Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Electronic Supplementary Information

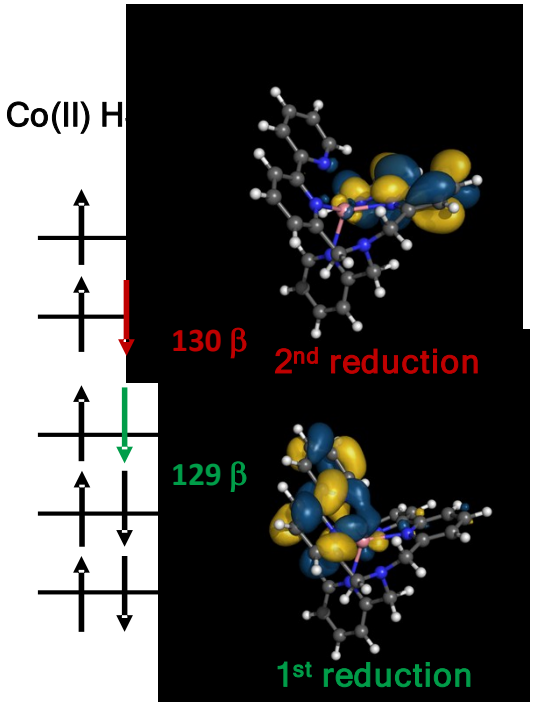
Computational details

All the electronic structure calculations have been carried out with the Gaussian09 package,[1] and, following the computational protocol employed in our previous work,[2] the B3LYP functional[3] in combination with a 6-311G** basis set was adopted. In agreement with the experimentally assessed and computationally confirmed ground state high spin configuration of the complex (charge +2 and spin multiplicity 4, see Ref. 2), all the reduced and protonated intermediates have been considered in their high-spin electronic configuration. Redox potentials in acetonitrile for the complex, "Co(II)", and its reduced species, "Co(I)" and Co(0), were calculated as free energy differences in solution.[4] The Gibbs free energy in solution of a species i (G^i_{solv}) is defined as $G^i_{solv} = G^i_{vac} + \Delta G^i_{solv}$, where G^i_{vac} is the Gibbs free energy in gas phase (the gas phase energy with zero point energy and thermal corrections) and ΔG^i_{solv} is the free energy of solvation. G^i_{vac} is obtained by performing a single point calculation at the optimized geometry *in vacuo*, followed by frequency calculations in order to include the vibrational contribution to the total partition function. The solvation free energy, $\Delta G^i_{solv,}$ was obtained by a single-point calculation in solution and a reference calculation in gas phase at the geometry optimized in solution, by using the IEFPCM approach and the gaussian03 default settings as implemented in Gaussian09.[1] Similarly to the procedure reported in Ref. [5] to calculate the relative free energies for the considered reaction steps, we used values of $G^*(H^+_{(s)})$=-266.5 Kcal/mol[6] and $G^0(e^-_{(g)})$=-0.868 Kcal/mol[7] and a value of -4.44 eV for the *vacuum* level with respect to the Normal Hydrogen Electrode (NHE) in acetonitrile. Excited states calculation on the complex and on the possible catalytic intermediates were also performed at TD-DFT (UB3LYP/6-311G**/C-PCM) level of theory on top of the geometries optimized in solution (water). The calculated spectra were obtained by Gaussian convolution (σ=0.17 eV) of the calculated vertical excitation energies.

Using the same level of theory (B3LYP/6-311G** in acetonitrile), each minimum energy path depicted in Figure 10 of the main text were calculated as follow: the transition state was firstly determined by a frequency calculation, followed by the computation of Intrinsic Reaction Coordinate (IRC)[8] pathways connecting the transition state with both –H···H– and ···H–H··· minima structures.

Moreover, a relaxed scan was performed along the H-Co distance to show the energy barrier associated with the first and limiting step in the conversion of Co(0)-BPY1/2H into Co(II)-H (Figure S2), and of Co(I)-BPY1/2H into Co(III)-H (Figure S3). As it can be seen, in all cases the proton transfer from a bipyridine ligand toward Co forms a high intermediate species, expected to subsequently relax through a strong structural rearrangement, that should involve a complex reorientation of (*i*) the pyridine moiety and of (*ii*) the bipyridine having just lost a proton.

Moreover, the possible decoordination step (of a pyridine or bi-pyridine ligand) prior protonation of Co(I) was assessed (Fig. S4 and Table S1), finding that only a bi-pyridine ligand can be decoordinated by reaching low-energy transition states (ca. 5 kcal/mol).



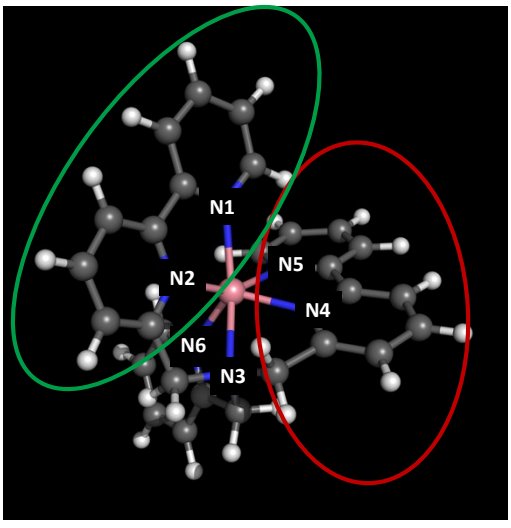


Figure S1. Left: Electronic configuration (high spin) and isodensity plots (isovalue 0.03) of the β manifold LUMO and LUMO+1 of complex **1** calculated in ACN at UB3LYP/6-311G* level of theory. Right: Atom labelling and bipyridine (BPY) ligands nomenclature.

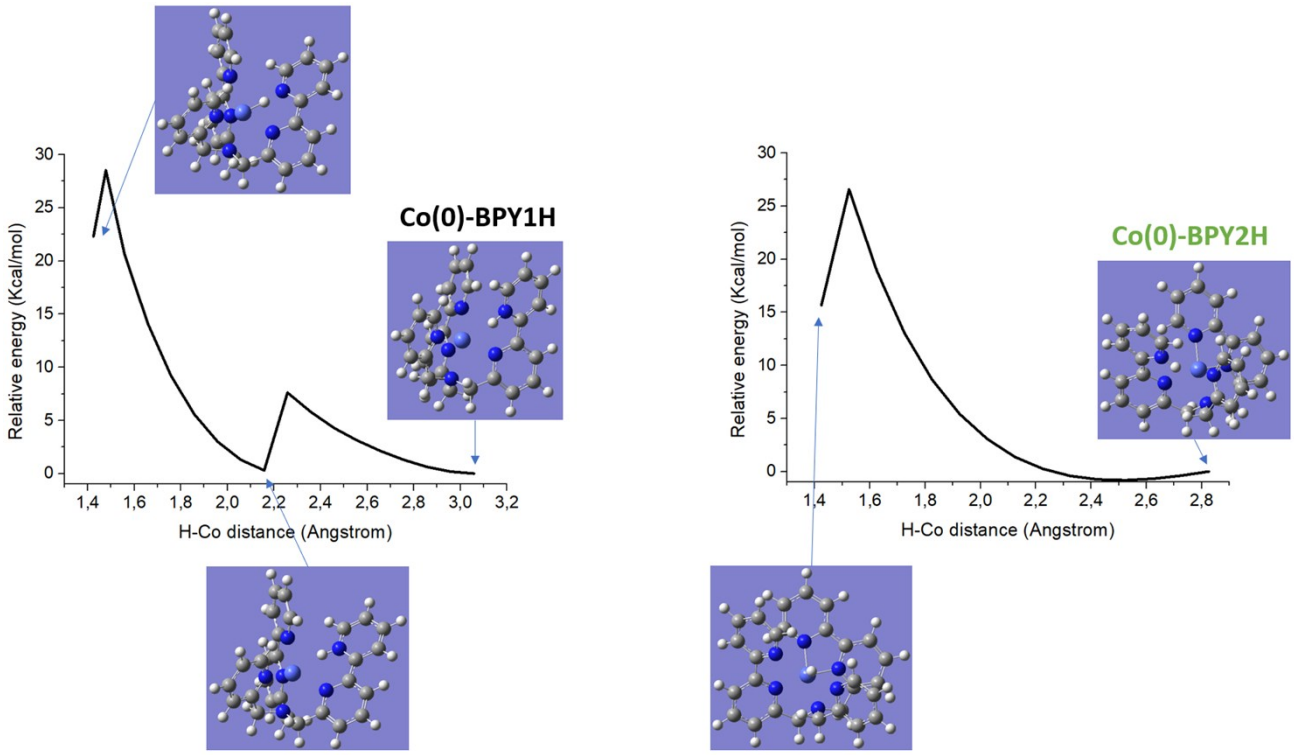


Figure S2. Calculated relaxed scan corresponding to the proton transfer from bipyridine (Co(0)-BPY1/2H) to the Co center, as first step in the conversion toward Co(II)-H. In the case of Co(0)-BPY1H (left), an additional minimum is found while approaching the proton, due to local reorientation of the BPY1H moiety. The energy profile only refers to the electronic energy and entropy is not taken into account.

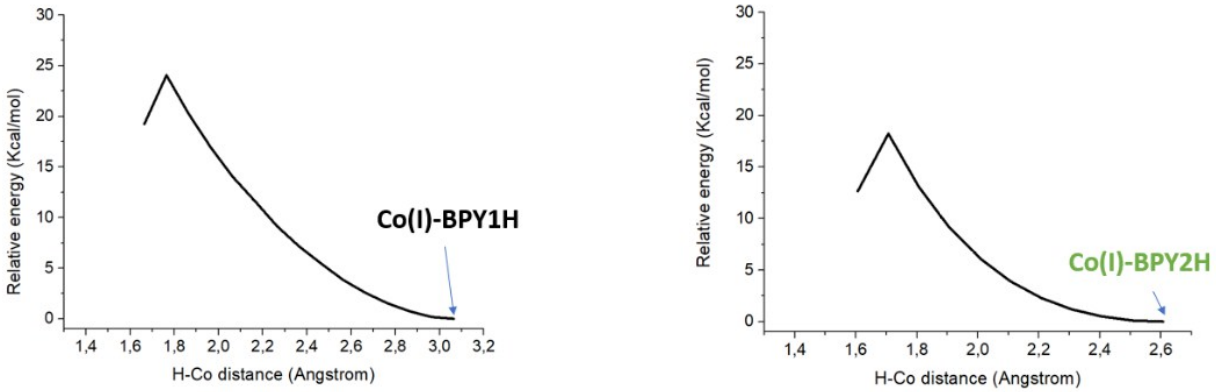


Figure S3. Calculated relaxed scan corresponding to the proton transfer from bipyridine (Co(I)-BPY1/2H) to the Co center, as first step in the conversion toward Co(III)-H. Only electronic energies are taken into account.

