

## Supporting Information

### **Electronic effects on the mechanism of the NAD<sup>+</sup> coenzyme reduction catalysed by non-organometallic ruthenium(II) polypyridyl amine complex in the presence of formate**

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**Table S1.** Values of the initial rate and pseudo-first order rate constant as a function of the  $[\text{HCOO}^-]$  for the catalysed reduction of  $\text{NAD}^+$  to 1,4-NADH in water/ethanol (1:9, v/v) solution,  $T = 36.8$  °C.

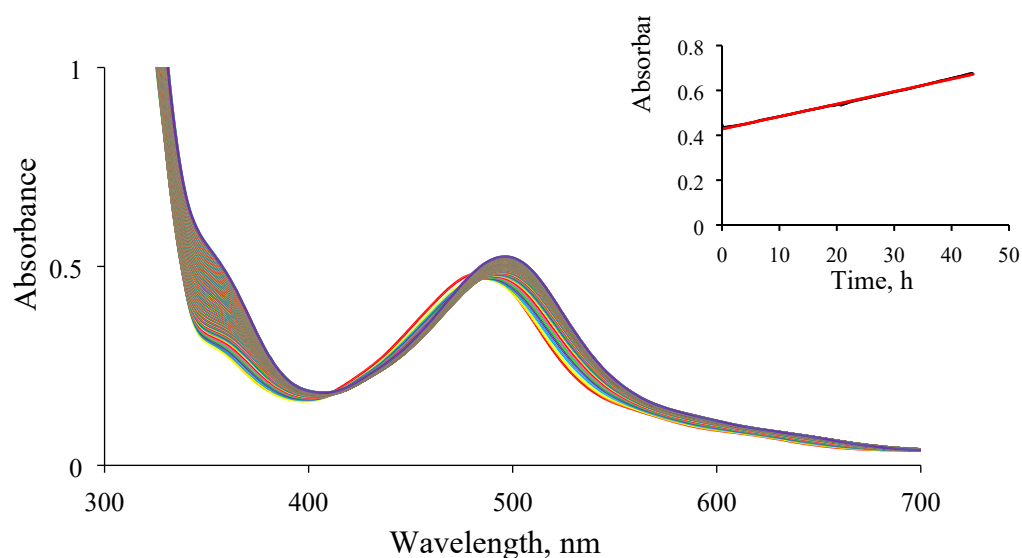
$[\text{HCOO}^-]$ , mM	$10^5 r$ , $\text{M h}^{-1}$ , 340 nm	$10^6 r$ , $\text{M h}^{-1}$ , 340 nm (10 points)	$10^6 k_{\text{obs}}$ , $\text{s}^{-1}$
58	$8.97 \pm 0.01$	-	-
43.5	$8.97 \pm 0.01$	-	-
29	$8.45 \pm 0.01$	-	-
22	$8.45 \pm 0.01$	-	-
14.5	$8.28 \pm 0.01$	-	-
7.2	$6.48 \pm 0.01$	-	-
2.2	-	$4.40 \pm 0.04$	-
1.65	-	$3.70 \pm 0.04$	-
1.35	-	$3.21 \pm 0.03$	$9.1 \pm 0.1$
1.1	-	$2.79 \pm 0.03$	$10.4 \pm 0.1$
0.86	-	$2.48 \pm 0.02$	$9.5 \pm 0.2$
0.56	-	$1.59 \pm 0.01$	$13.2 \pm 0.8$

**Table S2.** Values of the initial rate and pseudo-first order rate constants as a function of the  $[\text{Ru(II)}]$  for the catalysed reduction of  $\text{NAD}^+$  to 1,4-NADH in water/ethanol (1:9, v/v) solution,  $T = 36.8$  °C.

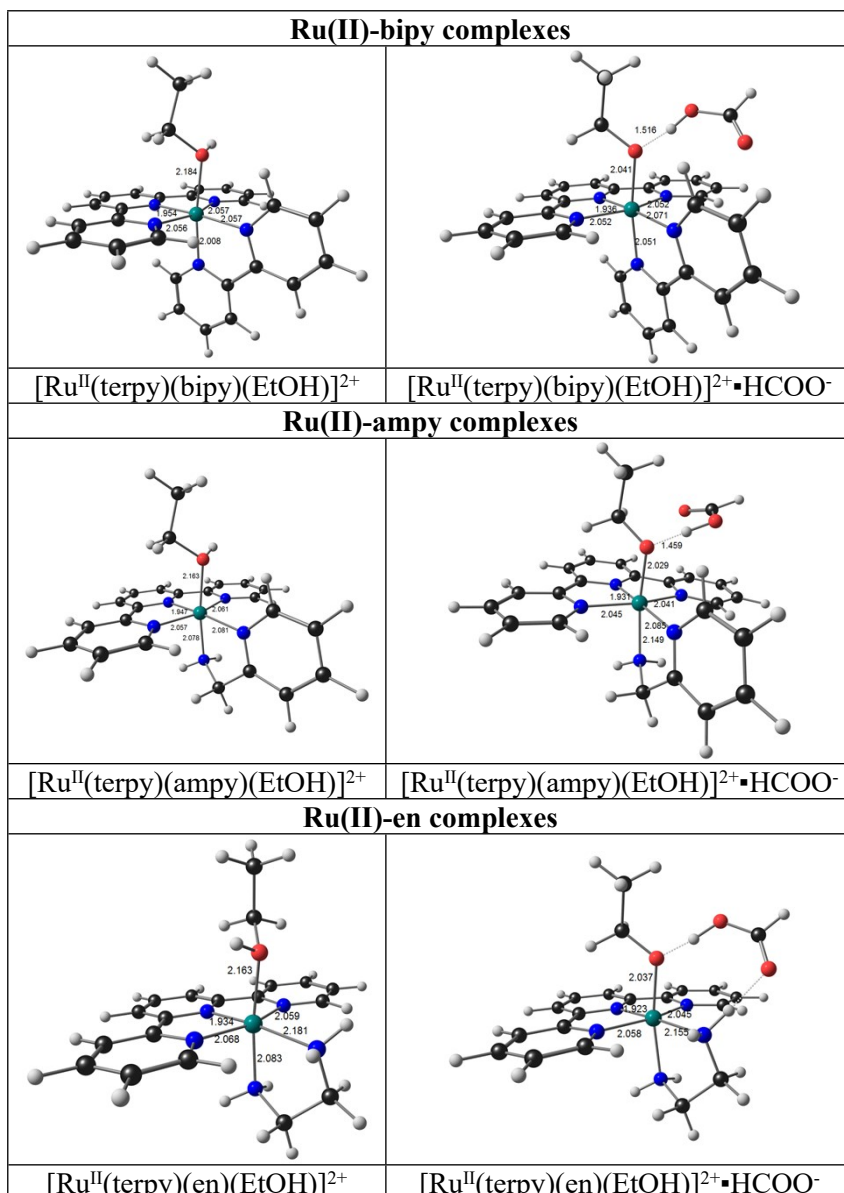
$10^3 [\text{NAD}^+]$ , mM	$10^3 [\text{Ru(II)}]$ , mM	$[\text{HCOO}^-]$ , mM		
		1.1		43.5
		$10^6 r$ , $\text{M h}^{-1}$ 10 points	$10^6 k_{\text{obs}}$ , $\text{s}^{-1}$	$10^5 r$ , $\text{M h}^{-1}$
310	106	$5.04 \pm 0.06$	$9.9 \pm 0.1$	$1.99 \pm 0.03$
	79	$4.50 \pm 0.06$	$9.6 \pm 0.1$	$1.44 \pm 0.01$
	63.6	$3.62 \pm 0.05$	$9.9 \pm 0.2$	$1.15 \pm 0.01$
	53	$2.78 \pm 0.03$	$10.1 \pm 0.1$	$0.90 \pm 0.01$
	42.4	$2.49 \pm 0.03$	$9.9 \pm 0.2$	$0.71 \pm 0.01$
	26.5	$1.68 \pm 0.03$	$9.7 \pm 0.3$	$0.46 \pm 0.01$

**Table S3.** Values of the initial rate and pseudo-first order rate constants as a function of the  $[\text{NAD}^+]$  for the catalysed reduction of  $\text{NAD}^+$  to 1,4-NADH in water/ethanol (1:9, v/v) solution,  $T = 36.8\text{ }^\circ\text{C}$ .

[Ru(II)], mM	[NAD <sup>+</sup> ], mM	[HCOO <sup>-</sup> ], mM		
		1.1		43.5
		$10^6 r, \text{M h}^{-1}$ 10 points	$10^6 k_{\text{obs}}, \text{s}^{-1}$	$10^5 r, \text{M h}^{-1}$
0.053	0.40	$2.97 \pm 0.05$	$15.0 \pm 0.4$	$0.89 \pm 0.01$
	0.31	$2.78 \pm 0.03$	$10.1 \pm 0.1$	$0.90 \pm 0.01$
	0.25	$3.03 \pm 0.03$	$7.95 \pm 0.06$	$0.89 \pm 0.01$
	0.20	$3.06 \pm 0.04$	$6.84 \pm 0.01$	$0.91 \pm 0.01$
	0.15	$2.97 \pm 0.06$	$6.0 \pm 0.2$	$0.88 \pm 0.01$



**Figure S1.** Spectral changes observed during the reduction of  $\text{NAD}^+$  to 1,4-NADH in the presence of formate in water/ethanol (1:9, v/v) solution catalysed by  $[\text{Ru}(\text{terpy})(\text{bipy})(\text{H}_2\text{O}/\text{EtOH})]^{2+}$ . Experimental conditions:  $[\text{HCOO}^-] = 58\text{ mM}$ ;  $[\text{Ru}(\text{II})] = 0.053\text{ mM}$ ,  $[\text{NAD}^+] = 0.31\text{ mM}$ ,  $T = 36.8\text{ }^\circ\text{C}$ ; spectra recorded every 15 min. Inset: kinetic trace recorded at 340 nm.



**Figure S2.** Structures of [Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)(EtOH)]<sup>2+</sup> and {[Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)(EtOH)]<sup>2+</sup>·HCOO<sup>-</sup>} complexes predicted for the conversion of [Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)(EtOH)]<sup>2+</sup> into [Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)H]<sup>+</sup> by DFT calculations. Colour scheme used for atoms (online version): Ru (green), O (red), C (black), N (blue), and H (white).

Optimized Cartesian coordinates (Å)

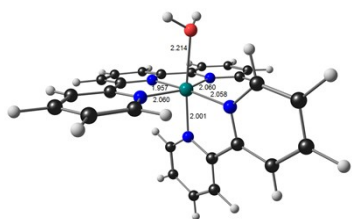


All compounds were optimized by the ZORA Hamiltonian, ZORA/TZ2P basis set, all electron, OLYP functional.

