sigma->0) = -85.13661027

H C N O			
1.0000000000000000			
25.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	25.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	25.0000000000000000	
H C N O			
5	6	1	1
Direct			
0.6859509430565729	0.7491629966983924	0.3930548545461731	
0.7152032864021154	0.8450885273853311	0.3854662776829054	
0.6799794122477156	0.9016658271756098	0.3117702655758433	
0.6160163568571222	0.8644818708632993	0.2453177350555803	
0.5864557745708397	0.7685181955786424	0.2535636655906663	
0.6347353354264764	0.7543735117668631	0.3236316277324949	
0.6146028710565894	0.7862089139395365	0.2818427304631109	
0.6711550402369355	0.7751386017085120	0.3613003940779769	
0.6310769446454745	0.8393107592463502	0.2775273375464279	
0.6871350856540800	0.8281218901039250	0.3567469066420066	
0.6671539497073121	0.8601201283756486	0.3149694936317762	
0.6155006007536683	0.7007595084191480	0.3241857374681412	
0.6331746676526651	0.6716896035639635	0.3604755019978993	



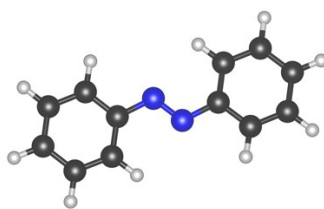
energy(sigma->0) = -93.59992676

H C N O			
1.0000000000000000			
25.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	25.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	25.0000000000000000	
H C N O			
7	6	1	1
Direct			
0.6931244721046462	0.7705854355634433	0.3907450585146455	
0.7251498840070350	0.8621029438561580	0.3684098872323381	
0.6852299451861068	0.9122044388285085	0.2917422550991000	
0.6132104110268803	0.8691942887296430	0.2373427263370217	
0.5814537427778649	0.7778362820323910	0.2594741631867801	
0.5974934423462521	0.6993284990296469	0.3084554780158371	
0.6365592370103061	0.6768071672351065	0.4005669606477431	
0.6347660443955042	0.7687089482821756	0.3271645396046787	
0.6126178845483952	0.7966779511379429	0.2835450336019012	
0.6755622860095364	0.7926297430362620	0.3575632049160601	
0.6306245317651044	0.8480403519235920	0.2712862788327346	
0.6933827813120529	0.8440000403408754	0.3445821332892628	
0.6710819172741267	0.8721805871529626	0.3016586546440541	
0.6129456179728342	0.7187999303699525	0.3408628767559433	
0.6509236825715856	0.6830469523820564	0.3648404879664151	



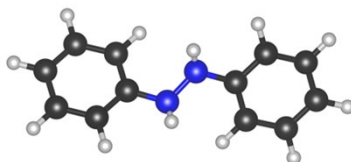
energy(sigma->0) = -166.10430360

H 10 C 12 N 2 O 1			
1.0000000000000000			
25.0000000000000000	0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000	0.0000000000000000
H C N O			
10	12	2	1
Direct			
0.6436560480528377	0.7215427113509019	0.4218852558968747	
0.6832843944706208	0.7774718736474382	0.4945875308202047	
0.7635419225780589	0.8337486052923931	0.4758675891816762	
0.8037342598681386	0.8339173613337996	0.3845992686734279	
0.7642543914447223	0.7775890136340065	0.3125494752359346	
0.7246649981458070	0.6779297018425687	0.1024344944753429	
0.7459800033536876	0.7230892519955751	0.1885470532343517	
0.6121233753134269	0.6440549601676347	0.2636669078772755	
0.6465648500612504	0.6156607681152964	0.0970838739575803	
0.5907199184571077	0.5996229360029844	0.1779593606157325	
0.7018855416230533	0.7466788654670764	0.3636470677012239	
0.7469088507528000	0.7780091777731539	0.3524077234126962	
0.6787277412477295	0.7461928098331252	0.4145211745490416	
0.7687647640942352	0.8093293590372993	0.3930880512500851	
0.7011782369897486	0.7776507789596525	0.4548461565705476	
0.7461412179601191	0.8092260428332941	0.4443171125406015	
0.6809553608422246	0.6867836745909471	0.2320930519984600	
0.7121111363482272	0.6957599355783206	0.1856088214966055	
0.6366408546194281	0.6515501167452453	0.2287191114036623	
0.6999758298853045	0.6704804890576582	0.1376093782179499	
0.6248972430598103	0.6266382457822111	0.1801315422403117	
0.6561514506435729	0.6356592691914790	0.1346127072144086	
0.6773953618248334	0.7131290072300798	0.3221344099385945	
0.6996537835021586	0.7159193352136309	0.2758811645617008	
0.6371384648610992	0.6850937093242208	0.3356225169357272	