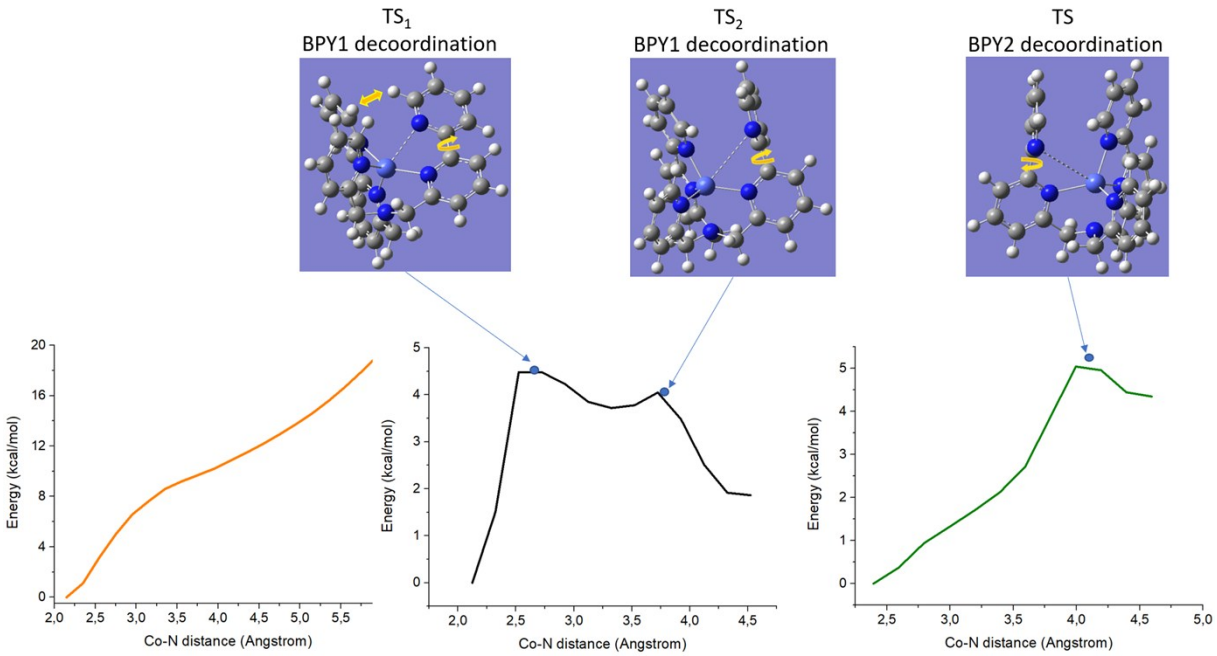


Figure S4. Calculated relaxed scan starting from the Co(I) structure (taken as reference energy) and showing decoordination of pyridine (left), BPY1 (center) or BPY2 (right), as plausible preparatory steps allowing further protonation of the decoordinated ligand. The calculated transition states are also shown (light blue dots) with the corresponding structures. The graphs indicate the electronic energy.

Table S1. Characterization of the transition states involved in decoordination of the Co(I) structure (refer to the geometries shown in Figure S4): calculated Free energies, imaginary frequencies and related normal mode.

Transition state	Free energy (Hartree)	ν (cm^{-1})	Normal mode
TS_1 BPY1 decoordination	-2792.534266	-43.37	Coupled rotations of BPY1 and BPY2 moieties, due to steric clash
TS_2 BPY1 decoordination	-2792.535228	-31.60	Rotation of BPY1 pyridine moiety
TS BPY2 decoordination	-2792.533100	-30.86	Rotation of BPY2 pyridine moiety

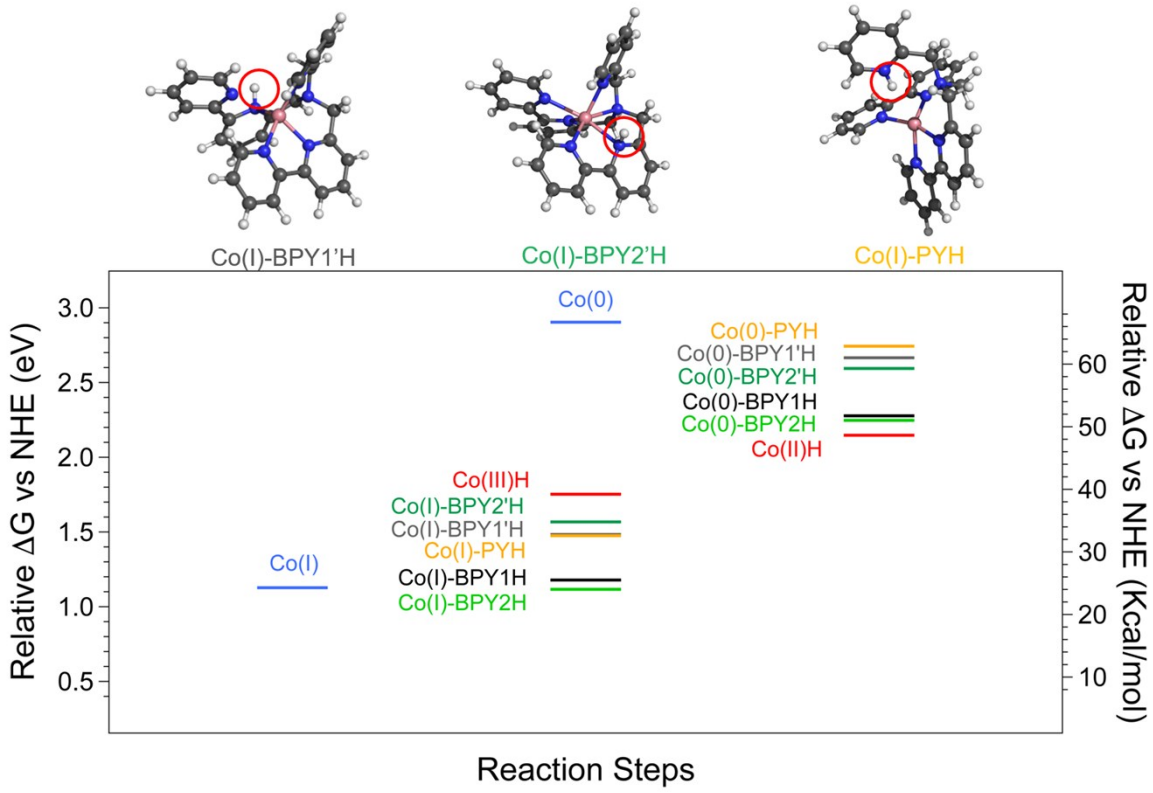


Figure S5. Top: optimized molecular structure of three possible N-H intermediates after reduction and the protonation step. Bottom: Calculated free energies differences (in eV et Kcal/mol) in acetonitrile for all the possible reaction steps involved in the proposed mechanism.

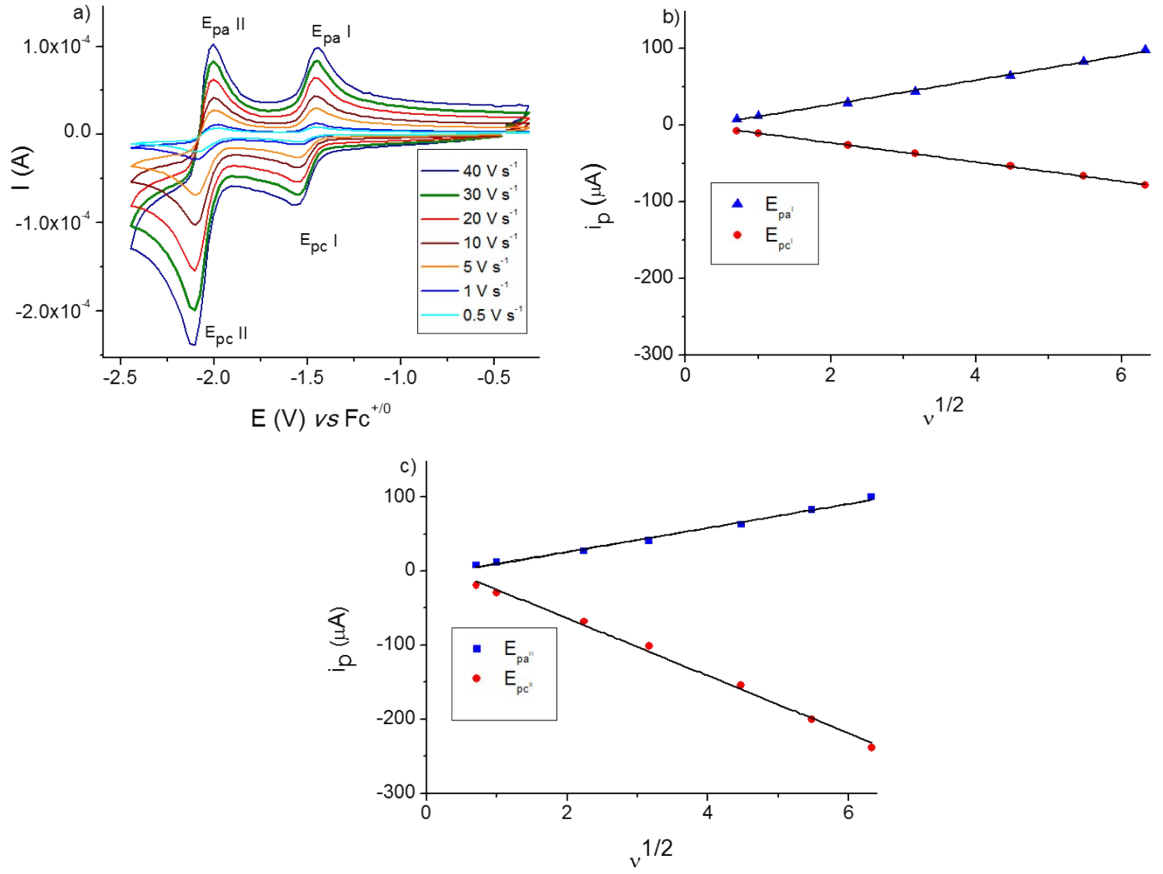


Figure S6. a) Cyclic voltammograms of Complex **1** at different scan rates (ν) in ACN with 0.1 M *n*Bu_4NPF_6 and glassy carbon as working electrode. b) Plot of i_p *vs* square root of scan rate ($\nu^{1/2}$) for anodic and cathodic waves of the first (E_{pa}^{I} and E_{pc}^{I}) and second (E_{pa}^{II} and E_{pc}^{II}) electrochemical signal. The slope of E_{pc}^{I} in b) allows the calculation of the diffusion coefficient (D cm^2 s^{-1}). Equation: Slope = $0.446\ FSC_{cat}\ (FD_{cat}/RT)^{1/2}$ with Slope = -1.2x10^{-5} (R^2 =0.999), F: Faraday constant, S: electrode surface area (0.02 cm^2), C_{cat} : concentration of the catalyst, D_{cat} : diffusion coefficient of the catalyst, R: Gas constant, T: temperature. For more details see equation (S4). D_{cat} = 5x10 $^{-12}$ cm^2 s^{-1}.

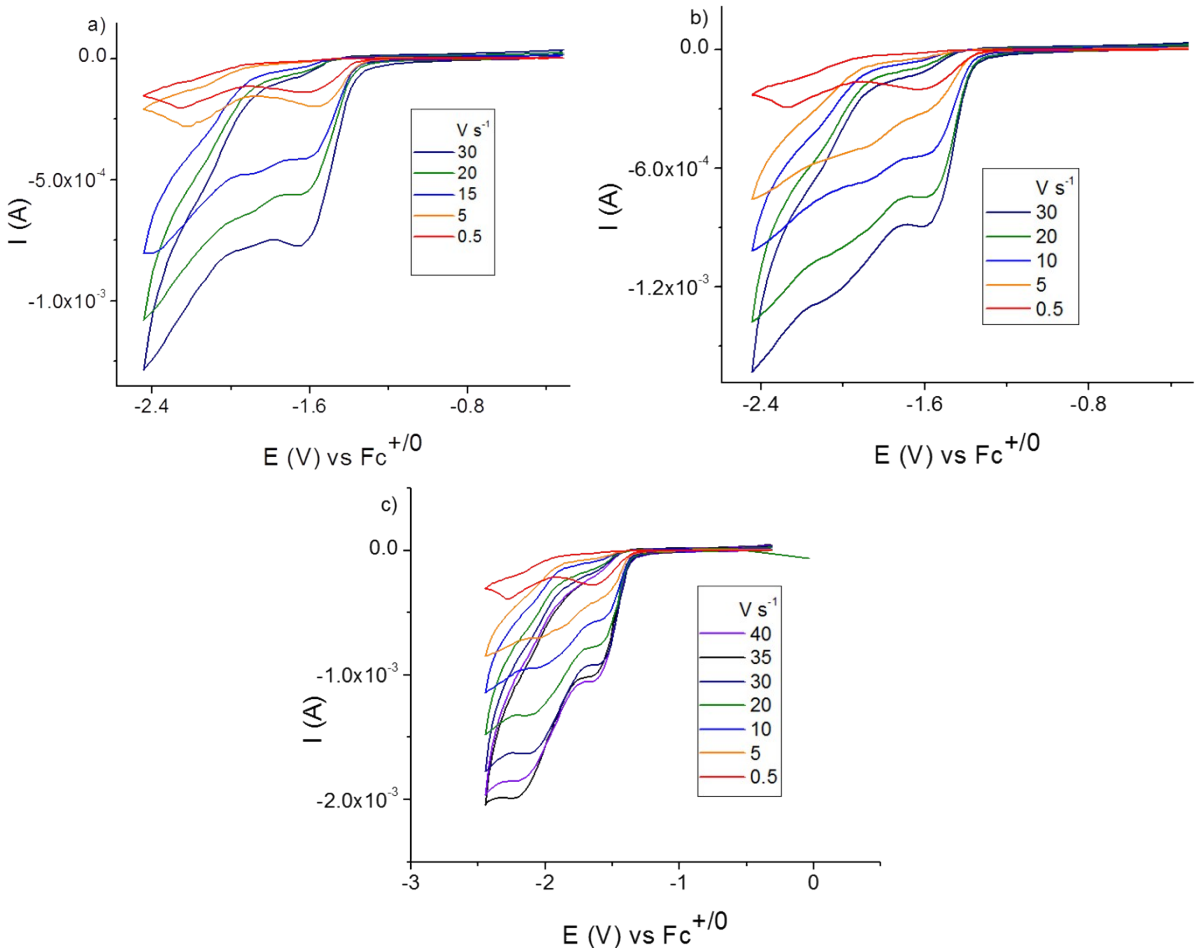


Figure S7. Cyclic voltammograms of Complex **1** (1 mM in ACN), nBu$_4$NPF$_6$ (0.1 M) on glassy carbon electrode with 10 mM (a) 15 mM (b) and 20 mM (c) TFA at different scan rates (0.5-40 Vs^{-1}).