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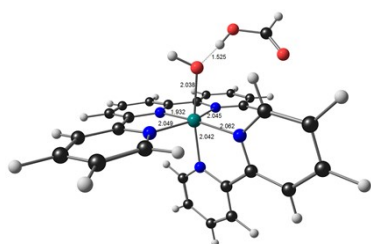
1.  $[\text{Ru}^{\text{II}}(\text{terpy})(\text{bipy})(\text{H}_2\text{O})]^{2+}$



Ru	-3.454626000	2.823203000	2.912004000
N	-3.066911000	0.826610000	3.238611000
C	-3.229206000	0.130467000	4.381008000
H	-3.590641000	0.696330000	5.232786000
C	-2.950513000	-1.228506000	4.476957000
H	-3.098421000	-1.741859000	5.422487000
C	-2.482283000	-1.903231000	3.350177000
H	-2.256688000	-2.965188000	3.392415000
C	-2.308707000	-1.194750000	2.163722000
H	-1.949768000	-1.699507000	1.273526000
C	-2.602045000	0.167790000	2.120988000
C	-2.462372000	1.006018000	0.921919000
C	-1.935971000	0.635924000	-0.316109000
H	-1.578709000	-0.373487000	-0.486006000
C	-1.865455000	1.587411000	-1.334919000
H	-1.451272000	1.315168000	-2.301457000
C	-2.324650000	2.887322000	-1.116932000
H	-2.270625000	3.625546000	-1.909143000
C	-2.842676000	3.222350000	0.134590000
N	-2.887088000	2.283810000	1.118754000
C	-3.346491000	4.531066000	0.572049000
C	-3.463064000	5.643841000	-0.260268000
H	-3.170420000	5.573398000	-1.302168000
C	-3.958216000	6.841292000	0.250140000
H	-4.052327000	7.713143000	-0.391326000
C	-4.332007000	6.899359000	1.592104000
H	-4.723567000	7.812480000	2.030547000
C	-4.195954000	5.761260000	2.379563000
H	-4.468856000	5.762525000	3.429400000
N	-3.718395000	4.596810000	1.897574000
N	-3.877301000	3.414495000	4.836967000
C	-5.089907000	3.395372000	5.430699000
H	-5.913032000	3.048187000	4.816888000
C	-5.283599000	3.790646000	6.747095000
H	-6.280501000	3.754694000	7.176309000
C	-4.186999000	4.228176000	7.491728000
H	-4.305444000	4.544326000	8.524195000
C	-2.935001000	4.253447000	6.887878000
H	-2.070240000	4.589371000	7.448141000
C	-2.797991000	3.843074000	5.559377000
C	-1.536983000	3.825395000	4.819425000
N	-1.631105000	3.370440000	3.528149000

O	-5.572168000	2.309602000	2.519987000
H	-5.986606000	2.816459000	1.805554000
H	-5.732974000	1.377964000	2.307143000
C	-0.514161000	3.327897000	2.768065000
C	-0.307535000	4.235566000	5.340471000
C	0.726865000	3.725968000	3.241860000
C	0.835665000	4.189447000	4.552388000
H	-0.632212000	2.963709000	1.757121000
H	-0.247193000	4.594059000	6.361218000
H	1.590561000	3.671470000	2.585875000
H	1.793296000	4.509835000	4.952904000

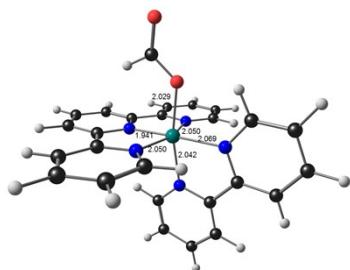
## 2. $[\text{Ru}^{\text{II}}(\text{terpy})(\text{bipy})(\text{H}_2\text{O})]^{2+} \bullet \text{HCOO}^-$



Ru	-3.424361000	2.586234000	2.888780000
N	-2.981675000	0.615202000	3.228804000
C	-3.112037000	-0.069433000	4.381835000
H	-3.515718000	0.490861000	5.217715000
C	-2.753174000	-1.405151000	4.504633000
H	-2.872420000	-1.907784000	5.459752000
C	-2.245636000	-2.074988000	3.389718000
H	-1.955904000	-3.120022000	3.453511000
C	-2.118132000	-1.383136000	2.190253000
H	-1.732392000	-1.881467000	1.307662000
C	-2.487463000	-0.038334000	2.121633000
C	-2.393689000	0.788612000	0.917245000
C	-1.909262000	0.415796000	-0.335571000
H	-1.545758000	-0.591317000	-0.506751000
C	-1.899371000	1.354159000	-1.369403000
H	-1.522674000	1.077414000	-2.349397000
C	-2.377554000	2.646156000	-1.145455000
H	-2.377116000	3.376144000	-1.947157000
C	-2.853134000	2.990580000	0.118997000
N	-2.838019000	2.064398000	1.123085000
C	-3.360959000	4.288765000	0.560320000
C	-3.513275000	5.399036000	-0.269912000
H	-3.260860000	5.324360000	-1.321843000
C	-3.999416000	6.591103000	0.255656000
H	-4.132587000	7.458249000	-0.384942000
C	-4.318715000	6.648861000	1.612208000
H	-4.714806000	7.553388000	2.063227000
C	-4.150135000	5.515417000	2.396068000

H	-4.433267000	5.502233000	3.439576000
N	-3.689191000	4.354899000	1.896002000
N	-3.891381000	3.176213000	4.808651000
C	-5.120805000	3.098147000	5.354730000
H	-5.889343000	2.704146000	4.703430000
C	-5.378925000	3.524545000	6.650033000
H	-6.389804000	3.455217000	7.039501000
C	-4.338034000	4.049644000	7.415781000
H	-4.511988000	4.395184000	8.430804000
C	-3.066760000	4.129190000	6.857046000
H	-2.242421000	4.532956000	7.433099000
C	-2.861356000	3.684961000	5.549133000
C	-1.573710000	3.702061000	4.855387000
N	-1.604331000	3.200863000	3.580185000
O	-5.380721000	2.122326000	2.557049000
H	-6.334828000	3.191445000	2.036654000
H	-5.480680000	1.297288000	2.066756000
C	-7.314391000	4.787644000	2.570399000
O	-7.016534000	3.874251000	1.660284000
O	-6.824593000	4.898493000	3.682707000
H	-8.086491000	5.482068000	2.187533000
C	-0.455153000	3.166187000	2.869523000
C	-0.380611000	4.173103000	5.410950000
C	0.753085000	3.619689000	3.374283000
C	0.794107000	4.135469000	4.671267000
H	-0.528227000	2.764600000	1.866564000
H	-0.374975000	4.569397000	6.419474000
H	1.644484000	3.570637000	2.755844000
H	1.724030000	4.502862000	5.095842000

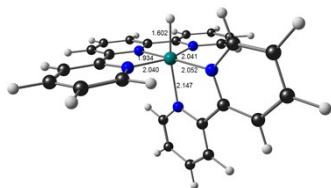
### 3. [Ru<sup>II</sup>(terpy)(bipy)(HCOO)]<sup>+</sup>



Ru	-3.423143000	2.868397000	2.957125000
N	-3.082330000	0.869754000	3.260679000
C	-3.204642000	0.182984000	4.413845000
H	-3.515235000	0.761844000	5.276274000
C	-2.960114000	-1.180720000	4.501469000
H	-3.077290000	-1.687090000	5.454950000
C	-2.577639000	-1.874571000	3.351943000
H	-2.384713000	-2.943052000	3.387599000
C	-2.453341000	-1.177801000	2.154866000
H	-2.164442000	-1.694900000	1.246785000
C	-2.709390000	0.194016000	2.119676000

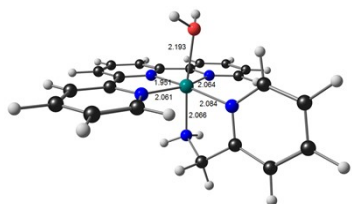
C	-2.633692000	1.021484000	0.915040000
C	-2.375416000	0.603352000	-0.388550000
H	-2.166585000	-0.439518000	-0.598799000
C	-2.417411000	1.536675000	-1.426196000
H	-2.232192000	1.219070000	-2.447791000
C	-2.714180000	2.873503000	-1.156125000
H	-2.767519000	3.595744000	-1.962922000
C	-2.968581000	3.263822000	0.157387000
N	-2.925251000	2.334817000	1.159058000
C	-3.357429000	4.591085000	0.635658000
C	-3.472837000	5.721813000	-0.175183000
H	-3.258905000	5.647965000	-1.235544000
C	-3.868777000	6.933913000	0.379591000
H	-3.965829000	7.817677000	-0.244664000
C	-4.144805000	6.993303000	1.746884000
H	-4.463106000	7.917469000	2.219899000
C	-4.017847000	5.840317000	2.509467000
H	-4.234370000	5.834638000	3.571909000
N	-3.631874000	4.660582000	1.983848000
N	-3.879185000	3.443518000	4.891067000
C	-5.121741000	3.432097000	5.423430000
H	-5.904991000	3.099236000	4.749153000
C	-5.364727000	3.816421000	6.735050000
H	-6.380298000	3.789876000	7.119086000
C	-4.296724000	4.230133000	7.534683000
H	-4.457879000	4.536360000	8.564574000
C	-3.017335000	4.244327000	6.991115000
H	-2.173599000	4.560339000	7.593889000
C	-2.825094000	3.846993000	5.664582000
C	-1.531480000	3.812193000	4.981338000
N	-1.583037000	3.376648000	3.681124000
O	-5.393661000	2.484211000	2.663621000
C	-5.968718000	1.966142000	1.600587000
O	-7.155970000	1.720126000	1.516084000
H	-5.281870000	1.762246000	0.751546000
C	-0.432324000	3.308327000	2.973200000
C	-0.315851000	4.179531000	5.565387000
C	0.797038000	3.660994000	3.506596000
C	0.859771000	4.106226000	4.829108000
H	-0.526562000	2.958515000	1.951984000
H	-0.292214000	4.521968000	6.593358000
H	1.689062000	3.586404000	2.891607000
H	1.807906000	4.390531000	5.276549000