energy(sigma->0) = -160.23343243

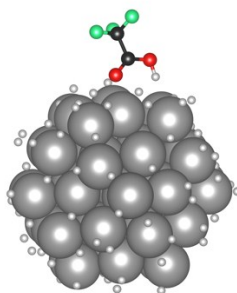
H C N		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C N		
10	12	2
Direct		
0.6802690848242406	0.6855832843312117	0.3909015247230087
0.7420457887571908	0.7232095994873828	0.4603453780320934
0.7625214732076676	0.8208069276902665	0.4603872945771327
0.7216352455432903	0.8804046876737240	0.3919043394321101
0.6597439961849993	0.8425960201778744	0.3232215221648275
0.4973286527137933	0.7811734018968286	0.1409252705167948
0.5587718983200685	0.8183108798993490	0.2109113603159835
0.5888005384574081	0.6593498559453994	0.2698688525736230
0.4820932898752604	0.6827729623733749	0.1359768739020218
0.5277106450932907	0.6218912112762000	0.2001993963299161
0.6664529944617394	0.7617987963921613	0.3532476736636142
0.6780429477486259	0.8169842611838225	0.3533396071895632
0.6897309717367652	0.7281678154977116	0.3918572923036272
0.7125018570694520	0.8377473316716040	0.3917868884018117
0.7241635586338300	0.7493523596587207	0.4303768949997878
0.7356313629802155	0.8041267033717888	0.4303955916448948
0.5770472988299008	0.7411265056791975	0.2444133865434548
0.5513702327906599	0.7754095451624955	0.2079647747030352
0.5684850861237795	0.6854636524578870	0.2415337039237249
0.5172069287848595	0.7544772748252769	0.1690959685840959
0.5344308713741360	0.6649240209690387	0.2026025217651995
0.5086802941062382	0.6992537961841371	0.1663477958690077
0.6322507143751871	0.7360856847222895	0.3161771983345983
0.6107929408073881	0.7667438072554005	0.2819315104736905



energy(sigma->0) = -168.39802528

H C N		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H C N		
12	12	2
Direct		
0.6713470093796606	0.6960810046552116	0.4220756381806623
0.6971208993098761	0.7621772595729268	0.4912002131859609
0.7466365522094095	0.8453753852542051	0.4657590500470565
0.7683302234157335	0.8616134295419328	0.3696138870000571
0.7421818114499931	0.7956583607324111	0.3001482373703671
0.7169591902645012	0.6437504042693627	0.0973584841516038
0.7602011907691777	0.6835198525769119	0.1771284800058146
0.6108149510709165	0.6739989488794270	0.2631896119850107
0.6202093776056254	0.6180614345012864	0.0997524116779951
0.5677341253533534	0.6338282859862537	0.1832485999287926
0.6856605282747137	0.6653253359885779	0.3342807320539370
0.7548663132645982	0.6971790398356988	0.2703505312429931
0.7052887221540400	0.7413018538499482	0.3564089906187177
0.7324320494247253	0.7884777394690292	0.3419990429180730
0.6926447017259395	0.7324816301097757	0.4107040670405659
0.7469020141190983	0.8254670397863845	0.3814066956942914
0.7072089177407090	0.7698009500007258	0.4494284330778495
0.7347695118074014	0.8165476642726573	0.4352597925865859
0.6884531579096822	0.6813225754029284	0.2256511033172689
0.7179501427860778	0.6724719163183837	0.1783083528892584
0.6339202683621674	0.6673229799847077	0.2268593734607000
0.6934420910375412	0.6501389741129956	0.1335616111254006
0.6099455630726237	0.6448142857290303	0.1815579849692144
0.6391860781733858	0.6359097779309515	0.1347327061463647
0.6895959861868832	0.7029818493279735	0.3188958151842691
0.7147075830627245	0.7045196676611887	0.2690093499722001