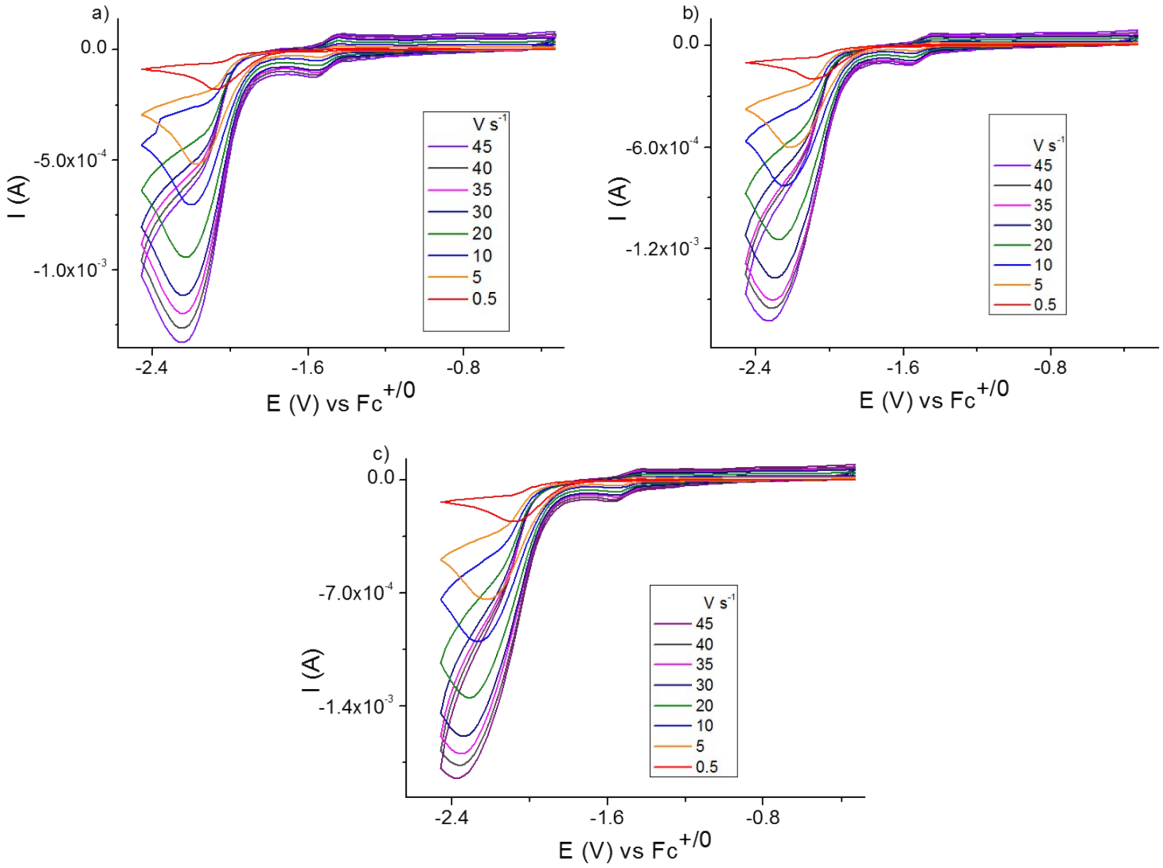


Figure S8. Cyclic voltammograms of Complex **1** (1 mM in ACN), nBu$_4$NPF$_6$ (0.1 M) on glassy carbon electrode with 15 mM (a) 20 mM (b) and 25 mM (c) Et$_3$NHBF$_4$ at different scan rates (0.5-45 Vs^{-1}).

FOWA analysis

The first rate constant of the proton transfer was gained plotting the ratio (i_{cat}/i_p) of the catalytic current (i_{cat}) and the peak current of a non-catalytic wave in the absence of acid (i_p) versus 1/ {1 + exp [F/RT(E - E_{cat})]} [9, 10] with E_{cat} being the potential at half of the catalytic current. The slope of the fit in the linear part of the plot (near the foot of the catalytic wave) provides the first rate constant k_1 = 1.5(±0.2)x10^7 $M^{-1}s^{-1}$ according to equation (S1) for an ECEC process. The average value of k_1 was calculated from CVs performed at 10, 15 and 20 mM TFA and 0.5–50 V s^{-1} (Figure S4).

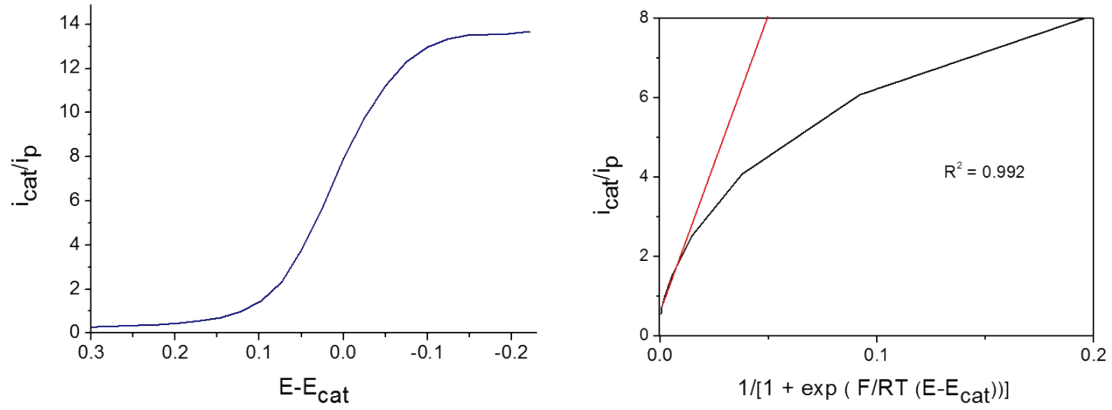


Figure S9. Left: Normalized CV of complex **1** (1 mM), TFA 20 mM at 30 V s^{-1} in CAN, nBu$_4$NPF$_6$ 0.1 M on glassy carbon electrode. Right: Example of FOWA plot (black line) and linear fit near the foot of the catalytic wave (red line) for complex **1** (1 mM), TFA 20 mM at 30 V s^{-1} in ACN nBu$_4$NPF$_6$ 0.1 M on glassy carbon electrode.

The second rate constant (k_2) was extracted from equation (S2). Figure S7 shows the values of k_2 obtained at different conditions (10, 15, 20 mM and 5-50 V s^{-1}) with an average value of k_2 = 8.5(±0.7)x10^5 $M^{-1}s^{-1}$.
The reliability of the rate constant was tested with equation (S3). The k_2 was used to calculate the expected plateau current (i_{pl}). For instance, at 30 V s^{-1} and 20 mM of TFA an i_{pl} = -1.1 mA was obtained, which is slightly higher than the experimental one (i_{cat} = -0.9 mA).[11]

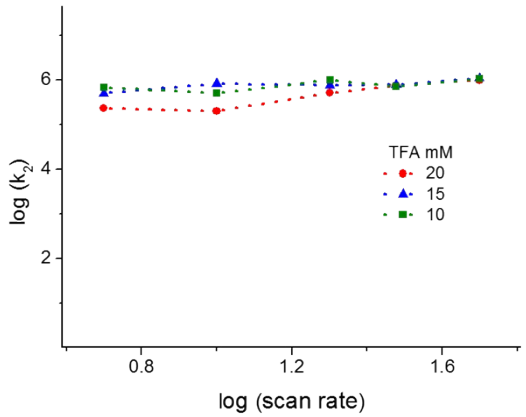


Figure S10. Logarithm of k_2 calculated from FOWA for three concentrations of TFA versus logarithm of the scan rates.

$$\frac{i_{cat}}{i} = \frac{4{,}48\sqrt{\frac{k_1 C_A^0 RT}{F\,v}}}{F}$$

$$E_{cat} = E_{CoII/I} + \frac{RT}{F} ln\left(1 + \sqrt{\frac{k_1 C_A^0}{}}\right)$$

$$i_{pl} = 2FSC_{cat}\sqrt{D_{cat}}\sqrt{k_2 C_Z^0} \qquad \text{equation (S3)}$$

The diffusion coefficient D_{cat} can be calculated from equation (S4):

$$i_p = 0.446FSC_{cat}\sqrt{\frac{Fv\,D_{cat}}{RT}}$$

$$\frac{i_{pl}}{i_p} = \frac{2}{0.4463}\sqrt{\frac{RT}{Fv}}\frac{1}{\frac{1}{\sqrt{k_1 C_A^0}} + \frac{1}{\sqrt{k_2 C_Z^0}}} \qquad \text{equation (S5)}$$

For the Equations:

F : Faraday Constant;
S : electrode surface area;
C_{cat} : concentration of the catalyst;
D_{cat} : Diffusion coefficient of the catalyst;
R: Gas constant;
T: temperature;
C_Z^0 : C_A^0 : concentration of acid;
k_1 : first protonation rate constant;
k_2 : second protonation rate constant;
ν : scan rate;
E : electrode potential;
E_{cat} : half-wave potential of the catalytic wave;
$E_{CoII/I}$: potential of $Co^{II/I}$ in the absence of acid;
i_{cat} : catalytic current;
i_p : peak current of a non-catalytic wave.

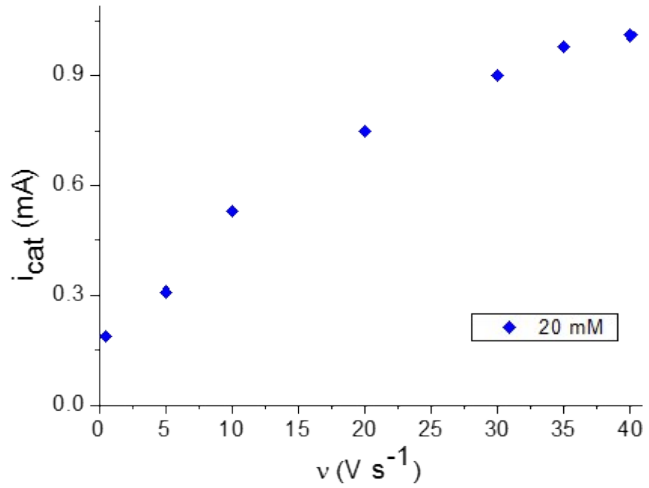


Figure S11. Catalytic current versus scan rate in CVs of 1 mM of complex **1** in ACN and 20 mM of TFA with a glassy carbon electrode.