#### 4. Ru<sup>II</sup> (terpy) (bipy) (H) ]<sup>+</sup>



Ru	-3.358920000	2.758066000	2.883829000
N	-3.054497000	0.762144000	3.173598000
C	-3.223731000	0.062744000	4.315595000
H	-3.572720000	0.634044000	5.168502000
C	-2.977839000	-1.299485000	4.406166000
H	-3.134857000	-1.810671000	5.351366000
C	-2.532632000	-1.986960000	3.273963000
H	-2.333145000	-3.053894000	3.313400000
C	-2.349150000	-1.279129000	2.092331000
H	-2.004549000	-1.784795000	1.197044000
C	-2.612980000	0.091564000	2.052922000
C	-2.478624000	0.928338000	0.863948000
C	-2.067700000	0.538091000	-0.409333000
H	-1.788018000	-0.491594000	-0.601765000
C	-2.025233000	1.483772000	-1.434935000
H	-1.707370000	1.191457000	-2.430966000
C	-2.396071000	2.804648000	-1.180055000
H	-2.371494000	3.543072000	-1.973562000
C	-2.799762000	3.166521000	0.104075000
N	-2.829682000	2.229497000	1.100386000
C	-3.231708000	4.482441000	0.565756000
C	-3.323247000	5.616525000	-0.243935000
H	-3.054327000	5.550027000	-1.292334000
C	-3.756719000	6.821229000	0.296294000
H	-3.830989000	7.708685000	-0.325519000
C	-4.090392000	6.867526000	1.652520000
H	-4.430109000	7.787380000	2.119366000
C	-3.984470000	5.712550000	2.413442000
H	-4.237198000	5.703167000	3.467917000
N	-3.569873000	4.534237000	1.901482000
N	-3.866064000	3.321538000	4.790847000
C	-5.135876000	3.320250000	5.269484000
H	-5.894357000	3.002527000	4.564472000
C	-5.454305000	3.693697000	6.564835000
H	-6.491169000	3.668650000	6.886809000
C	-4.433330000	4.095261000	7.430677000
H	-4.650256000	4.394680000	8.451906000
C	-3.129404000	4.103387000	6.954612000
H	-2.318270000	4.411256000	7.604174000
C	-2.859482000	3.715335000	5.638308000
C	-1.515520000	3.689255000	5.055958000
N	-1.469395000	3.286133000	3.756492000
H	-4.891517000	2.436421000	2.544917000
C	-0.279349000	3.225717000	3.131592000
C	-0.345642000	4.037399000	5.742991000
C	0.914773000	3.558408000	3.756602000
C	0.879340000	3.972091000	5.090792000
H	-0.302694000	2.897389000	2.096928000
H	-0.390011000	4.354601000	6.778177000
H	1.850614000	3.492913000	3.209299000
H	1.793500000	4.238968000	5.614125000

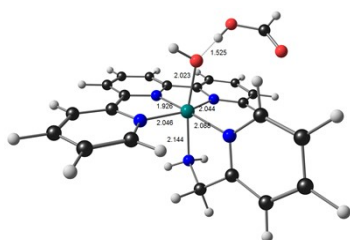
5. [Ru<sup>II</sup>(terpy)(ampy)(H<sub>2</sub>O)]<sup>2+</sup>



Ru	-3.497521000	2.881454000	2.879224000
N	-2.934430000	0.931543000	3.240238000
C	-3.015474000	0.238341000	4.396495000
H	-3.413321000	0.784669000	5.245492000
C	-2.618569000	-1.089041000	4.507984000
H	-2.706403000	-1.597939000	5.463522000
C	-2.116131000	-1.741805000	3.381884000
H	-1.798234000	-2.779400000	3.436362000
C	-2.031054000	-1.042389000	2.180720000
H	-1.648423000	-1.530781000	1.291044000
C	-2.442561000	0.289530000	2.120526000
C	-2.401058000	1.112501000	0.903316000
C	-1.914115000	0.746594000	-0.353043000
H	-1.506945000	-0.244118000	-0.521816000
C	-1.951061000	1.676850000	-1.392949000
H	-1.571991000	1.406814000	-2.374528000
C	-2.467925000	2.955286000	-1.175576000
H	-2.490598000	3.678471000	-1.983058000
C	-2.946879000	3.288344000	0.092375000
N	-2.904100000	2.364917000	1.094150000
C	-3.510772000	4.575806000	0.525563000
C	-3.687556000	5.676321000	-0.312885000
H	-3.402892000	5.611415000	-1.357458000
C	-4.230246000	6.855311000	0.193360000
H	-4.371614000	7.716252000	-0.454229000
C	-4.587620000	6.909784000	1.540119000
H	-5.013302000	7.809036000	1.975837000
C	-4.391047000	5.785710000	2.335396000
H	-4.655156000	5.783842000	3.387545000
N	-3.868816000	4.636149000	1.858135000
N	-3.938426000	3.515175000	4.814893000
C	-5.168494000	3.724356000	5.336308000
H	-6.004955000	3.469745000	4.694897000
C	-5.358456000	4.231141000	6.615802000
H	-6.367842000	4.374616000	6.990290000
C	-4.244750000	4.555266000	7.390238000
H	-4.362087000	4.963173000	8.390312000
C	-2.972382000	4.346616000	6.855733000
H	-2.080188000	4.588407000	7.426388000
C	-2.852516000	3.818628000	5.576593000

C	-1.528639000	3.489298000	4.945789000
H	-1.267669000	2.448859000	5.166615000
H	-0.728404000	4.131945000	5.325257000
N	-1.647241000	3.596349000	3.456259000
H	-0.866688000	3.101712000	3.023152000
H	-1.556901000	4.574863000	3.176708000
O	-5.568033000	2.237836000	2.550767000
H	-5.984227000	2.588045000	1.748576000
H	-5.691189000	1.277123000	2.512158000

6.  $[\text{Ru}^{\text{II}}(\text{terpy})(\text{ampy})(\text{H}_2\text{O})]^{2+} \bullet \text{HCOO}^-$

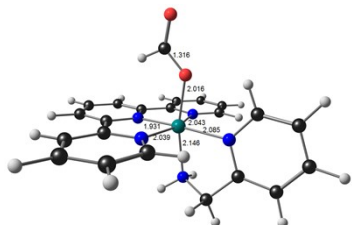


Ru	-3.414469000	2.773594000	2.897082000
N	-2.758522000	0.875253000	3.285569000
C	-2.742552000	0.220322000	4.467821000
H	-3.150892000	0.767549000	5.310530000
C	-2.246031000	-1.067565000	4.609831000
H	-2.254105000	-1.541658000	5.586912000
C	-1.749190000	-1.731271000	3.485248000
H	-1.350817000	-2.738775000	3.564841000
C	-1.778257000	-1.080852000	2.256951000
H	-1.405277000	-1.574772000	1.366360000
C	-2.284736000	0.217794000	2.165706000
C	-2.354604000	0.995639000	0.929029000
C	-1.978235000	0.593087000	-0.351485000
H	-1.574074000	-0.399230000	-0.518520000
C	-2.136694000	1.478019000	-1.419345000
H	-1.847835000	1.176033000	-2.421421000
C	-2.675727000	2.746874000	-1.201702000
H	-2.813365000	3.431492000	-2.031034000
C	-3.043656000	3.123827000	0.089244000
N	-2.860288000	2.251934000	1.127909000
C	-3.608634000	4.399902000	0.521887000
C	-3.902528000	5.463430000	-0.329801000
H	-3.740996000	5.358252000	-1.396880000
C	-4.411108000	6.647857000	0.192298000
H	-4.656988000	7.476112000	-0.465908000
C	-4.607527000	6.748035000	1.569727000
H	-5.015726000	7.647437000	2.020225000
C	-4.316328000	5.655763000	2.374571000
H	-4.518818000	5.668696000	3.437451000
N	-3.838580000	4.496044000	1.880711000



N	-3.913109000	3.365753000	4.836295000
C	-5.175280000	3.452700000	5.309659000
H	-5.953626000	3.186239000	4.606809000
C	-5.444565000	3.882490000	6.603409000
H	-6.475731000	3.935713000	6.939389000
C	-4.390149000	4.253445000	7.435061000
H	-4.574523000	4.604498000	8.446619000
C	-3.086756000	4.174713000	6.941381000
H	-2.236481000	4.460087000	7.554502000
C	-2.881797000	3.718489000	5.646642000
C	-1.511751000	3.518428000	5.056044000
H	-1.177098000	2.495802000	5.262611000
H	-0.786153000	4.209494000	5.498460000
N	-1.580358000	3.654206000	3.574266000
H	-0.743741000	3.250231000	3.156987000
H	-1.587013000	4.641693000	3.317605000
O	-5.312699000	2.134936000	2.614438000
H	-6.259187000	3.027400000	1.818698000
H	-5.347606000	1.200894000	2.374531000
C	-7.340624000	4.625546000	2.032637000
O	-6.899269000	3.631797000	1.276904000
O	-7.023609000	4.861681000	3.186347000
H	-8.051512000	5.257980000	1.467474000

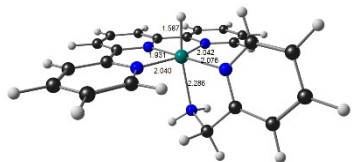
### 7. [Ru<sup>II</sup>(terpy)(ampy)(HCOO)]<sup>+</sup>



Ru	-3.469255000	2.955796000	2.917614000
N	-2.937911000	1.016349000	3.255255000
C	-2.999647000	0.328540000	4.415807000
H	-3.356441000	0.888146000	5.273571000
C	-2.651535000	-1.010502000	4.515637000
H	-2.725945000	-1.514314000	5.474943000
C	-2.226978000	-1.688244000	3.369834000
H	-1.956257000	-2.739142000	3.414516000
C	-2.170900000	-0.997629000	2.164296000
H	-1.859218000	-1.503426000	1.257151000
C	-2.530869000	0.350662000	2.115654000
C	-2.535014000	1.164302000	0.900194000
C	-2.214695000	0.764665000	-0.396290000
H	-1.897566000	-0.253264000	-0.593288000
C	-2.328622000	1.682085000	-1.442273000
H	-2.095753000	1.376723000	-2.457863000
C	-2.753087000	2.988359000	-1.188391000