2.5.2. Hydrogen Evolution Reaction



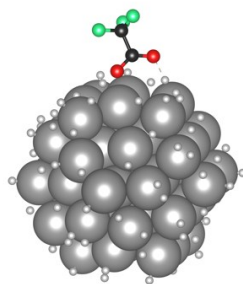
energy(sigma->0) = -851.32336537

H 89 C 2 O 2 F 3 Ru 57		
1.0000000000000000		
25.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000
H	C	O F Ru
89	2 2	3 57
Direct		
0.5484514803628082	0.7190774488604716	0.5045685726359552
0.4877837565156712	0.7544854658043685	0.4591293401799550
0.4099830793258649	0.7216525083574640	0.4834619698421254
0.3211201693097754	0.6681541587864613	0.4923423897002748
0.2411320678099490	0.6345155471297417	0.4777289569924999
0.2427818601929117	0.6345017603520721	0.5145972916134671
0.2844326320433058	0.5521176804281884	0.6297683343181405
0.2706365976581674	0.5276999920912866	0.6096063799472317
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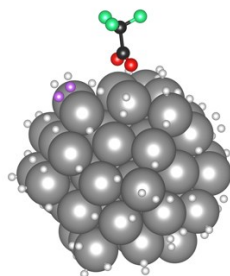
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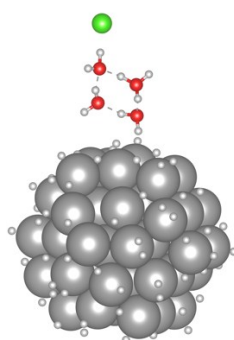
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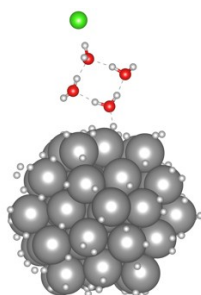
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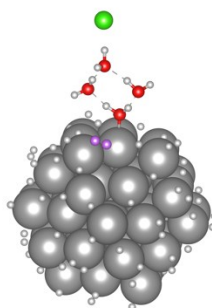
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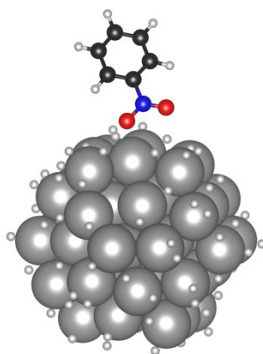
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2.5.3. Hydride transfer processes



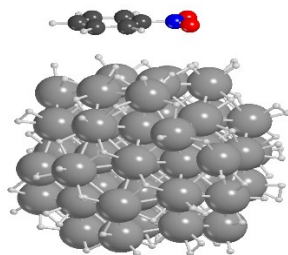
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H 93 C 6 N 1 O 2 Ru 57				
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H C N O Ru				
93	6	1	2	57
Direct				
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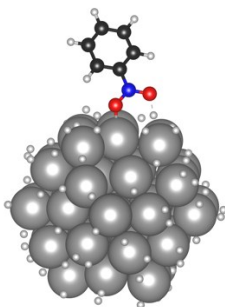
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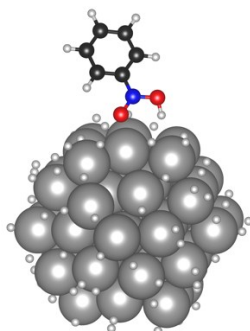
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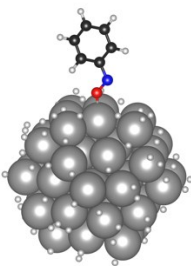
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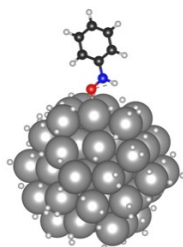
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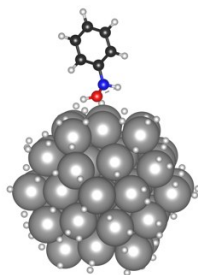
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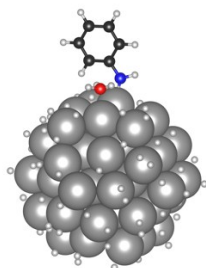
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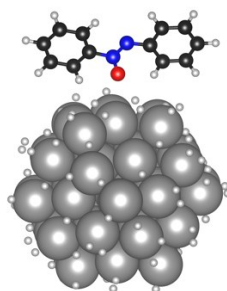
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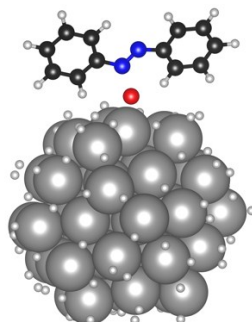
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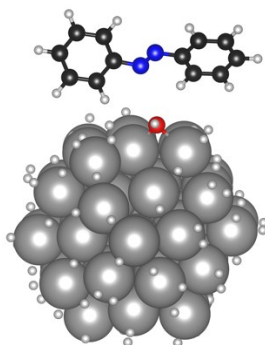
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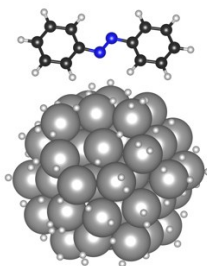
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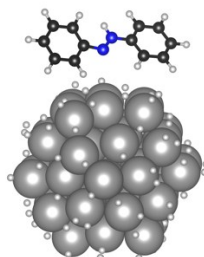
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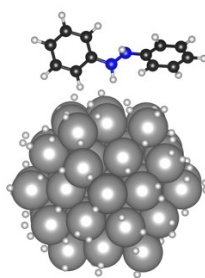
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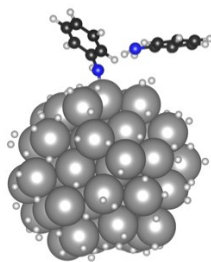
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