FOWA analysis was also performed for the CVs of Figure S5. In this case the addition of Et_3NH^+ triggers the catalytic wave at E_{cat} = -2.06 V *vs* $Fc^{+/0}$ corresponding to the potential of the second reduction signal in the absence of acid. Therefore, we assumed an EEC process on the basis of the experimental behavior. Plotting i_{cat}/i_p versus 1/ {1 + exp [F/RT(E - E_{cat})]}, we calculated an average value of k_1 = 2(±0.1)x10^5 $M^{-1}s^{-1}$ for different concentrations of acid (15, 20, 25 mM) and at different scan rate (0.5–50 V s^{-1}) (Figure S10).

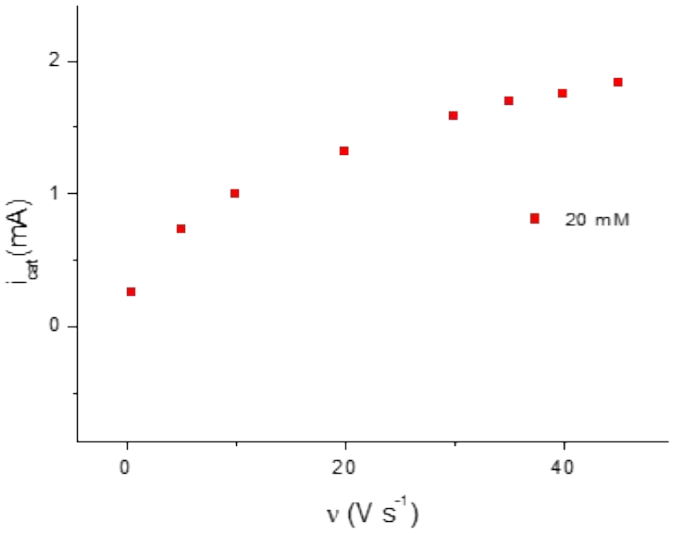


Figure S12. Catalytic current versus scan rate in CVs of 1 mM of complex **1** in ACN and 20 mM of Et_3NH^+ with a glassy carbon electrode.

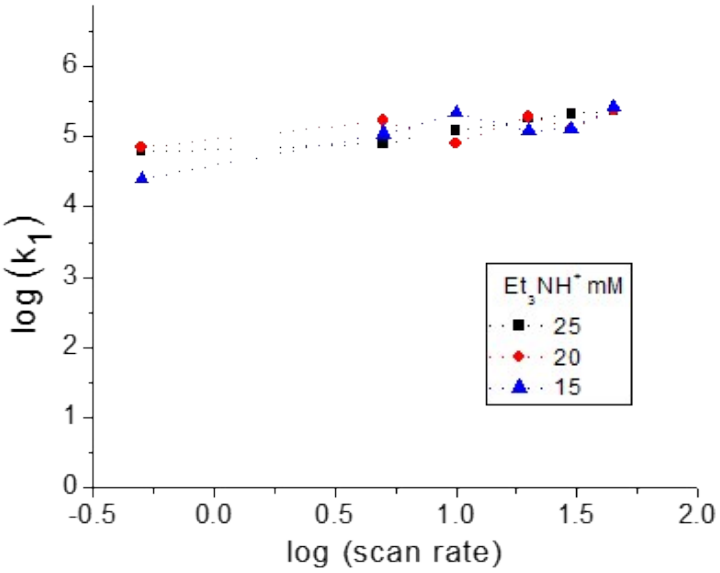


Figure S13. Logarithm of k_1 calculated from FOWA for three concentrations of Et_3NH^+ versus logarithm of the scan rates.

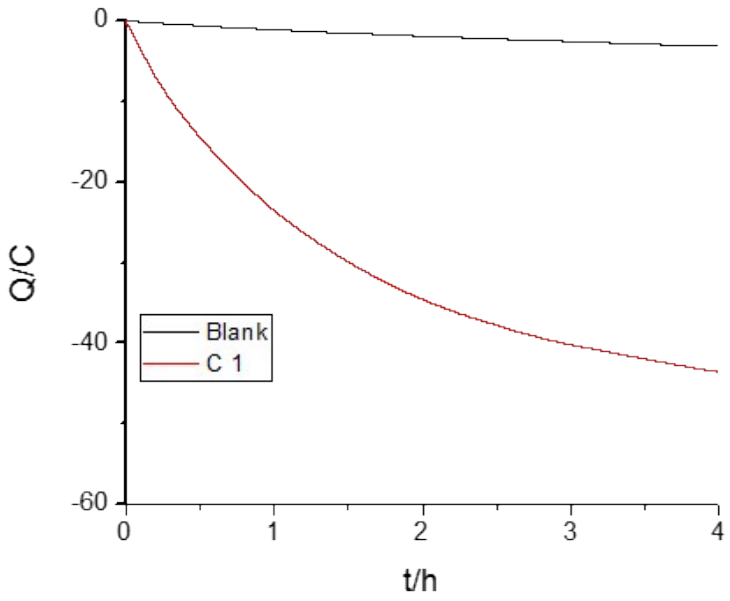


Figure S14. Coulometry of the bulk electrolysis performed at -1.53 V *vs* $Fc^{+/0}$ in the presence of Complex **1** (1 mM), nBu$_4$NPF$_6$ (0.1 M), and TFA (100 mM) in 8 mL solution ACN with a pool mercury as working electrode.

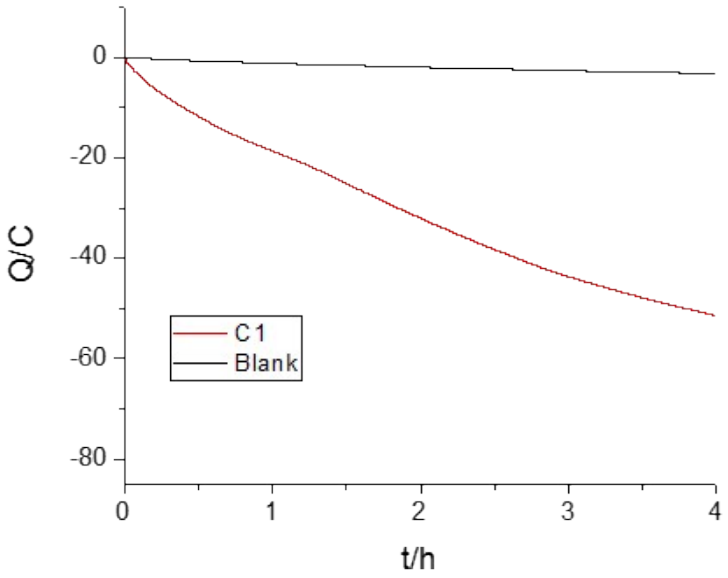


Figure S15. Coulometry of the bulk electrolysis performed at -2.1 V vs $Fc^{+/0}$ in the presence of Complex **1** (1 mM), nBu$_4$NPF$_6$ (0.1 M), and Et_3NH^+ (100 mM) in 8 mL solution of ACN with a pool mercury as working electrode.

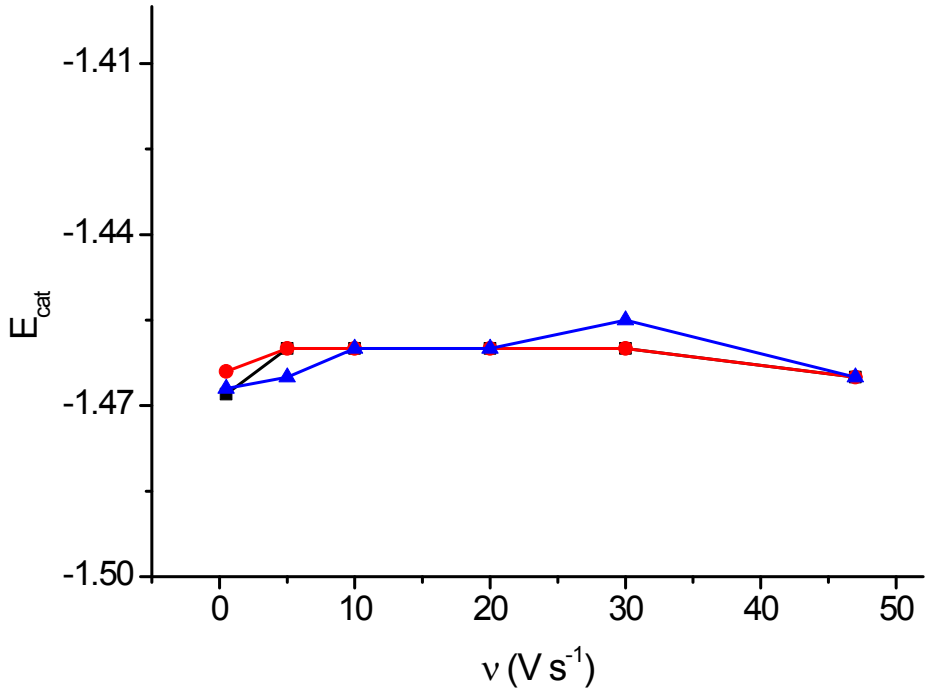
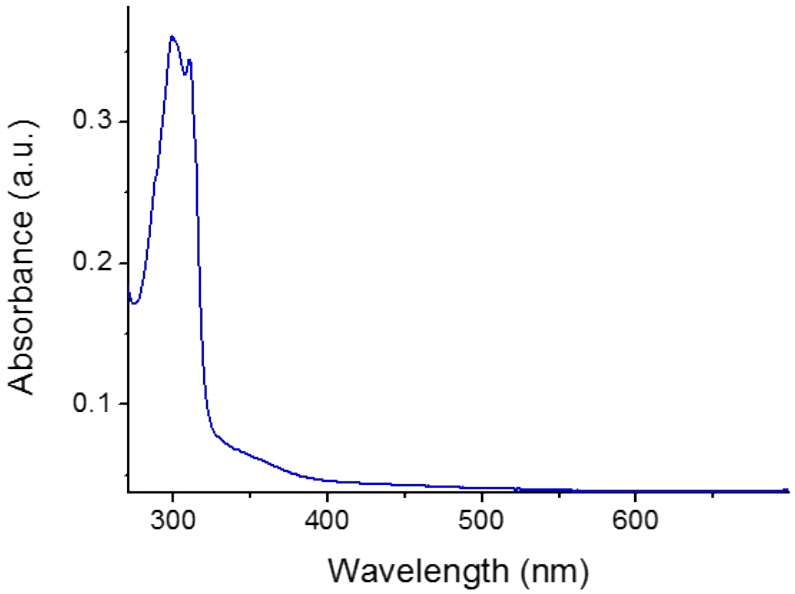


Figure S16. E_{cat} versus scan rate with 20 mM TFA (black), 15 mM TFA (red), 10 mM TFA (blue).



FigureS17. UV-Vis spectrum of complex **2** in H_2O.