H	-2.854818000	3.698442000	-2.001377000
C	-3.065509000	3.361738000	0.117143000
N	-2.955112000	2.446005000	1.127888000
C	-3.566372000	4.654374000	0.585643000
C	-3.784419000	5.763212000	-0.233425000
H	-3.576455000	5.695456000	-1.295560000
C	-4.276354000	6.944360000	0.312445000
H	-4.454010000	7.809659000	-0.319827000
C	-4.544845000	6.993846000	1.682067000
H	-4.938408000	7.892145000	2.148886000
C	-4.314217000	5.863727000	2.454385000
H	-4.527465000	5.851068000	3.517606000
N	-3.832521000	4.712447000	1.939536000
N	-3.913130000	3.557129000	4.863573000
C	-5.162007000	3.726228000	5.354183000
H	-5.963099000	3.445122000	4.677600000
C	-5.388829000	4.215507000	6.634962000
H	-6.409661000	4.331191000	6.987465000
C	-4.302276000	4.553612000	7.441377000
H	-4.451668000	4.949022000	8.442280000
C	-3.013104000	4.373702000	6.937120000
H	-2.138623000	4.620431000	7.532733000
C	-2.852224000	3.864631000	5.655202000
C	-1.505681000	3.554122000	5.058358000
H	-1.261462000	2.504843000	5.259299000
H	-0.722035000	4.177951000	5.501201000
N	-1.567819000	3.700210000	3.576962000
H	-0.771422000	3.224939000	3.155754000
H	-1.489001000	4.684920000	3.322405000
O	-5.400201000	2.411913000	2.715665000
C	-5.986676000	1.962951000	1.626320000
O	-7.170785000	1.703116000	1.547172000
H	-5.308936000	1.827918000	0.756480000

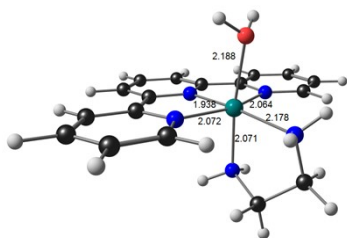
### 8. Ru<sup>II</sup> (terpy) (ampy) (H) ]<sup>+</sup>



Ru	-3.374017000	2.884867000	2.825233000
N	-2.831356000	0.951436000	3.181553000
C	-2.846367000	0.283172000	4.357489000
H	-3.209459000	0.846996000	5.209827000
C	-2.446527000	-1.038795000	4.481343000
H	-2.484681000	-1.521568000	5.453550000
C	-2.011322000	-1.726518000	3.344999000
H	-1.696560000	-2.764103000	3.408834000
C	-1.993317000	-1.057740000	2.126573000

H	-1.664285000	-1.566503000	1.227159000
C	-2.402613000	0.275119000	2.053923000
C	-2.426593000	1.067935000	0.826910000
C	-2.064726000	0.663211000	-0.457347000
H	-1.714398000	-0.347624000	-0.634365000
C	-2.159233000	1.570368000	-1.513751000
H	-1.880877000	1.265463000	-2.517985000
C	-2.614861000	2.869002000	-1.279903000
H	-2.692280000	3.576876000	-2.097621000
C	-2.973908000	3.245345000	0.013377000
N	-2.871176000	2.345316000	1.040605000
C	-3.478107000	4.542485000	0.458280000
C	-3.684577000	5.640574000	-0.378510000
H	-3.462167000	5.556698000	-1.436695000
C	-4.176029000	6.831642000	0.143567000
H	-4.342717000	7.688699000	-0.502537000
C	-4.448334000	6.902475000	1.512200000
H	-4.832429000	7.811760000	1.965560000
C	-4.225757000	5.784535000	2.302933000
H	-4.435545000	5.794667000	3.367036000
N	-3.754892000	4.616159000	1.811052000
N	-3.908609000	3.488606000	4.738020000
C	-5.189381000	3.655940000	5.155430000
H	-5.951544000	3.398940000	4.429172000
C	-5.512588000	4.124058000	6.421151000
H	-6.557322000	4.232997000	6.697500000
C	-4.489809000	4.450453000	7.311616000
H	-4.711607000	4.827364000	8.305819000
C	-3.170751000	4.283563000	6.890678000
H	-2.339924000	4.526802000	7.547315000
C	-2.911483000	3.796064000	5.615753000
C	-1.511372000	3.523875000	5.131664000
H	-1.277919000	2.467032000	5.307686000
H	-0.788642000	4.125352000	5.695365000
N	-1.428982000	3.738602000	3.670661000
H	-0.576332000	3.320495000	3.306458000
H	-1.388450000	4.734168000	3.459781000
H	-4.856552000	2.395390000	2.541687000

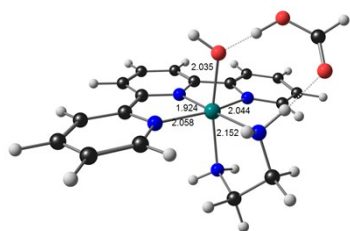
9.  $[\text{Ru}^{\text{II}}(\text{terpy})(\text{en})(\text{H}_2\text{O})]^{2+}$



Ru	-3.431406000	2.702861000	2.867896000
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N	-2.789801000	0.769353000	3.243812000
C	-2.815399000	0.066224000	4.396590000
H	-3.225670000	0.574316000	5.262772000
C	-2.352550000	-1.239565000	4.505945000
H	-2.407051000	-1.751265000	5.462526000
C	-1.826945000	-1.864611000	3.375273000
H	-1.455009000	-2.884272000	3.424809000
C	-1.798565000	-1.161242000	2.174494000
H	-1.404693000	-1.629339000	1.278966000
C	-2.285734000	0.145428000	2.118194000
C	-2.325281000	0.952300000	0.892207000
C	-1.872583000	0.586063000	-0.376572000
H	-1.432694000	-0.390442000	-0.545143000
C	-1.990237000	1.492913000	-1.430370000
H	-1.641014000	1.219880000	-2.422147000
C	-2.553676000	2.750995000	-1.212606000
H	-2.640283000	3.458135000	-2.029911000
C	-2.999404000	3.085578000	0.066835000
N	-2.880892000	2.183422000	1.084141000
C	-3.608363000	4.351485000	0.493915000
C	-3.874059000	5.418819000	-0.365074000
H	-3.615756000	5.343506000	-1.415754000
C	-4.478355000	6.573378000	0.124869000
H	-4.691202000	7.407049000	-0.538812000
C	-4.805292000	6.637354000	1.479160000
H	-5.280402000	7.515872000	1.905839000
C	-4.510086000	5.550355000	2.293394000
H	-4.751816000	5.571089000	3.350436000
N	-3.923253000	4.421973000	1.837948000
N	-3.851084000	3.374530000	4.897129000
C	-2.706972000	4.234229000	5.329089000
C	-1.425706000	3.607038000	4.811346000
H	-1.286286000	2.610074000	5.237740000
H	-0.555206000	4.221289000	5.062828000
N	-1.553033000	3.444138000	3.327054000
H	-0.800506000	2.842912000	2.987686000
H	-1.415306000	4.351029000	2.876791000
O	-5.506481000	2.029046000	2.698215000
H	-6.033196000	2.445070000	1.998969000
H	-5.637215000	1.074497000	2.592888000
H	-2.668899000	4.346699000	6.417180000
H	-2.845273000	5.224456000	4.885529000
H	-3.939847000	2.597541000	5.551056000
H	-4.722465000	3.894909000	4.995089000

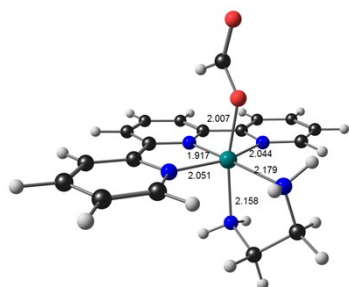
10.  $[\text{Ru}^{\text{II}}(\text{terpy})(\text{en})(\text{H}_2\text{O})]^{2+} \bullet \text{HCOO}^-$



Ru	-3.462064000	2.720558000	2.793789000
N	-2.779350000	0.823699000	3.208563000
C	-2.779983000	0.150093000	4.379678000
H	-3.250926000	0.650732000	5.217769000
C	-2.222388000	-1.110389000	4.537659000
H	-2.253817000	-1.594214000	5.509415000
C	-1.632965000	-1.732195000	3.435274000
H	-1.181626000	-2.716047000	3.524983000
C	-1.638692000	-1.067249000	2.215178000
H	-1.193301000	-1.526473000	1.339489000
C	-2.215511000	0.200030000	2.110270000
C	-2.272170000	0.972790000	0.870972000
C	-1.866282000	0.569192000	-0.400311000
H	-1.438020000	-0.415029000	-0.553192000
C	-2.034035000	1.437734000	-1.479961000
H	-1.727779000	1.131929000	-2.475791000
C	-2.608578000	2.692618000	-1.281621000
H	-2.754263000	3.365387000	-2.119193000
C	-2.998252000	3.073796000	0.002137000
N	-2.813999000	2.216412000	1.053986000
C	-3.568687000	4.349736000	0.417641000
C	-3.828111000	5.411801000	-0.448889000
H	-3.660225000	5.287636000	-1.512930000
C	-4.304477000	6.617540000	0.050572000
H	-4.528022000	7.442470000	-0.619510000
C	-4.484797000	6.743975000	1.428547000
H	-4.848873000	7.666435000	1.870796000
C	-4.227678000	5.654319000	2.246076000
H	-4.427440000	5.703252000	3.305476000
N	-3.812133000	4.458177000	1.775861000
N	-4.244228000	3.266262000	4.722497000
C	-3.258271000	4.078621000	5.468321000
C	-1.855423000	3.590456000	5.135838000
H	-1.719414000	2.563303000	5.482715000
H	-1.098433000	4.222796000	5.613482000
N	-1.695615000	3.575394000	3.650548000
H	-0.840478000	3.078279000	3.404819000
H	-1.582384000	4.531055000	3.310770000
O	-5.356437000	2.054916000	2.463173000
H	-6.313969000	3.081980000	2.199505000
H	-5.402000000	1.327690000	1.830341000
C	-7.147609000	4.736269000	2.910060000
O	-7.038878000	3.831085000	1.975157000

O	-6.497274000	4.822306000	3.952227000
H	-7.919716000	5.487234000	2.662942000
H	-4.500264000	2.436079000	5.251685000
H	-5.121625000	3.786912000	4.558978000
H	-3.423630000	4.043698000	6.551086000
H	-3.369665000	5.119048000	5.151141000

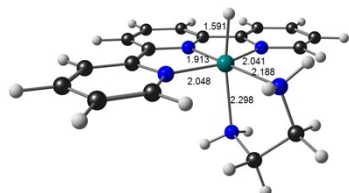
### 11. [Ru<sup>II</sup>(terpy)(en)(HCOO)]<sup>+</sup>



Ru	-3.410100000	2.954853000	2.774660000
N	-2.837945000	1.000795000	3.022678000
C	-2.797615000	0.260972000	4.151585000
H	-3.069516000	0.769502000	5.069724000
C	-2.449491000	-1.081305000	4.174118000
H	-2.447947000	-1.620676000	5.116896000
C	-2.121286000	-1.713956000	2.972803000
H	-1.850717000	-2.765682000	2.953612000
C	-2.159686000	-0.973327000	1.797603000
H	-1.921392000	-1.441041000	0.848781000
C	-2.522209000	0.375024000	1.830339000
C	-2.627629000	1.225900000	0.648492000
C	-2.400245000	0.870025000	-0.680159000
H	-2.086902000	-0.137410000	-0.929914000
C	-2.594054000	1.815657000	-1.687224000
H	-2.426430000	1.545350000	-2.725251000
C	-3.016073000	3.106234000	-1.361673000
H	-3.182512000	3.839908000	-2.142349000
C	-3.242343000	3.436012000	-0.028006000
N	-3.040770000	2.496713000	0.950472000
C	-3.749145000	4.698089000	0.504238000
C	-4.099553000	5.798932000	-0.279986000
H	-3.977110000	5.750964000	-1.356270000
C	-4.617244000	6.942981000	0.316481000
H	-4.899642000	7.800116000	-0.287725000
C	-4.782733000	6.960549000	1.702922000
H	-5.199112000	7.824448000	2.212673000
C	-4.421114000	5.839933000	2.435644000
H	-4.559782000	5.816362000	3.510502000
N	-3.905002000	4.723579000	1.877674000
N	-3.764384000	3.512682000	4.851047000
C	-2.621686000	4.323866000	5.340794000

C	-1.337638000	3.726904000	4.783811000
H	-1.218601000	2.698493000	5.136420000
H	-0.468244000	4.309305000	5.109386000
N	-1.444205000	3.675389000	3.297079000
H	-0.696726000	3.093205000	2.921389000
H	-1.303230000	4.609562000	2.912400000
O	-5.346277000	2.425880000	2.784495000
C	-6.076655000	2.119278000	1.732607000
O	-7.274422000	1.929683000	1.767262000
H	-5.503890000	2.034310000	0.783330000
H	-2.746140000	5.342963000	4.962745000
H	-2.578439000	4.368503000	6.434821000
H	-4.644096000	4.020677000	4.928277000
H	-3.884941000	2.688977000	5.437346000

## 12. Ru<sup>II</sup> (terpy) (en) (H) ]<sup>+</sup>



Ru	-3.700255000	2.988358000	2.402981000
N	-3.681892000	0.941816000	2.472480000
C	-4.219953000	0.107195000	3.391229000
H	-4.737628000	0.578523000	4.219458000
C	-4.146659000	-1.274860000	3.312127000
H	-4.609472000	-1.882440000	4.084399000
C	-3.478199000	-1.856486000	2.231783000
H	-3.401873000	-2.935729000	2.138506000
C	-2.911419000	-1.021895000	1.276614000
H	-2.386241000	-1.442116000	0.425964000
C	-3.020062000	0.365189000	1.400350000
C	-2.482364000	1.318883000	0.437220000
C	-1.779404000	1.040365000	-0.733481000
H	-1.566008000	0.014014000	-1.010643000
C	-1.350847000	2.090704000	-1.546186000
H	-0.803628000	1.883417000	-2.460584000
C	-1.630390000	3.408164000	-1.182269000
H	-1.302530000	4.229540000	-1.809610000
C	-2.336608000	3.661037000	-0.008217000
N	-2.747929000	2.619249000	0.785930000
C	-2.732460000	4.957299000	0.528516000
C	-2.464403000	6.179948000	-0.090718000
H	-1.919591000	6.195631000	-1.028239000
C	-2.896448000	7.366657000	0.487938000
H	-2.694636000	8.320492000	0.009471000
C	-3.599812000	7.303091000	1.693751000
H	-3.964364000	8.201158000	2.184064000

C	-3.843435000	6.063763000	2.265792000
H	-4.398024000	5.986314000	3.194366000
N	-3.428496000	4.894686000	1.725233000
N	-4.784493000	3.427615000	4.252529000
C	-3.851974000	3.878005000	5.323204000
C	-2.595231000	3.022815000	5.278768000
H	-2.855016000	1.971446000	5.436220000
H	-1.907976000	3.329047000	6.077017000
N	-1.991199000	3.136944000	3.931783000
H	-1.280236000	2.420157000	3.804012000
H	-1.522392000	4.036016000	3.835628000
H	-5.092803000	2.947629000	1.635146000
H	-3.589739000	4.920578000	5.119190000
H	-4.312983000	3.829370000	6.316526000
H	-5.495482000	4.138492000	4.092386000
H	-5.297034000	2.611019000	4.580020000

### 13. [Ru<sup>II</sup>(terpy)(bipy)(EtOH)]<sup>2+</sup>

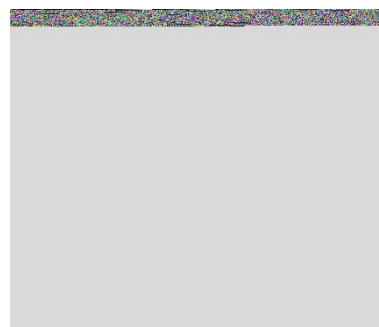


Ru	-3.389428000	2.733742000	2.925591000
N	-2.890546000	0.765782000	3.252595000
C	-2.989763000	0.071858000	4.402278000
H	-3.369911000	0.621980000	5.256059000
C	-2.631045000	-1.267798000	4.501826000
H	-2.731344000	-1.782123000	5.452911000
C	-2.145275000	-1.922642000	3.370613000
H	-1.855769000	-2.968797000	3.415470000
C	-2.034719000	-1.213793000	2.177029000
H	-1.659879000	-1.701934000	1.284214000
C	-2.409548000	0.128133000	2.131081000
C	-2.348230000	0.961177000	0.923404000
C	-1.871080000	0.598938000	-0.336165000
H	-1.488694000	-0.399330000	-0.516929000
C	-1.884059000	1.543101000	-1.364879000
H	-1.510551000	1.276073000	-2.349248000
C	-2.372181000	2.829739000	-1.132563000
H	-2.379658000	3.563247000	-1.931036000
C	-2.842988000	3.157016000	0.139627000
N	-2.816147000	2.222926000	1.129273000
C	-3.370147000	4.450860000	0.592256000
C	-3.514995000	5.569741000	-0.227496000
H	-3.238357000	5.512639000	-1.274514000



C	-4.011665000	6.757708000	0.302792000
H	-4.125386000	7.634511000	-0.328809000
C	-4.358224000	6.801089000	1.653018000
H	-4.747215000	7.707324000	2.107756000
C	-4.199565000	5.656660000	2.426274000
H	-4.453518000	5.645855000	3.480662000
N	-3.720264000	4.500477000	1.924980000
N	-3.844170000	3.325826000	4.842007000
C	-5.057773000	3.255465000	5.429769000
H	-5.848905000	2.824203000	4.827189000
C	-5.289049000	3.704734000	6.722394000
H	-6.285576000	3.626368000	7.147004000
C	-4.230163000	4.249989000	7.450527000
H	-4.379605000	4.614146000	8.462887000
C	-2.975162000	4.318988000	6.856309000
H	-2.138400000	4.736185000	7.404398000
C	-2.798657000	3.849527000	5.552234000
C	-1.528617000	3.864197000	4.827050000
N	-1.587320000	3.360769000	3.552454000
O	-5.462167000	2.173676000	2.524858000
H	-5.895424000	2.880821000	2.024808000
C	-0.458993000	3.332362000	2.809586000
C	-0.323708000	4.341284000	5.349003000
C	0.759781000	3.793273000	3.284395000
C	0.831819000	4.309371000	4.577947000
H	-0.550522000	2.928262000	1.810640000
H	-0.291237000	4.737201000	6.357030000
H	1.634725000	3.746714000	2.642828000
H	1.771230000	4.679499000	4.978850000
C	-5.807543000	0.909608000	1.858692000
H	-5.213106000	0.832534000	0.943720000
H	-5.488498000	0.137995000	2.560029000
C	-7.289905000	0.849927000	1.574915000
H	-7.591229000	1.643911000	0.880329000
H	-7.527995000	-0.110035000	1.103133000
H	-7.871261000	0.937285000	2.497651000

**14. [Ru<sup>II</sup>(terpy)(bipy)(EtOH)]<sup>2+</sup>•HCOO<sup>-</sup>**



Ru	-3.501302000	2.745308000	3.039612000
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N	-3.135978000	0.755445000	3.360898000
C	-3.213426000	0.083627000	4.526204000
H	-3.498815000	0.672331000	5.390683000
C	-2.960759000	-1.277206000	4.625281000
H	-3.040790000	-1.770338000	5.589300000
C	-2.614765000	-1.985946000	3.473005000
H	-2.416088000	-3.053149000	3.515649000
C	-2.525044000	-1.302602000	2.265694000
H	-2.256713000	-1.828051000	1.355983000
C	-2.782985000	0.068262000	2.222044000
C	-2.715590000	0.885947000	1.012326000
C	-2.350789000	0.478713000	-0.267983000
H	-2.090069000	-0.555606000	-0.462068000
C	-2.328199000	1.417503000	-1.301128000
H	-2.051004000	1.111210000	-2.305169000
C	-2.664906000	2.745544000	-1.044503000
H	-2.659260000	3.475964000	-1.844889000
C	-3.031931000	3.119466000	0.245741000
N	-3.050209000	2.188923000	1.241608000
C	-3.444216000	4.442519000	0.705985000
C	-3.604230000	5.552189000	-0.123173000
H	-3.391197000	5.465802000	-1.182511000
C	-4.061215000	6.751812000	0.409008000
H	-4.201013000	7.617710000	-0.231863000
C	-4.348817000	6.820445000	1.773061000
H	-4.718922000	7.734016000	2.228093000
C	-4.169902000	5.688355000	2.554501000
H	-4.395407000	5.687859000	3.614891000
N	-3.729349000	4.522123000	2.049265000
N	-3.787432000	3.338743000	4.989194000
C	-4.978661000	3.329659000	5.625274000
H	-5.814587000	3.018500000	5.006022000
C	-5.107018000	3.692512000	6.957572000
H	-6.087002000	3.671640000	7.425381000
C	-3.970425000	4.079936000	7.672598000
H	-4.040178000	4.367012000	8.717957000
C	-2.743083000	4.095784000	7.020982000
H	-1.847411000	4.393019000	7.554318000
C	-2.669103000	3.723821000	5.675661000
C	-1.438432000	3.694592000	4.885017000
N	-1.597464000	3.247184000	3.600278000
O	-5.521497000	2.476236000	2.847340000
C	-6.027732000	1.183286000	2.537237000
H	-5.673325000	0.872864000	1.544814000
H	-5.668585000	0.452925000	3.274662000
H	-6.143150000	3.408464000	1.848740000
C	-7.550189000	1.198024000	2.555026000
H	-7.943464000	1.879662000	1.797383000
H	-7.930450000	0.190294000	2.349381000
H	-7.917973000	1.516495000	3.536962000
C	-6.453301000	3.671308000	-0.053262000