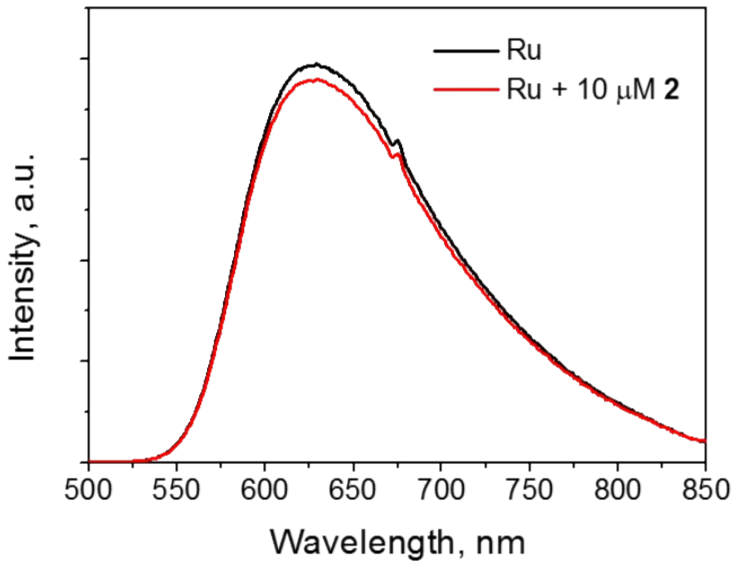
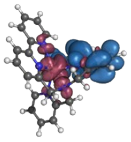
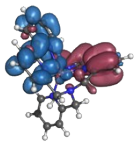
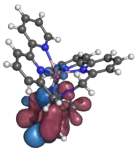
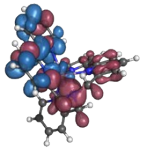
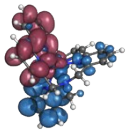
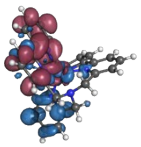
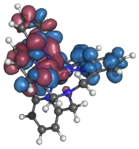
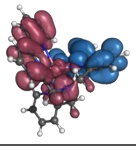


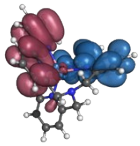
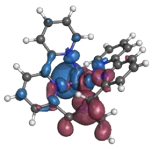
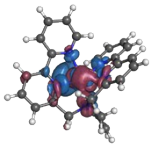
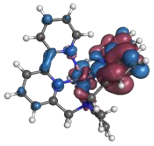
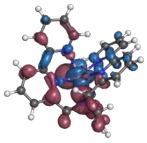
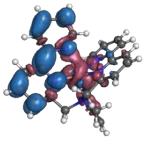
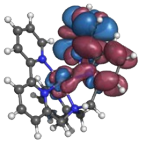
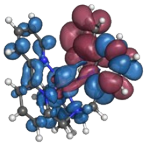
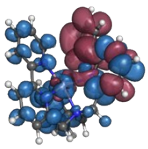
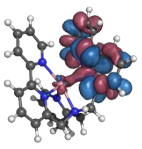
Figure S18. Emission spectra of 50 μM $Ru(bpy)_3^{2+}$ in 1 M acetate buffer (pH 4) in the absence (black trace) and presence of 10 μM complex **2**.

Table S2. Calculated (UB3LYP/6-311G*/ACN) Mulliken charges on the Cobalt and Nitrogen atoms for the complex and its mono e doubly reduced species. The Co-Nx bond lengths (Å) are also reported. The atom labelling is displayed in Figure S1.

Atom	*Mulliken charges (a.u.)*		
	Complex 1	**[Complex 1]$^{-}$**	**[Complex 1]$^{2-}$**
Co1	+1.44	+1.39	+1.41
N1	-0.56	-0.64	-0.63
N2	-0.64	-0.69	-0.68
N3	-0.47	-0.45	-0.43
N4	-0.63	-0.61	-0.68
N5	-0.51	-0.44	-0.63
N6	-0.56	-0.52	-0.51
Bond	**Length (Å)**		
Co1-N1	2.282	2.124	2.147
Co1-N2	2.131	2.055	2.084
Co1-N3	2.309	2.352	2.387
Co1-N4	2.115	2.137	2.081
Co1-N5	2.274	2.394	2.323
Co1-N6	2.153	2.151	2.176

Table S3. Calculated vertical excitation energies (nm) and oscillator strengths of some representative energy portions of the absorption spectrum of Co(II), Co(I), Co(III)-H and Co(I)-BPY2H. The isodensity plots of the density difference between the excited and the ground state are also shown.

State	E_{exc} (nm)	Oscillator Strength	Nature
Co(II)			
9	349	0.0153	
23	298	0.1299	
25	294	0.1814	
28	289	0.2470	
Co(I)			
13	642	0.0120	
14	608	0.0283	
20	416	0.0519	
25	361	0.1953	

31	330	0.0144	
Co(III)-H			
8	449	0.0121	
11	374	0.0156	
28	307	0.0250	
36	292	0.1091	
38	289	0.1309	
Co(I)-BPY2H			
6	823	0.0137	
9	741	0.0197	
11	604	0.0115	
17	440	0.0673	

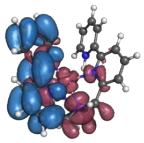
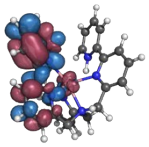
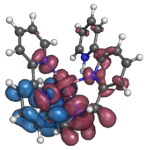
21	479	0.3338	
34	378	0.1034	
35	376	0.1121	

Table S4. Calculated free energy differences in acetonitrile for the possible reaction steps involved in the proposed mechanism. All the values are in eV.

Mechanism	ΔG	ΔG vs NHE	Sum of ΔG vs NHE
ECEC			
$Co(II) + e^- \rightarrow Co(I)$	-3.313	1.127	1.127
$Co(I) + H^+ \rightarrow Co(III)\text{-}H$	0.626	0.626	1,753
$Co(I) + H^+ \rightarrow Co(I)\text{-}BPY1H$	0,051	0,051	1,178
$Co(I) + H^+ \rightarrow Co(I)\text{-}BPY2H$	-0,011	-0,011	1,116
$Co(III)\text{-}H + e^- \rightarrow CO(II)\text{-}H$	-4,046	0,394	2,147
$Co(I)\text{-}BPY1H + e^- \rightarrow Co(0)\text{-}BPY1H$	-3,341	1,099	2,277
$Co(I)\text{-}BPY2H + e^- \rightarrow Co(0)\text{-}BPY2H$	-3,309	1,131	2,247
EECC			
$Co(II) + e^- \rightarrow Co(I)$	-3.313	1.127	1.127
$Co(I) + e^- \rightarrow Co(0)$	-2,663	1,777	2,904

Computational details
The xyz coordinates of the calculated intermediates along with their energies.

Co(II)

Electronic+Thermal Energy= -2792.143997 a.u.

C	7.302630	2.991799	4.069050
C	8.561942	2.554469	3.662011
N	8.776648	2.160881	2.389962
C	7.752206	2.046592	1.535636
C	6.464449	2.444083	1.882535
C	6.251494	2.960337	3.156629
C	9.719073	2.349935	4.565489
N	10.804394	1.790172	3.982689
C	11.852241	1.479988	4.754912
C	11.887050	1.710861	6.125937
C	10.782780	2.310469	6.722206
C	9.684556	2.633374	5.931950
Co	10.738465	1.830291	1.697950
N	9.334757	0.629536	0.304715
C	8.095231	1.422546	0.201724
N	11.260315	2.391314	-0.289565
C	12.055208	3.464405	-0.485846
C	12.487813	3.808639	-1.766087
C	12.068526	3.046392	-2.851623
C	11.225050	1.962908	-2.639580
C	10.847701	1.659771	-1.334612
C	12.389133	4.240428	0.734416
N	11.901481	3.756204	1.903658
C	12.135002	4.459441	3.021827
C	12.859252	5.644986	3.048410
C	13.375626	6.130712	1.854466
C	13.133457	5.419537	0.685021
C	9.983712	0.463479	-1.007414
N	11.468986	-0.185414	1.730265
C	10.560258	-1.141737	1.442816
C	10.875140	-2.494678	1.506084
C	12.165005	-2.877590	1.864025
C	13.111611	-1.890985	2.124264
C	12.720005	-0.562031	2.045108
C	9.188843	-0.648867	1.025583
H	7.252549	0.824340	-0.167677
H	8.264890	2.212429	-0.536413
H	5.647195	2.342001	1.177926
H	5.263947	3.294108	3.453956
H	7.124817	3.325235	5.082770
H	8.813446	3.089885	6.383598
H	10.770245	2.516994	7.786287
H	12.758996	1.429357	6.703628
H	12.700668	1.027587	4.255978
H	9.251593	0.283216	-1.803325
H	10.622672	-0.422534	-0.974635
H	10.868503	1.361712	-3.468050
H	12.389956	3.304758	-3.854127
H	13.135038	4.658849	-1.930340
H	13.518105	5.793906	-0.253754

H	13.950993	7.048947	1.827543
H	13.010472	6.166512	3.985508
H	11.726138	4.056676	3.937097
H	8.673108	-1.408271	0.425162
H	8.577027	-0.473345	1.913988
H	10.123224	-3.238323	1.267411
H	12.430540	-3.927230	1.918483
H	14.134278	-2.142492	2.377293
H	13.433026	0.236295	2.221949

Co(I)

Electronic+Thermal Energy= -2792.399520 a.u.

C	7.265162	3.028413	4.003234
C	8.544790	2.627995	3.605835
N	8.789215	2.242674	2.326031
C	7.749773	2.044728	1.494559
C	6.452182	2.390690	1.838033
C	6.216212	2.944827	3.100444
C	9.665743	2.418337	4.533113
N	10.693121	1.697245	4.021409
C	11.685791	1.336987	4.842251
C	11.732694	1.675266	6.188480
C	10.700271	2.459738	6.706048
C	9.658517	2.834676	5.871915
Co	10.732452	1.859738	1.665984
N	11.509676	-0.130515	1.688290
C	10.613805	-1.110273	1.451800
C	10.958288	-2.454250	1.557162
C	12.260149	-2.798482	1.910485
C	13.189032	-1.784967	2.126439
C	12.768956	-0.467017	2.002177
C	9.220508	-0.660521	1.041178
N	9.317250	0.586097	0.279702
C	8.093300	1.389257	0.175760
N	11.219285	2.373014	-0.280450
C	12.003538	3.472756	-0.472931
C	12.353863	3.880349	-1.773517
C	11.889562	3.171840	-2.862035
C	11.075300	2.043814	-2.650061
C	10.780940	1.678442	-1.352781
C	12.403697	4.150881	0.747074
N	11.994950	3.563353	1.923385
C	12.338335	4.193222	3.071041
C	13.069506	5.360962	3.132550
C	13.488101	5.956386	1.933514
C	13.147372	5.343521	0.745872
C	9.983507	0.435298	-1.021155
H	7.236896	0.804127	-0.188741
H	8.283649	2.165919	-0.571210
H	5.638681	2.223001	1.141350
H	5.216452	3.245574	3.391670
H	7.079373	3.354876	5.018457
H	8.850193	3.444184	6.256007
H	10.707467	2.769199	7.745259
H	12.557420	1.343688	6.807689
H	12.482297	0.751198	4.395934
H	9.270654	0.199416	-1.822218
H	10.671463	-0.411529	-0.961319

H	10.691960	1.466738	-3.484083
H	12.147067	3.481404	-3.868424
H	12.982867	4.747403	-1.927181
H	13.449070	5.790381	-0.192628
H	14.060001	6.877219	1.936118
H	13.305215	5.798840	4.095071
H	12.004754	3.725583	3.985394
H	8.713028	-1.464201	0.487785
H	8.627245	-0.465809	1.939189
H	10.218470	-3.220480	1.353556
H	12.548029	-3.840360	1.996077
H	14.219436	-2.006618	2.377156
H	13.457709	0.359595	2.140947

Co(0)

Electronic+Thermal Energy= -2792.541273 a.u.

C	7.252691	3.014110	4.025775
C	8.550760	2.571212	3.652811
N	8.780207	2.205765	2.334182
C	7.730963	2.021641	1.514136
C	6.433688	2.341733	1.858125
C	6.211573	2.920817	3.137888
C	9.636525	2.338885	4.548116
N	10.761410	1.757257	3.990865
C	11.769751	1.425902	4.802590
C	11.789119	1.641521	6.171150
C	10.663941	2.277530	6.744234
C	9.603432	2.620913	5.943057
Co	10.725340	1.936137	1.680856
N	11.476492	-0.096808	1.707872
C	10.584909	-1.076723	1.467871
C	10.931190	-2.420347	1.585207
C	12.230444	-2.760930	1.949998
C	13.155834	-1.744619	2.165229
C	12.732444	-0.428295	2.030693
C	9.196967	-0.630257	1.041829
N	9.294781	0.594962	0.259694
C	8.082030	1.414017	0.171959
N	11.232530	2.372190	-0.286841
C	12.039321	3.475369	-0.489181
C	12.399991	3.849970	-1.806950
C	11.933291	3.135978	-2.882544
C	11.091483	2.016933	-2.657928
C	10.792087	1.677003	-1.356867
C	12.434130	4.167951	0.702100
N	11.966074	3.641848	1.896607
C	12.274898	4.305299	3.033297
C	13.043824	5.447111	3.085606
C	13.549072	5.971279	1.875287
C	13.239522	5.333026	0.699853
C	9.972974	0.443850	-1.026885
H	7.224762	0.848624	-0.225788
H	8.295874	2.211650	-0.546344
H	5.615969	2.161651	1.169453
H	5.216682	3.245861	3.424942
H	7.076486	3.393821	5.025767
H	8.733834	3.102226	6.375464
H	10.634593	2.490147	7.808634

H	12.644693	1.345055	6.766092
H	12.629494	0.967558	4.320124
H	9.268243	0.218436	-1.840919
H	10.650525	-0.412019	-0.961540
H	10.695704	1.435956	-3.483902
H	12.199556	3.427872	-3.893031
H	13.038296	4.709936	-1.969935
H	13.608524	5.727499	-0.239288
H	14.163965	6.865556	1.870405
H	13.243753	5.921690	4.039032
H	11.872792	3.879965	3.942135
H	8.688262	-1.449575	0.507913
H	8.607121	-0.410901	1.935940
H	10.191815	-3.187326	1.381114
H	12.518974	-3.802269	2.046142
H	14.184686	-1.961578	2.427557
H	13.415947	0.401754	2.173036

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Co(III)-H

Electronic+Thermal Energy= -2792.667245 a.u.