O	-6.613631000	4.077353000	1.196672000
O	-5.842829000	2.683305000	-0.423434000
H	-6.945496000	4.369426000	-0.757800000
C	-0.513318000	3.185641000	2.796851000
C	-0.181787000	4.082915000	5.359591000
C	0.753929000	3.558280000	3.217340000
C	0.926776000	4.016143000	4.525016000
H	-0.687650000	2.827392000	1.790046000
H	-0.073878000	4.438247000	6.377650000
H	1.589120000	3.490433000	2.526445000
H	1.906514000	4.317303000	4.885070000

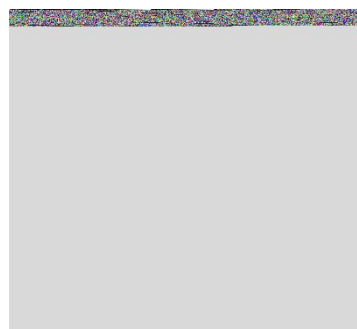
15. [Ru<sup>II</sup>(terpy)(ampy)(EtOH)]<sup>2+</sup>



Ru	-3.513742000	2.860845000	2.985426000
N	-2.925506000	0.924659000	3.356780000
C	-2.960479000	0.253769000	4.526813000
H	-3.321911000	0.816490000	5.381073000
C	-2.570290000	-1.074745000	4.644314000
H	-2.621639000	-1.566677000	5.611218000
C	-2.119614000	-1.750220000	3.509365000
H	-1.809013000	-2.789656000	3.567379000
C	-2.078127000	-1.070678000	2.294606000
H	-1.737877000	-1.576072000	1.397418000
C	-2.482630000	0.262586000	2.229927000
C	-2.500565000	1.060688000	0.997076000
C	-2.067400000	0.675491000	-0.272006000
H	-1.656634000	-0.313854000	-0.439137000
C	-2.160637000	1.584409000	-1.327876000
H	-1.823077000	1.298543000	-2.319790000
C	-2.679295000	2.861994000	-1.111797000
H	-2.744478000	3.569877000	-1.930513000
C	-3.101977000	3.215889000	0.170480000
N	-3.007299000	2.312281000	1.187068000
C	-3.634469000	4.513386000	0.608209000
C	-3.831904000	5.606002000	-0.236366000
H	-3.606150000	5.519606000	-1.293567000
C	-4.313439000	6.805883000	0.280891000
H	-4.465757000	7.662075000	-0.370479000
C	-4.592285000	6.888708000	1.645067000
H	-4.966865000	7.805804000	2.090428000
C	-4.385093000	5.770349000	2.444372000

H	-4.592104000	5.790272000	3.508982000
N	-3.918107000	4.600403000	1.957574000
N	-3.859867000	3.555702000	4.916420000
C	-5.067046000	3.806764000	5.471278000
H	-5.926820000	3.511841000	4.879625000
C	-5.202948000	4.401234000	6.719298000
H	-6.195203000	4.578706000	7.123582000
C	-4.057241000	4.763896000	7.427609000
H	-4.132482000	5.239432000	8.401568000
C	-2.808320000	4.503102000	6.861726000
H	-1.892502000	4.769449000	7.381731000
C	-2.742637000	3.891661000	5.616601000
C	-1.448090000	3.510828000	4.954326000
H	-1.200239000	2.474219000	5.206119000
H	-0.622606000	4.149797000	5.282451000
N	-1.619118000	3.564201000	3.468184000
H	-0.865755000	3.037753000	3.024996000
H	-1.521588000	4.529341000	3.148677000
O	-5.585251000	2.280831000	2.757399000
C	-5.967082000	0.922734000	2.336159000
H	-5.376014000	0.662975000	1.453031000
H	-5.669145000	0.285545000	3.169526000
H	-6.023691000	2.894070000	2.149250000
C	-7.451838000	0.856694000	2.064193000
H	-7.731027000	1.515168000	1.232035000
H	-7.720635000	-0.166846000	1.779708000
H	-8.027347000	1.132420000	2.952992000

**16. [Ru<sup>II</sup>(terpy)(ampy)(EtOH)]<sup>2+</sup>•HCOO<sup>-</sup>**



Ru	-3.490700000	2.816233000	2.968074000
N	-2.883984000	0.904274000	3.365017000
C	-2.867249000	0.268303000	4.555037000
H	-3.226431000	0.846866000	5.399421000
C	-2.439677000	-1.044465000	4.701421000
H	-2.449661000	-1.506411000	5.684302000
C	-2.014917000	-1.747230000	3.572114000
H	-1.677444000	-2.776521000	3.652473000
C	-2.036615000	-1.108310000	2.336076000
H	-1.720771000	-1.633999000	1.441744000

C	-2.474896000	0.212632000	2.241750000
C	-2.567412000	0.970595000	0.992465000
C	-2.302484000	0.519792000	-0.298862000
H	-1.967795000	-0.497480000	-0.468118000
C	-2.495900000	1.387404000	-1.375962000
H	-2.312619000	1.041962000	-2.388843000
C	-2.928890000	2.695208000	-1.154570000
H	-3.089040000	3.368308000	-1.988846000
C	-3.174482000	3.122208000	0.148869000
N	-3.006957000	2.249587000	1.186929000
C	-3.614235000	4.442593000	0.589527000
C	-3.790098000	5.538245000	-0.253851000
H	-3.620942000	5.427730000	-1.318610000
C	-4.204970000	6.756159000	0.269548000
H	-4.358557000	7.610972000	-0.382568000
C	-4.424877000	6.858653000	1.645091000
H	-4.755235000	7.789192000	2.097308000
C	-4.233345000	5.741265000	2.443112000
H	-4.424248000	5.769031000	3.509473000
N	-3.842983000	4.548181000	1.946662000
N	-3.924225000	3.515469000	4.883377000
C	-5.170578000	3.708467000	5.370639000
H	-5.976213000	3.366592000	4.731572000
C	-5.396532000	4.305739000	6.604301000
H	-6.416774000	4.440077000	6.951659000
C	-4.310057000	4.730565000	7.368641000
H	-4.458750000	5.212101000	8.331123000
C	-3.022209000	4.525208000	6.870815000
H	-2.147423000	4.838031000	7.434320000
C	-2.862726000	3.907683000	5.637469000
C	-1.516101000	3.576642000	5.052997000
H	-1.254442000	2.546778000	5.321093000
H	-0.738992000	4.239492000	5.448421000
N	-1.591735000	3.624438000	3.566467000
H	-0.791504000	3.135550000	3.169157000
H	-1.532974000	4.591758000	3.247301000
O	-5.417298000	2.204769000	2.792550000
C	-5.775265000	1.111419000	1.961838000
H	-5.679170000	1.401161000	0.906230000
H	-5.108888000	0.259940000	2.149452000
H	-6.275195000	3.318495000	2.402827000
C	-7.211845000	0.702725000	2.258642000
H	-7.894858000	1.533768000	2.061995000
H	-7.498458000	-0.142572000	1.622060000
H	-7.313582000	0.405117000	3.308253000
C	-7.026601000	4.375743000	0.936920000
O	-6.932223000	4.122884000	2.229793000
O	-6.441571000	3.789663000	0.045332000
H	-7.715952000	5.221157000	0.745913000

17. [Ru<sup>II</sup>(terpy)(en)(EtOH)]<sup>2+</sup>



Ru	-3.418924000	2.770291000	2.847815000
N	-2.837836000	0.815764000	3.192185000
C	-2.883078000	0.094197000	4.333622000
H	-3.287354000	0.597010000	5.205668000
C	-2.443345000	-1.220723000	4.425161000
H	-2.507895000	-1.745416000	5.374031000
C	-1.927451000	-1.839183000	3.286470000
H	-1.573575000	-2.865753000	3.322200000
C	-1.879617000	-1.117798000	2.097570000
H	-1.490358000	-1.579530000	1.196907000
C	-2.338202000	0.199620000	2.059501000
C	-2.344645000	1.029934000	0.849960000
C	-1.886252000	0.679127000	-0.421059000
H	-1.463931000	-0.302667000	-0.603412000
C	-1.975577000	1.606937000	-1.458456000
H	-1.623358000	1.344975000	-2.451889000
C	-2.509774000	2.874651000	-1.220294000
H	-2.568332000	3.600380000	-2.023587000
C	-2.954242000	3.197015000	0.061690000
N	-2.872001000	2.270364000	1.061354000
C	-3.536529000	4.466854000	0.509803000
C	-3.808296000	5.542470000	-0.335276000
H	-3.565490000	5.474804000	-1.390043000
C	-4.402074000	6.694541000	0.172907000
H	-4.620132000	7.534785000	-0.480455000
C	-4.710939000	6.747829000	1.531961000
H	-5.175743000	7.624845000	1.972749000
C	-4.412689000	5.650593000	2.330649000
H	-4.645219000	5.659754000	3.389654000
N	-3.841294000	4.524259000	1.855313000
N	-3.815513000	3.427131000	4.889751000
C	-2.644823000	4.245045000	5.329712000
C	-1.382648000	3.578758000	4.814094000
H	-1.282595000	2.572078000	5.228790000
H	-0.493673000	4.158267000	5.083346000
N	-1.505265000	3.439219000	3.328726000
H	-0.777327000	2.810221000	2.986561000
H	-1.327092000	4.344121000	2.889179000
O	-5.483272000	2.158035000	2.641624000
H	-5.571884000	1.210737000	2.823434000

H	-2.605949000	4.353394000	6.418443000
H	-2.747424000	5.240835000	4.888799000
H	-3.927564000	2.647867000	5.537228000
H	-4.670814000	3.973355000	4.989777000
C	-6.230290000	2.415368000	1.398147000
H	-6.305374000	3.501627000	1.345813000
H	-5.626308000	2.053712000	0.560210000
C	-7.585030000	1.749550000	1.450027000
H	-8.169073000	2.112826000	2.300940000
H	-7.488116000	0.658594000	1.514810000
H	-8.132685000	1.977986000	0.528546000

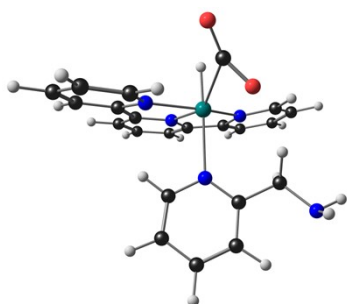
**18. [Ru<sup>II</sup>(terpy)(en)(EtOH)]<sup>2+</sup>•HCOO<sup>-</sup>**



Ru	-3.500762000	2.788950000	2.867085000
N	-2.940480000	0.861017000	3.321327000
C	-3.004238000	0.208803000	4.501124000
H	-3.424085000	0.763614000	5.332145000
C	-2.570512000	-1.098130000	4.676014000
H	-2.647095000	-1.563787000	5.654228000
C	-2.050594000	-1.789650000	3.580539000
H	-1.701630000	-2.813248000	3.681727000
C	-1.995490000	-1.144155000	2.350490000
H	-1.607663000	-1.660344000	1.479362000
C	-2.442491000	0.172487000	2.230258000
C	-2.443993000	0.925603000	0.978344000
C	-2.023802000	0.484071000	-0.274774000
H	-1.637566000	-0.521173000	-0.400957000
C	-2.110192000	1.345383000	-1.369637000
H	-1.790486000	1.010277000	-2.351563000
C	-2.600314000	2.640399000	-1.198808000
H	-2.659980000	3.317301000	-2.043760000
C	-3.009417000	3.058249000	0.066270000
N	-2.937653000	2.194458000	1.127400000
C	-3.504498000	4.373867000	0.452951000
C	-3.645711000	5.447040000	-0.427873000
H	-3.409933000	5.312279000	-1.477737000
C	-4.088705000	6.678356000	0.038773000
H	-4.209545000	7.515204000	-0.642917000
C	-4.378236000	6.811169000	1.398144000
H	-4.736024000	7.749511000	1.811508000

C	-4.226530000	5.714572000	2.233547000
H	-4.493679000	5.774223000	3.278895000
N	-3.809653000	4.504547000	1.797345000
N	-4.024336000	3.497519000	4.833785000
C	-2.913409000	4.305589000	5.380683000
C	-1.594025000	3.668330000	4.972082000
H	-1.514867000	2.662750000	5.393877000
H	-0.743022000	4.263192000	5.322875000
N	-1.584699000	3.523474000	3.486186000
H	-0.812463000	2.921524000	3.202824000
H	-1.415233000	4.433779000	3.057567000
O	-5.458047000	2.233833000	2.767876000
C	-5.851488000	1.217729000	1.852861000
H	-5.828701000	1.607987000	0.822512000
H	-5.139369000	0.384620000	1.903126000
H	-6.333087000	3.283090000	2.701485000
C	-7.246802000	0.715323000	2.192845000
H	-7.976638000	1.527256000	2.131134000
H	-7.538299000	-0.072907000	1.488374000
H	-7.263845000	0.303809000	3.207964000
C	-7.130687000	4.944988000	3.532815000
O	-7.099182000	4.060775000	2.577825000
O	-6.348723000	5.058368000	4.482646000
H	-7.968196000	5.656765000	3.414107000
H	-2.966417000	4.404442000	6.470796000
H	-2.985043000	5.309410000	4.951844000
H	-4.898844000	4.049840000	4.771440000
H	-4.231329000	2.722125000	5.458820000

**19. Reaction intermediate 1: [Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)(H)(CO<sub>2</sub>)]<sup>+</sup> ( $\Delta E = 0.32$  eV)**

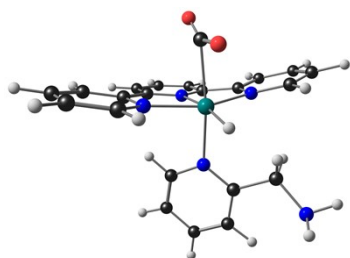


Ru	-3.849495000	2.981844000	2.535601000
N	-3.501464000	0.940726000	2.585809000
C	-3.765963000	0.071976000	3.582457000
H	-4.203364000	0.492683000	4.479314000
C	-3.524122000	-1.291211000	3.477904000
H	-3.773745000	-1.941748000	4.310701000
C	-2.980915000	-1.796910000	2.297506000
H	-2.796645000	-2.860787000	2.179447000
C	-2.670260000	-0.910119000	1.272668000
H	-2.229534000	-1.269729000	0.349633000



C	-2.924705000	0.451534000	1.434882000
C	-2.579901000	1.474786000	0.450461000
C	-1.944038000	1.294735000	-0.778943000
H	-1.662289000	0.301969000	-1.110193000
C	-1.671487000	2.407693000	-1.571344000
H	-1.174731000	2.282781000	-2.528794000
C	-2.045995000	3.682565000	-1.143058000
H	-1.851414000	4.547591000	-1.766043000
C	-2.694115000	3.829473000	0.081644000
N	-2.925351000	2.727651000	0.854224000
C	-3.281001000	5.060215000	0.626166000
C	-3.267495000	6.291537000	-0.028394000
H	-2.718898000	6.405394000	-0.956426000
C	-3.981303000	7.362753000	0.500931000
H	-3.980796000	8.324547000	-0.003773000
C	-4.709521000	7.172310000	1.674941000
H	-5.300481000	7.972561000	2.110369000
C	-4.669010000	5.932874000	2.300224000
H	-5.204485000	5.737240000	3.221718000
N	-3.953003000	4.901642000	1.814690000
N	-1.844360000	3.304330000	3.751496000
C	-0.918814000	2.339565000	3.575693000
H	-1.161206000	1.564239000	2.861352000
C	0.292266000	2.294454000	4.252973000
H	0.987087000	1.480777000	4.066348000
C	0.574116000	3.304645000	5.168959000
H	1.505856000	3.307062000	5.729382000
C	-0.357279000	4.321280000	5.342315000
H	-0.182483000	5.150439000	6.018200000
C	-1.552526000	4.304759000	4.618942000
C	-2.547567000	5.434986000	4.762897000
H	-3.551600000	5.003012000	4.802467000
H	-2.494374000	6.025245000	3.840934000
N	-2.227387000	6.319573000	5.880781000
H	-2.495952000	5.884543000	6.760284000
H	-2.763926000	7.178228000	5.804737000
O	-5.132409000	3.419399000	4.267526000
C	-5.609476000	2.473426000	3.630267000
O	-6.429909000	1.620084000	3.552100000
H	-5.135655000	2.779578000	1.653345000

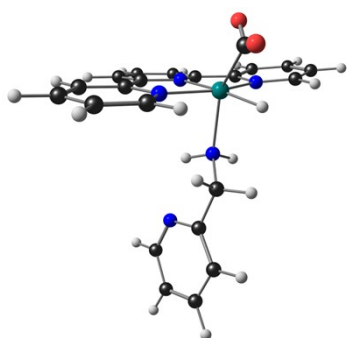
20. Reaction intermediate 2:  $[\text{Ru}^{\text{II}}(\text{terpy})(\text{N}^{\wedge}\text{N})(\text{H})(\text{CO}_2)]^+$  ( $\Delta E = 1.00 \text{ eV}$ )



Ru	-3.751403000	3.022775000	2.861907000
N	-3.544343000	0.978323000	2.769232000
C	-4.045523000	0.072398000	3.631163000
H	-4.505291000	0.485594000	4.522086000
C	-3.992434000	-1.298871000	3.397108000
H	-4.424876000	-1.981798000	4.122416000
C	-3.386381000	-1.765781000	2.231916000
H	-3.331667000	-2.829676000	2.019222000
C	-2.860785000	-0.840168000	1.332476000
H	-2.401026000	-1.174768000	0.409035000
C	-2.953108000	0.523504000	1.603640000
C	-2.488473000	1.566314000	0.668539000
C	-1.820733000	1.390526000	-0.547585000
H	-1.542551000	0.404269000	-0.901016000
C	-1.531264000	2.521800000	-1.314190000
H	-1.013366000	2.407579000	-2.262379000
C	-1.921223000	3.795530000	-0.892495000
H	-1.719108000	4.661254000	-1.512749000
C	-2.593990000	3.915256000	0.327933000
N	-2.806618000	2.811844000	1.065477000
C	-3.244072000	5.117647000	0.885030000
C	-3.343204000	6.316885000	0.179704000
H	-2.824762000	6.429664000	-0.765801000
C	-4.148203000	7.345633000	0.663573000
H	-4.246287000	8.273806000	0.107779000
C	-4.847898000	7.145424000	1.852786000
H	-5.514817000	7.903467000	2.252928000
C	-4.680245000	5.947341000	2.538555000
H	-5.184439000	5.752458000	3.478075000
N	-3.886716000	4.953194000	2.094993000
N	-1.798183000	3.314865000	3.689237000
C	-0.854711000	2.387588000	3.406455000
H	-1.137911000	1.601679000	2.724856000
C	0.418479000	2.386183000	3.952793000
H	1.114154000	1.597792000	3.681577000
C	0.758530000	3.398221000	4.847081000
H	1.743914000	3.438034000	5.303980000
C	-0.196809000	4.363113000	5.136803000
H	0.002810000	5.186074000	5.813870000
C	-1.465443000	4.314708000	4.552621000
C	-2.469332000	5.396818000	4.877144000

H	-3.456981000	4.919574000	4.942393000
H	-2.507656000	6.070050000	4.014058000
N	-2.085695000	6.183520000	6.044361000
H	-2.300971000	5.674752000	6.898309000
H	-2.625156000	7.043113000	6.069876000
O	-5.875115000	2.803300000	2.656729000
C	-5.400474000	2.691939000	1.528813000
O	-5.544339000	2.520615000	0.361181000
H	-4.216248000	3.170523000	4.400292000

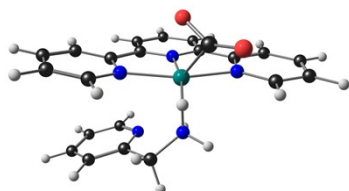
**21. Reaction intermediate 3: [Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)(H)(CO<sub>2</sub>)]<sup>+</sup> ( $\Delta E = 0.44$  eV)**



Ru	-3.832433000	2.932580000	2.644849000
N	-3.557778000	0.894790000	2.883352000
C	-4.032484000	0.115655000	3.879196000
H	-4.641560000	0.622697000	4.618008000
C	-3.800237000	-1.252303000	3.940796000
H	-4.220708000	-1.826593000	4.760841000
C	-3.045832000	-1.860986000	2.938329000
H	-2.854508000	-2.930084000	2.954803000
C	-2.542544000	-1.071005000	1.910420000
H	-1.951004000	-1.514825000	1.117242000
C	-2.801012000	0.299389000	1.892550000
C	-2.296455000	1.205603000	0.852821000
C	-1.440279000	0.899517000	-0.209502000
H	-1.080191000	-0.111319000	-0.363318000
C	-1.036489000	1.928050000	-1.060710000
H	-0.363294000	1.711125000	-1.885233000
C	-1.477049000	3.238796000	-0.855219000
H	-1.149515000	4.035199000	-1.513686000
C	-2.337348000	3.495476000	0.212946000
N	-2.719202000	2.478452000	1.020858000
C	-2.948833000	4.784927000	0.584581000
C	-2.853059000	5.934060000	-0.197845000
H	-2.254310000	5.920843000	-1.101787000
C	-3.547547000	7.084127000	0.168716000
H	-3.482855000	7.981099000	-0.440636000
C	-4.333187000	7.056761000	1.319082000
H	-4.902259000	7.925218000	1.636738000