C	12.790683	5.660973	0.624107
C	12.156230	4.417592	0.666852
N	11.596094	3.943464	1.801238
C	11.627213	4.720294	2.891957
C	12.218653	5.977426	2.922390
C	12.826858	6.450617	1.766275
C	11.991168	3.565281	-0.530710
N	11.299157	2.423235	-0.335050
C	10.968179	1.656642	-1.384513
C	11.369969	1.965470	-2.679978
C	12.142687	3.101563	-2.884632
C	12.441592	3.920640	-1.802185
Co	10.949668	1.739174	1.660059
N	9.420138	0.653226	0.201869
C	10.119606	0.451255	-1.072976
N	9.007649	2.094784	2.342178
C	8.822915	2.361665	3.651227
C	7.571885	2.751113	4.129716
C	6.505288	2.832825	3.239706
C	6.694372	2.476871	1.907831
C	7.968156	2.097989	1.496717
C	10.023580	2.160614	4.494520
N	11.151632	1.820117	3.823932
C	12.287577	1.663627	4.517018
C	12.359271	1.794913	5.898731
C	11.198455	2.114189	6.594312
C	10.019374	2.307447	5.882265
C	8.289971	1.595372	0.107972
N	11.259037	-0.424059	1.837194
C	10.277945	-1.260326	1.442741
C	10.381517	-2.641694	1.578408
C	11.532670	-3.188830	2.132846
C	12.560138	-2.330621	2.512320
C	12.383476	-0.966326	2.341808
C	9.052054	-0.618110	0.841612
H	7.405969	1.137000	-0.352547
H	8.585332	2.430907	-0.531851

H	5.867557	2.476296	1.207087
H	5.526408	3.138210	3.591228
H	7.417321	2.978792	5.175957
H	9.110500	2.567324	6.408931
H	11.208757	2.219221	7.673132
H	13.303958	1.651365	6.408707
H	13.176498	1.441319	3.941288
H	9.425477	0.244443	-1.897633
H	10.762090	-0.428426	-0.977284
H	11.078231	1.329521	-3.507810
H	12.486117	3.363174	-3.878842
H	13.005870	4.829364	-1.959057
H	13.246553	6.021575	-0.287937
H	13.313490	7.418965	1.748100
H	12.203300	6.561486	3.834422
H	11.159873	4.324607	3.782722
H	8.561525	-1.302782	0.138848
H	8.328298	-0.414465	1.634442
H	9.569883	-3.278317	1.244484
H	11.633670	-4.262126	2.246695
H	13.489574	-2.707670	2.921181
H	13.175686	-0.277963	2.601600
H	12.392880	1.585236	1.434987

Co(I)-BPY1H

Electronic+Thermal Energy= -2792.686528 a.u.

C	13.195421	5.420086	0.058087
N	12.439628	4.356971	0.394711
C	12.112270	4.173227	1.695392
C	12.527863	5.059960	2.681849
C	13.297801	6.164897	2.325502
C	13.641256	6.347399	0.988202
Co	11.905347	2.813715	-0.910050
N	9.875271	5.254600	-1.632062
C	9.150110	4.342354	-2.392819
C	8.586748	4.848544	-3.588551
C	8.734816	6.165323	-3.949538
C	9.457514	7.063395	-3.110575
C	9.998187	6.580639	-1.959909
C	8.995676	3.002066	-1.906848
N	9.850336	2.554076	-0.908917
C	9.512624	1.411747	-0.244904
C	8.408462	0.653468	-0.565422
C	7.617844	1.032332	-1.666836
C	7.913518	2.196812	-2.332762
C	10.450369	0.930888	0.850111
N	11.574100	1.855876	1.083505
C	11.246091	2.966440	1.995375
N	12.714637	2.970703	-2.882440
C	13.613475	1.988699	-3.166446
C	14.178908	1.871921	-4.434213
C	13.829501	2.779829	-5.429117
C	12.920801	3.788437	-5.131672
C	12.388225	3.841281	-3.849356
C	13.962944	1.080655	-2.041072
N	13.314951	1.345415	-0.889963
C	13.547950	0.645677	0.227066

C	14.455009	-0.409351	0.233249
C	15.127619	-0.709103	-0.949013
C	14.890092	0.041972	-2.098877
C	12.815598	1.145781	1.458893
H	9.889121	0.739973	1.773269
H	10.869007	-0.031023	0.543511
H	8.171867	-0.235611	0.007768
H	6.766342	0.431440	-1.963468
H	7.269612	2.533929	-3.134199
H	8.041011	4.175704	-4.236416
H	8.293425	6.525428	-4.871045
H	9.569427	8.108354	-3.366721
H	10.544029	7.190730	-1.252038
H	12.621339	0.329910	2.163789
H	13.473454	1.851841	1.974783
H	14.635912	-0.979968	1.136752
H	15.839848	-1.525874	-0.976808
H	15.423896	-0.189806	-3.010801
H	14.887337	1.083960	-4.653053
H	14.264160	2.698375	-6.418751
H	12.624175	4.519902	-5.873088
H	11.670326	4.606498	-3.581882
H	11.335259	2.676913	3.048759
H	10.198543	3.233267	1.830378
H	12.256505	4.886095	3.716887
H	13.633703	6.865008	3.082067
H	14.251579	7.184374	0.671732
H	13.451732	5.511849	-0.991783
H	10.163115	4.956613	-0.710150

Co(I)-BPY2H

Electronic+Thermal Energy= -2792.687640 a.u.

C	12.328031	5.734406	0.101803
N	11.995152	4.493865	0.505759
C	12.050980	4.208277	1.823903
C	12.475870	5.147567	2.758360
C	12.829636	6.423483	2.331652
C	12.745833	6.726566	0.974914
Co	11.492731	2.926672	-0.785906
N	10.395591	3.835882	-2.406617
C	9.075104	3.511079	-2.403388
C	8.196886	4.037228	-3.349781
C	8.672796	4.914351	-4.318169
C	10.023202	5.243729	-4.319944
C	10.840907	4.679937	-3.349201
C	8.638156	2.568436	-1.340376
N	9.626264	2.139620	-0.530447
C	9.385940	1.282596	0.470434
C	8.099271	0.817409	0.724682
C	7.064206	1.250169	-0.099247
C	7.329546	2.130799	-1.145960
C	10.615042	0.819622	1.225076
N	11.683337	1.841386	1.183941
C	11.533936	2.849630	2.248162
N	14.250226	3.857828	-2.743814
C	13.875684	2.678460	-3.365022
C	13.941350	2.670337	-4.776313
C	14.377178	3.774039	-5.471258

C	14.784184	4.946404	-4.777878
C	14.719687	4.950465	-3.415584
C	13.535124	1.564545	-2.525757
N	13.193426	1.840977	-1.212941
C	13.313333	0.820914	-0.299674
C	13.608176	-0.470197	-0.658922
C	13.773074	-0.783451	-2.029813
C	13.739510	0.231430	-2.954475
C	13.039118	1.243078	1.121060
H	10.366277	0.529048	2.251661
H	10.990067	-0.080515	0.727985
H	7.910786	0.130485	1.541525
H	6.050974	0.904959	0.071960
H	6.521614	2.464595	-1.782991
H	7.148725	3.769438	-3.339740
H	7.998133	5.330144	-5.057638
H	10.439483	5.921227	-5.055194
H	11.899755	4.906252	-3.327033
H	13.152832	0.410042	1.822307
H	13.754517	2.016778	1.410261
H	13.710936	-1.238117	0.098607
H	13.971536	-1.802666	-2.338890
H	13.955320	0.021726	-3.994706
H	13.632399	1.781957	-5.311444
H	14.420435	3.747150	-6.553643
H	15.152418	5.815570	-5.306192
H	15.030383	5.786376	-2.802120
H	12.006899	2.527968	3.183230
H	10.465722	2.957309	2.462071
H	12.519558	4.884737	3.809207
H	13.159357	7.169394	3.045876
H	12.995730	7.711962	0.601124
H	12.238132	5.931827	-0.960729
H	14.308227	3.827066	-1.732716

Co(II)-H

Electronic+Thermal Energy= -2792.949554 a.u.

C	12.795924	5.745543	0.630034
C	12.111447	4.527488	0.704329
N	11.505791	4.131734	1.839190
C	11.533639	4.946773	2.898066
C	12.173788	6.179886	2.899047
C	12.830511	6.578782	1.740128
C	11.955818	3.616268	-0.455326
N	11.286949	2.455556	-0.230228
C	10.999920	1.673453	-1.285580
C	11.433972	1.970492	-2.577595
C	12.180662	3.115763	-2.797360
C	12.422900	3.960677	-1.723499
Co	11.098851	1.953169	1.811371
N	9.307538	0.536275	0.085827
C	10.163523	0.430600	-1.067612
N	9.098746	2.103881	2.303821
C	8.895431	2.333754	3.623633
C	7.629777	2.634454	4.131531
C	6.546083	2.667129	3.265745
C	6.746396	2.340274	1.929125
C	8.032661	2.046770	1.484888

C	10.101115	2.188388	4.461330
N	11.231235	1.874104	3.774308
C	12.376510	1.729494	4.465938
C	12.449112	1.857534	5.845353
C	11.290888	2.164982	6.553803
C	10.106475	2.337025	5.850048
C	8.292199	1.566728	0.070921
N	11.160103	-0.547915	1.764592
C	10.169907	-1.363216	1.374839
C	10.232611	-2.747025	1.543963
C	11.358401	-3.307231	2.136205
C	12.398568	-2.465556	2.518503
C	12.252311	-1.099743	2.306956
C	8.959286	-0.715851	0.721089
H	7.340897	1.246100	-0.384509
H	8.653361	2.403893	-0.532261
H	5.913631	2.290776	1.236681
H	5.554722	2.904533	3.634891
H	7.485233	2.828077	5.186204
H	9.195806	2.583376	6.380454
H	11.308885	2.271815	7.632371
H	13.399045	1.721345	6.348158
H	13.253605	1.516244	3.872092
H	9.614976	0.210400	-1.999820
H	10.841819	-0.413208	-0.909719
H	11.176283	1.305497	-3.394288
H	12.541350	3.365437	-3.788810
H	12.956991	4.886764	-1.883104
H	13.302167	6.049367	-0.276147
H	13.358554	7.524795	1.697149
H	12.161326	6.801599	3.786433
H	11.025746	4.593382	3.788441
H	8.489960	-1.434497	0.028320
H	8.211280	-0.514985	1.494614
H	9.413557	-3.373463	1.205871
H	11.430092	-4.380128	2.278860
H	13.307966	-2.856652	2.959893
H	13.045623	-0.407022	2.562920
H	12.587746	1.791587	1.696528

Co(0)-BPY1H

Electronic+Thermal Energy= -2792.951681 a.u.

C	13.243403	5.366920	0.019807
N	12.466998	4.319379	0.353099
C	12.083660	4.180389	1.643371
C	12.462432	5.094075	2.620115
C	13.250893	6.186526	2.265330
C	13.651659	6.323262	0.938340
Co	11.926645	2.771366	-0.950268
N	9.938993	5.171140	-1.678990
C	9.089942	4.305030	-2.374572
C	8.462292	4.844987	-3.519201
C	8.661576	6.147785	-3.905556
C	9.514350	6.998468	-3.133488
C	10.120817	6.484534	-2.032848
C	8.915854	2.976407	-1.871509
N	9.807407	2.519994	-0.918396
C	9.504120	1.384667	-0.245062

C	8.381314	0.623798	-0.514417
C	7.539100	1.015655	-1.569042
C	7.802094	2.185244	-2.240916
C	10.481191	0.904610	0.819708
N	11.567800	1.852133	1.075407
C	11.209954	2.976361	1.946197
N	12.727703	2.991015	-2.842223
C	13.676152	2.032257	-3.133511
C	14.283440	1.980288	-4.398881
C	13.953496	2.906649	-5.367253
C	13.003551	3.894694	-5.060732
C	12.427265	3.889404	-3.807911
C	13.998232	1.124788	-2.044992
N	13.365759	1.430464	-0.873529
C	13.560634	0.670689	0.228518
C	14.388904	-0.428870	0.219484
C	15.058416	-0.757505	-0.979849
C	14.861894	0.017424	-2.106447
C	12.835191	1.190343	1.455837
H	9.931378	0.649146	1.736952
H	10.936730	-0.025226	0.467594
H	8.175975	-0.270435	0.062836
H	6.671438	0.419431	-1.828207
H	7.120494	2.530910	-3.007191
H	7.826208	4.203338	-4.114865
H	8.173589	6.531539	-4.793097
H	9.677476	8.031990	-3.408617
H	10.775502	7.055869	-1.387494
H	12.673877	0.394751	2.193805
H	13.468224	1.942536	1.934901
H	14.528201	-1.025262	1.114296
H	15.715809	-1.618318	-1.017309
H	15.362097	-0.239967	-3.031981
H	15.022236	1.217195	-4.610840
H	14.422878	2.872444	-6.343780
H	12.713473	4.644269	-5.787042
H	11.676372	4.625352	-3.547318
H	11.269487	2.719664	3.012704
H	10.167433	3.237328	1.742248
H	12.149152	4.947917	3.647933
H	13.558594	6.907839	3.013913
H	14.281942	7.145385	0.621051
H	13.550308	5.412430	-1.019341
H	10.323681	4.840118	-0.806696

Co(0)-BPY2H

Electronic+Thermal Energy= -2792.948767 a.u.

C	12.162232	5.720110	0.035421
N	11.878331	4.474651	0.458212
C	12.041243	4.188742	1.767697
C	12.531006	5.128294	2.668252
C	12.840979	6.409790	2.220320
C	12.640911	6.714359	0.876590
Co	11.433627	2.886499	-0.825184
N	10.399515	3.765341	-2.384084
C	9.044610	3.502229	-2.360413
C	8.179010	4.074684	-3.306228
C	8.668481	4.925679	-4.276360

C	10.046273	5.198961	-4.295240
C	10.850782	4.601542	-3.348794
C	8.603554	2.610649	-1.302954
N	9.614376	2.175914	-0.495345
C	9.355738	1.325487	0.522740
C	8.076818	0.909672	0.822302
C	7.016776	1.357888	0.006585
C	7.282918	2.194832	-1.059505
C	10.600775	0.807013	1.213310
N	11.689164	1.805827	1.175535
C	11.560510	2.825004	2.222581
N	14.180764	3.875973	-2.710763
C	13.958918	2.665194	-3.366071
C	14.148755	2.669656	-4.764537
C	14.555718	3.802344	-5.427493
C	14.807892	5.005176	-4.698497
C	14.623607	5.002580	-3.351622
C	13.616031	1.540433	-2.551753
N	13.230778	1.803793	-1.252838
C	13.302782	0.784769	-0.347163
C	13.594261	-0.512701	-0.699750
C	13.808537	-0.814275	-2.064964
C	13.827924	0.206669	-2.981699
C	13.027505	1.199023	1.081237
H	10.386800	0.473121	2.236547
H	10.948638	-0.070894	0.660018
H	7.893360	0.237926	1.653422
H	6.000745	1.040770	0.211210
H	6.473696	2.530535	-1.695970
H	7.120466	3.848056	-3.272825
H	8.003029	5.369600	-5.007754
H	10.481907	5.855340	-5.039107
H	11.919572	4.774574	-3.356264
H	13.149690	0.353608	1.769859
H	13.757113	1.961500	1.367077
H	13.650182	-1.286974	0.056143
H	13.999021	-1.834810	-2.376804
H	14.074205	0.001534	-4.016116
H	13.952955	1.761786	-5.320598
H	14.689085	3.783948	-6.502246
H	15.145241	5.904498	-5.196384
H	14.801128	5.863954	-2.720479
H	12.061781	2.528523	3.153233
H	10.496469	2.922135	2.459155
H	12.658517	4.860966	3.711474
H	13.221912	7.156170	2.908186
H	12.845950	7.703931	0.485776
H	11.972698	5.916560	-1.014306
H	14.143441	3.844096	-1.700736

Co(II)-H

Electronic+Thermal Energy= -2792.949554 a.u.

C	12.795924	5.745543	0.630034
C	12.111447	4.527488	0.704329
N	11.505791	4.131734	1.839190
C	11.533639	4.946773	2.898066
C	12.173788	6.179886	2.899047
C	12.830511	6.578782	1.740128

C	11.955818	3.616268	-0.455326
N	11.286949	2.455556	-0.230228
C	10.999920	1.673453	-1.285580
C	11.433972	1.970492	-2.577595
C	12.180662	3.115763	-2.797360
C	12.422900	3.960677	-1.723499
Co	11.098851	1.953169	1.811371
N	9.307538	0.536275	0.085827
C	10.163523	0.430600	-1.067612
N	9.098746	2.103881	2.303821
C	8.895431	2.333754	3.623633
C	7.629777	2.634454	4.131531
C	6.546083	2.667129	3.265745
C	6.746396	2.340274	1.929125
C	8.032661	2.046770	1.484888
C	10.101115	2.188388	4.461330
N	11.231235	1.874104	3.774308
C	12.376510	1.729494	4.465938
C	12.449112	1.857534	5.845353
C	11.290888	2.164982	6.553803
C	10.106475	2.337025	5.850048
C	8.292199	1.566728	0.070921
N	11.160103	-0.547915	1.764592
C	10.169907	-1.363216	1.374839
C	10.232611	-2.747025	1.543963
C	11.358401	-3.307231	2.136205
C	12.398568	-2.465556	2.518503
C	12.252311	-1.099743	2.306956
C	8.959286	-0.715851	0.721089
H	7.340897	1.246100	-0.384509
H	8.653361	2.403893	-0.532261
H	5.913631	2.290776	1.236681
H	5.554722	2.904533	3.634891
H	7.485233	2.828077	5.186204
H	9.195806	2.583376	6.380454
H	11.308885	2.271815	7.632371
H	13.399045	1.721345	6.348158
H	13.253605	1.516244	3.872092
H	9.614976	0.210400	-1.999820
H	10.841819	-0.413208	-0.909719
H	11.176283	1.305497	-3.394288
H	12.541350	3.365437	-3.788810
H	12.956991	4.886764	-1.883104
H	13.302167	6.049367	-0.276147
H	13.358554	7.524795	1.697149
H	12.161326	6.801599	3.786433
H	11.025746	4.593382	3.788441
H	8.489960	-1.434497	0.028320
H	8.211280	-0.514985	1.494614
H	9.413557	-3.373463	1.205871
H	11.430092	-4.380128	2.278860
H	13.307966	-2.856652	2.959893
H	13.045623	-0.407022	2.562920
H	12.587746	1.791587	1.696528

Co(II)-H-PYH
E(UB3LYP) = -2793.96321321 Hartree
Solvent: acetonitrile

C	12.401273	6.052305	0.591628

C	12.011152	4.718160	0.745256
N	11.762312	4.188342	1.959867
C	11.919373	4.966388	3.037558
C	12.315821	6.296224	2.969917
C	12.554829	6.850583	1.717312
C	11.846649	3.795914	-0.399187
N	11.267034	2.598111	-0.130024
C	11.062827	1.737961	-1.144940
C	11.446364	2.021066	-2.451897
C	12.074693	3.227223	-2.724970
C	12.268248	4.127264	-1.687178
Co	11.016510	2.114350	1.826097
N	9.587652	0.537958	0.392660
C	10.387806	0.425076	-0.829161
N	9.074864	2.402766	2.294544
C	8.840864	2.693168	3.592979
C	7.550044	2.934808	4.060176
C	6.485507	2.782381	3.178393
C	6.728520	2.305735	1.892454
C	8.044945	2.103624	1.490275
C	10.036327	2.534058	4.437108
N	11.099950	1.985540	3.782545
C	12.214118	1.717971	4.486305
C	12.318526	1.962154	5.849125
C	11.237587	2.529139	6.517303
C	10.083692	2.820283	5.799744
C	8.434074	1.454963	0.187061
N	11.426326	-1.154473	1.798886
C	10.251965	-1.669470	1.378227
C	10.090896	-3.048677	1.423441
C	11.118176	-3.853280	1.904060
C	12.317128	-3.277591	2.325431
C	12.447308	-1.907374	2.254721
C	9.142131	-0.755790	0.912015
H	7.578384	0.930386	-0.252424
H	8.729652	2.223075	-0.527560
H	5.912202	2.068382	1.221195
H	5.470892	2.962225	3.513445
H	7.369723	3.187856	5.096573
H	9.232139	3.270595	6.292678
H	11.290620	2.743912	7.577869
H	13.237444	1.717045	6.366450
H	13.039036	1.304968	3.924384
H	9.786737	0.103345	-1.689843
H	11.156110	-0.339583	-0.687928
H	11.251095	1.299978	-3.236494
H	12.398455	3.469440	-3.730216
H	12.751955	5.073973	-1.881604
H	12.572653	6.473747	-0.389101
H	12.854320	7.887076	1.614795
H	12.425777	6.875826	3.878133
H	11.720091	4.509130	3.998091
H	8.540122	-1.309340	0.178742
H	8.489055	-0.569791	1.770717
H	9.161660	-3.483900	1.079488
H	10.988158	-4.928047	1.940736
H	13.137885	-3.877784	2.693316
H	13.341128	-1.372142	2.542491
H	12.372112	1.405032	1.677324
H	11.580632	-0.125060	1.763091

TS [Co(II)-H-PYH → Co(II)-PY + H_2]
E(UB3LYP) = -2793.95153570 Hartree
Solvent: acetonitrile

C	12.404885	5.968394	0.662198
C	12.003112	4.635493	0.779909
N	11.837801	4.046964	1.982922
C	12.107180	4.761850	3.081654
C	12.528223	6.085791	3.048088
C	12.667794	6.703443	1.810977
C	11.756539	3.768248	-0.391472
N	11.187318	2.564659	-0.137084
C	10.962627	1.717202	-1.157340
C	11.293159	2.033803	-2.470518
C	11.884733	3.260132	-2.737681
C	12.116346	4.137439	-1.687297
Co	10.917329	2.033733	1.802223
N	9.561874	0.530809	0.427529
C	10.334401	0.390937	-0.810047
N	9.019876	2.445154	2.230555
C	8.784640	2.821260	3.507994
C	7.508872	3.185607	3.926014
C	6.454640	3.052589	3.025438
C	6.685924	2.468190	1.784257
C	7.993534	2.149812	1.424648
C	9.940173	2.569956	4.384069
N	10.955807	1.905628	3.762415
C	12.010740	1.509810	4.491889
C	12.103618	1.742034	5.858011
C	11.078327	2.435125	6.493313
C	9.983493	2.854369	5.745815
C	8.358794	1.370536	0.186508
N	11.603836	-1.017314	1.730361
C	10.417836	-1.593194	1.466123
C	10.275581	-2.974882	1.587050
C	11.358732	-3.746358	1.992751
C	12.579585	-3.128311	2.253768
C	12.659588	-1.754188	2.103826
C	9.223299	-0.748194	1.060428
H	7.506815	0.764909	-0.141135
H	8.576135	2.061580	-0.629036
H	5.866530	2.233619	1.115856
H	5.449234	3.326019	3.322535
H	7.325119	3.511197	4.941363
H	9.173065	3.395061	6.216471
H	11.126847	2.645899	7.554758
H	12.971388	1.391164	6.401468
H	12.799506	0.999777	3.957951
H	9.723380	0.030417	-1.646822
H	11.126355	-0.345179	-0.660045
H	11.084496	1.325373	-3.262824
H	12.160128	3.532875	-3.749471
H	12.585550	5.092133	-1.877937
H	12.505008	6.435630	-0.307602
H	12.978305	7.739015	1.737187
H	12.732101	6.611863	3.972320
H	11.985818	4.258093	4.031152