C	-4.380756000	5.891764000	2.077344000
H	-4.971486000	5.823325000	2.983724000
N	-3.703165000	4.775638000	1.740399000
N	0.312985000	2.352591000	4.768758000
C	1.570661000	2.187088000	5.205228000
H	2.300824000	1.867116000	4.462583000
C	1.957510000	2.402982000	6.528698000
H	2.990235000	2.252076000	6.830133000
C	0.991400000	2.820958000	7.443324000
H	1.252886000	3.008292000	8.481945000
C	-0.317425000	3.003794000	7.000937000
H	-1.098511000	3.335738000	7.680720000
C	-0.607735000	2.752705000	5.659081000
C	-2.020943000	2.875298000	5.127771000
H	-2.602136000	3.618815000	5.675629000
H	-2.533843000	1.916075000	5.231474000
N	-2.030371000	3.228469000	3.686269000
H	-1.255791000	2.697788000	3.273392000
H	-1.751905000	4.205940000	3.599925000
O	-5.831102000	2.776874000	1.885839000
C	-5.844268000	2.499895000	3.102655000
O	-6.506304000	2.067099000	3.994105000
H	-4.530522000	3.547995000	3.963858000

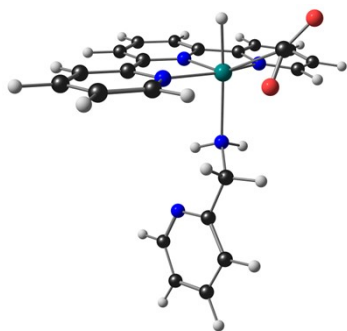
**22. Reaction intermediate 4: [Ru<sup>II</sup>(terpy)(N<sup>^</sup>N)(H)(CO<sub>2</sub>)]<sup>+</sup> ( $\Delta E = 0.34$  eV)**



Ru	-3.760314000	3.048480000	3.013180000
N	-2.846879000	1.353441000	3.743375000
C	-3.349757000	0.496476000	4.653053000
H	-4.271906000	0.809891000	5.129013000
C	-2.737728000	-0.712284000	4.966381000
H	-3.191307000	-1.367029000	5.704537000
C	-1.552057000	-1.055541000	4.321210000
H	-1.046298000	-1.990462000	4.545482000
C	-1.031279000	-0.186151000	3.366036000
H	-0.123882000	-0.442390000	2.830908000
C	-1.692767000	1.004040000	3.074116000
C	-1.273894000	1.924385000	2.001937000
C	-0.133045000	1.836296000	1.205180000
H	0.596596000	1.049397000	1.357831000
C	0.055042000	2.785275000	0.196878000
H	0.938199000	2.731377000	-0.433512000
C	-0.878853000	3.800172000	-0.010662000

H	-0.725889000	4.533814000	-0.793911000
C	-2.005412000	3.850422000	0.815731000
N	-2.159915000	2.922240000	1.784973000
C	-3.097453000	4.833644000	0.791928000
C	-3.179266000	5.876246000	-0.130070000
H	-2.411743000	5.982044000	-0.888698000
C	-4.245737000	6.768469000	-0.079448000
H	-4.319893000	7.576901000	-0.801357000
C	-5.213135000	6.601651000	0.910608000
H	-6.067396000	7.267910000	0.986105000
C	-5.092014000	5.544770000	1.805142000
H	-5.842618000	5.348616000	2.562366000
N	-4.069130000	4.664266000	1.759910000
N	-0.169108000	3.732865000	4.517598000
C	1.083988000	3.262103000	4.443309000
H	1.683515000	3.620718000	3.607471000
C	1.618640000	2.367552000	5.367971000
H	2.644893000	2.024460000	5.271296000
C	0.805476000	1.932669000	6.415921000
H	1.183101000	1.232469000	7.157101000
C	-0.499912000	2.408333000	6.496536000
H	-1.166447000	2.087512000	7.292952000
C	-0.939070000	3.314148000	5.529106000
C	-2.321983000	3.920701000	5.606438000
H	-2.296438000	4.762469000	6.312274000
H	-3.050020000	3.194106000	5.969433000
N	-2.743476000	4.406158000	4.269681000
H	-1.883509000	4.720777000	3.806499000
H	-3.355609000	5.210336000	4.378104000
O	-5.109799000	1.742038000	1.982922000
C	-5.774098000	2.611905000	2.581105000
O	-6.858252000	3.082385000	2.725206000
H	-4.856164000	3.066931000	4.199955000

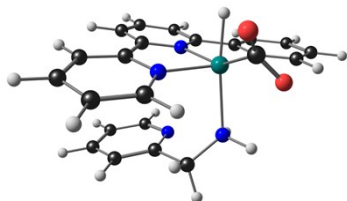
**23. Reaction intermediate 5: [Ru<sup>II</sup>(terpy)(N<sup>+</sup>N)(H)(CO<sub>2</sub>)]<sup>+</sup> ( $\Delta E = 0.13$  eV)**



Ru	-3.867824000	2.874625000	2.648624000
N	-3.560596000	0.870989000	2.949251000
C	-4.007830000	0.109111000	3.965114000

H	-4.591172000	0.627751000	4.717997000
C	-3.741602000	-1.252305000	4.045906000
H	-4.119937000	-1.822395000	4.889236000
C	-2.987811000	-1.856376000	3.040007000
H	-2.759344000	-2.917668000	3.078069000
C	-2.534727000	-1.078510000	1.978110000
H	-1.955864000	-1.527154000	1.178858000
C	-2.832724000	0.283244000	1.942191000
C	-2.466018000	1.184002000	0.843074000
C	-1.781432000	0.847257000	-0.322431000
H	-1.411284000	-0.161053000	-0.466760000
C	-1.589112000	1.816417000	-1.309050000
H	-1.065213000	1.559810000	-2.224872000
C	-2.063668000	3.111963000	-1.117941000
H	-1.908944000	3.871514000	-1.875513000
C	-2.724256000	3.426339000	0.070854000
N	-2.917091000	2.462667000	1.012417000
C	-3.221735000	4.730569000	0.498436000
C	-3.121061000	5.895559000	-0.262644000
H	-2.693484000	5.851724000	-1.258113000
C	-3.563454000	7.104580000	0.261350000
H	-3.496926000	8.016908000	-0.324278000
C	-4.082664000	7.120124000	1.555745000
H	-4.432937000	8.039755000	2.014797000
C	-4.172750000	5.929555000	2.264501000
H	-4.602586000	5.907338000	3.258308000
N	-3.777900000	4.741384000	1.758952000
N	0.345844000	2.404760000	4.945113000
C	1.593645000	2.221832000	5.400078000
H	2.329339000	1.885701000	4.669838000
C	1.966101000	2.439173000	6.727439000
H	2.992405000	2.274168000	7.043678000
C	0.993271000	2.874631000	7.625837000
H	1.242874000	3.061661000	8.667571000
C	-0.306586000	3.074489000	7.163459000
H	-1.091431000	3.420068000	7.831860000
C	-0.582672000	2.824328000	5.818016000
C	-1.985195000	2.964687000	5.260227000
H	-2.576071000	3.679948000	5.835446000
H	-2.491438000	1.996850000	5.335521000
N	-1.987333000	3.359690000	3.834274000
H	-1.178366000	2.886704000	3.421112000
H	-1.769389000	4.353069000	3.771717000
O	-5.037330000	3.055187000	4.473996000
C	-5.653046000	3.589470000	3.539852000
O	-6.586405000	4.233804000	3.190357000
H	-5.160892000	2.447222000	1.836348000

24. Reaction intermediate 6:  $[\text{Ru}^{\text{II}}(\text{terpy})(\text{N}^{\wedge}\text{N})(\text{H})(\text{CO}_2)]^+$  ( $\Delta E = 0.00 \text{ eV}$ )



Ru	-3.820076000	2.882583000	2.866725000
N	-3.092589000	1.156240000	3.750954000
C	-3.597878000	0.480649000	4.805553000
H	-4.521429000	0.862823000	5.220607000
C	-3.005347000	-0.660338000	5.327349000
H	-3.469291000	-1.161342000	6.171817000
C	-1.842099000	-1.154560000	4.736994000
H	-1.368485000	-2.058657000	5.108671000
C	-1.301190000	-0.465419000	3.659327000
H	-0.390189000	-0.812823000	3.185417000
C	-1.923545000	0.691685000	3.191301000
C	-1.381977000	1.542331000	2.140401000
C	-0.204353000	1.356426000	1.416570000
H	0.395834000	0.467224000	1.569427000
C	0.195906000	2.332450000	0.508939000
H	1.112799000	2.203559000	-0.058311000
C	-0.579859000	3.478891000	0.328960000
H	-0.272580000	4.242032000	-0.376564000
C	-1.763857000	3.623726000	1.046107000
N	-2.135711000	2.655424000	1.934664000
C	-2.735051000	4.715038000	0.925900000
C	-2.586739000	5.816678000	0.083754000
H	-1.688857000	5.923112000	-0.514185000
C	-3.594359000	6.774502000	0.015608000
H	-3.485702000	7.638601000	-0.633614000
C	-4.742259000	6.603789000	0.789517000
H	-5.554315000	7.324249000	0.764094000
C	-4.840841000	5.489411000	1.614175000
H	-5.711363000	5.306759000	2.234681000
N	-3.863236000	4.567129000	1.695705000
N	-0.501294000	4.257803000	4.333748000
C	0.774797000	4.121889000	3.948128000
H	1.121216000	4.813892000	3.181109000
C	1.639787000	3.162806000	4.474572000
H	2.668561000	3.101451000	4.130501000
C	1.148154000	2.291788000	5.446678000
H	1.785599000	1.523971000	5.878509000
C	-0.178013000	2.418583000	5.850843000
H	-0.602175000	1.753584000	6.598398000
C	-0.960727000	3.421545000	5.275434000
C	-2.383079000	3.651661000	5.730262000
H	-2.365547000	4.343477000	6.586213000

H	-2.829627000	2.715899000	6.071310000
N	-3.187607000	4.204652000	4.625513000
H	-2.648756000	4.974999000	4.228872000
H	-4.059910000	4.584157000	4.988252000
O	-5.819156000	3.299137000	3.612096000
C	-5.723723000	2.093042000	3.340571000
O	-6.224608000	1.017715000	3.353475000
H	-4.402616000	2.087533000	1.628260000