H	8.578254	-1.358666	0.414373
H	8.640491	-0.527664	1.960396
H	9.322301	-3.437622	1.361481
H	11.253646	-4.820373	2.092444
H	13.450042	-3.694747	2.558728
H	13.582048	-1.210139	2.275287
H	12.309554	1.226356	1.644298
H	11.881197	0.344088	1.669590

Co(II)-PY + H_2
E(UB3LYP) = -2793.96959124 Hartree
Solvent: acetonitrile

C	1.720226	4.028810	-1.137239
C	1.327598	2.694940	-1.052994
N	1.161955	2.073137	0.142307
C	1.427056	2.767542	1.259764
C	1.839574	4.093549	1.249568
C	1.975857	4.740550	0.028270
C	1.084647	1.847309	-2.231868
N	0.538273	0.637869	-1.957011
C	0.307017	-0.231197	-2.957238
C	0.613168	0.083059	-4.278694
C	1.172984	1.319250	-4.567508
C	1.410029	2.216705	-3.532451
Co	0.293503	0.212445	-0.028357
N	-1.084576	-1.388016	-1.345375
C	-0.297322	-1.553747	-2.571106
N	-1.694955	0.422226	0.469790
C	-1.919289	0.824121	1.733939
C	-3.189857	1.220695	2.138730
C	-4.236686	1.102535	1.224117
C	-4.009868	0.520544	-0.019753
C	-2.703738	0.172136	-0.360253
C	-0.747158	0.593066	2.603513
N	0.305975	0.018028	1.962079
C	1.370981	-0.375694	2.672032
C	1.447988	-0.210646	4.050238
C	0.391309	0.410558	4.708286
C	-0.722146	0.813263	3.977166
C	-2.297670	-0.571852	-1.609614
N	0.871454	-2.908859	0.042151
C	-0.269778	-3.522813	-0.298324
C	-0.417399	-4.912154	-0.251935
C	0.653272	-5.693143	0.167239
C	1.846083	-5.061879	0.509302
C	1.902945	-3.674200	0.426126
C	-1.449627	-2.667711	-0.716846
H	-3.127611	-1.189182	-1.971178
H	-2.076937	0.145136	-2.402403
H	-4.827507	0.320368	-0.701480
H	-5.238108	1.401982	1.510000
H	-3.378665	1.572173	3.144625
H	-1.562105	1.282053	4.472411
H	0.426589	0.572926	5.778822
H	2.325588	-0.551433	4.584131
H	2.180330	-0.823838	2.110012
H	-0.889038	-1.959316	-3.401689

H	0.509835	-2.261089	-2.372761
H	0.405909	-0.634910	-5.062338
H	1.421056	1.586347	-5.587730
H	1.854401	3.179842	-3.740257
H	1.820540	4.512435	-2.099076
H	2.279619	5.779246	-0.021285
H	2.039191	4.597903	2.186212
H	1.308786	2.248162	2.198103
H	-2.099966	-3.253857	-1.380499
H	-2.044154	-2.434180	0.171938
H	-1.356154	-5.369926	-0.543735
H	0.561859	-6.772730	0.213777
H	2.714162	-5.626004	0.829310
H	2.818563	-3.148341	0.680227
H	3.538719	-0.464696	-0.575899
H	3.108109	-1.061711	-0.678663

Co(0)-H-BPY1H
E(UB3LYP) = -2793.95999103 Hartree
Solvent: acetonitrile

C	11.467978	6.208640	0.803643
N	11.365409	4.874580	0.840610
C	11.649856	4.241333	1.989736
C	12.065223	4.918244	3.131873
C	12.166636	6.306379	3.088797
C	11.852523	6.965776	1.904459
Co	11.335457	3.497215	-0.833417
N	10.295752	4.617246	-2.059910
C	8.961092	4.324374	-2.092812
C	8.055496	5.120101	-2.787654
C	8.513930	6.246935	-3.461384
C	9.870470	6.550192	-3.417365
C	10.722218	5.714144	-2.705950
C	8.601188	3.100536	-1.355637
N	9.650430	2.587788	-0.680283
C	9.571036	1.410917	-0.046503
C	8.368437	0.715253	0.012223
C	7.257578	1.255684	-0.634447
C	7.369691	2.451392	-1.341408
C	10.897850	0.923314	0.482048
N	11.813416	2.085094	0.709294
C	11.379839	2.761300	1.977447
N	13.722943	2.960778	-3.621243
C	14.272636	1.729898	-3.761682
C	14.750760	1.364736	-5.015726
C	14.659950	2.259479	-6.076840
C	14.093688	3.519004	-5.885054
C	13.625278	3.844397	-4.627371
C	14.322618	0.902806	-2.535856
N	13.769293	1.486180	-1.468333
C	13.790618	0.867563	-0.292116
C	14.365892	-0.399502	-0.142467
C	14.935938	-1.012670	-1.253157
C	14.923617	-0.355934	-2.479643
C	13.217610	1.616357	0.889168
H	10.784816	0.323135	1.390561
H	11.346214	0.280004	-0.278152

H	8.302844	-0.227698	0.540779
H	6.307504	0.735645	-0.603831
H	6.518626	2.852491	-1.875934
H	7.002744	4.868751	-2.795056
H	7.821298	6.877407	-4.005928
H	10.272856	7.419759	-3.921480
H	11.781393	5.917421	-2.634149
H	13.280152	0.981237	1.779079
H	13.824254	2.504824	1.075300
H	14.367683	-0.891611	0.822648
H	15.389555	-1.992832	-1.165889
H	15.373900	-0.815746	-3.349410
H	15.191748	0.389451	-5.164739
H	15.033231	1.973361	-7.052635
H	14.014073	4.235623	-6.690787
H	13.172036	4.794923	-4.388143
H	11.826450	2.265865	2.843289
H	10.299013	2.633075	2.064561
H	12.298943	4.369091	4.036507
H	12.486438	6.860926	3.963677
H	11.913233	8.044398	1.825417
H	11.235487	6.683124	-0.142906
H	13.351373	3.214010	-2.683533
H	12.711837	4.082386	-1.265924

TS [Co(0)-H-BPY1H → Co(0)-BPY1 + H_2]
E(UB3LYP) = -2793.94709047 Hartree
Solvent: acetonitrile

C	11.688749	6.124711	0.475025
N	11.505665	4.807678	0.636261
C	11.771552	4.261950	1.834975
C	12.243824	5.014100	2.905396
C	12.426671	6.383471	2.734116
C	12.135941	6.951805	1.497832
Co	11.236536	3.315791	-0.892019
N	10.155719	4.386836	-2.128021
C	8.818010	4.121727	-2.074458
C	7.896456	4.877856	-2.789912
C	8.345998	5.931278	-3.579263
C	9.708443	6.200343	-3.630097
C	10.575536	5.407534	-2.888750
C	8.476592	2.970118	-1.225494
N	9.556281	2.464843	-0.591305
C	9.479796	1.351654	0.148484
C	8.260188	0.714044	0.348278
C	7.126624	1.244300	-0.262686
C	7.229148	2.375647	-1.070169
C	10.814990	0.865459	0.640100
N	11.771156	2.013455	0.729569
C	11.423010	2.804232	1.958292
N	13.868635	3.239703	-3.408636
C	14.398283	2.018384	-3.644133
C	15.060513	1.762827	-4.845274
C	15.182531	2.774568	-5.792069
C	14.647715	4.029788	-5.522338
C	13.993480	4.215180	-4.311827
C	14.268439	1.025345	-2.547626

N	13.825710	1.540992	-1.399806
C	13.672802	0.765902	-0.331621
C	13.982050	-0.595567	-0.355512
C	14.446829	-1.142998	-1.549872
C	14.589555	-0.331324	-2.670498
C	13.164952	1.484913	0.894102
H	10.736205	0.342902	1.597947
H	11.207167	0.152574	-0.088771
H	8.201655	-0.176786	0.960897
H	6.163279	0.769011	-0.122494
H	6.355537	2.772088	-1.569852
H	6.839981	4.651946	-2.729313
H	7.640695	6.530252	-4.142447
H	10.105068	7.009843	-4.229141
H	11.640023	5.587267	-2.893834
H	13.197114	0.829907	1.770561
H	13.807798	2.343635	1.091539
H	13.859034	-1.210568	0.528249
H	14.690467	-2.197475	-1.609197
H	14.935342	-0.753903	-3.605056
H	15.493988	0.790255	-5.035916
H	15.699895	2.584303	-6.725085
H	14.731448	4.847975	-6.225969
H	13.559752	5.172646	-4.048237
H	11.885391	2.353211	2.839180
H	10.342366	2.739497	2.101047
H	12.459777	4.536775	3.853784
H	12.792492	6.994010	3.551632
H	12.261628	8.012594	1.319716
H	11.469058	6.526205	-0.507097
H	13.114390	3.541450	-2.268782
H	12.652117	3.912393	-1.528041

Co(0)-BPY1 + H_2
E(UB3LYP) = -2793.95477821 Hartree
Solvent: acetonitrile

C	0.003430	3.096840	1.703029
N	-0.174601	1.778558	1.867135
C	0.121898	1.224412	3.055577
C	0.620495	1.972979	4.115195
C	0.804295	3.342291	3.940706
C	0.483132	3.917376	2.715223
Co	-0.406939	0.259345	0.361471
N	-1.440943	1.333327	-0.922351
C	-2.781709	1.076940	-0.890168
C	-3.685970	1.838416	-1.619490
C	-3.213603	2.882871	-2.408326
C	-1.846811	3.129136	-2.453424
C	-0.995397	2.332707	-1.695681
C	-3.142324	-0.074869	-0.050488
N	-2.071615	-0.594349	0.585559
C	-2.153329	-1.703135	1.331469
C	-3.377283	-2.332726	1.525219
C	-4.503372	-1.793872	0.907648
C	-4.393044	-0.661388	0.101768
C	-0.818616	-2.176655	1.832117
N	0.122762	-1.010037	1.919649

C	-0.212569	-0.237914	3.169087
N	2.254640	0.212992	-2.336915
C	2.787274	-1.005794	-2.536929
C	3.481804	-1.315314	-3.710982
C	3.631630	-0.336002	-4.688378
C	3.093182	0.926650	-4.469726
C	2.412068	1.144739	-3.274941
C	2.631547	-1.979554	-1.414343
N	2.157382	-1.466184	-0.274295
C	2.025583	-2.235210	0.805270
C	2.359315	-3.589660	0.803046
C	2.837992	-4.141269	-0.383832
C	2.978800	-3.334943	-1.506905
C	1.532075	-1.517908	2.039772
H	-0.890500	-2.692630	2.792824
H	-0.412231	-2.885479	1.107583
H	-3.445553	-3.222209	2.138336
H	-5.470255	-2.262824	1.043938
H	-5.263473	-0.257644	-0.397348
H	-4.745167	1.622577	-1.572232
H	-3.905195	3.489043	-2.980603
H	-1.433844	3.924507	-3.060034
H	0.073603	2.491852	-1.704275
H	1.592289	-2.170785	2.915116
H	2.167103	-0.650792	2.224884
H	2.246943	-4.194088	1.695462
H	3.100199	-5.192032	-0.432404
H	3.348180	-3.761501	-2.430338
H	3.916642	-2.294520	-3.863982
H	4.170821	-0.557890	-5.602458
H	3.195002	1.722323	-5.197992
H	1.978678	2.118713	-3.064742
H	0.271559	-0.698699	4.032002
H	-1.289983	-0.317050	3.327298
H	0.860589	1.493624	5.056418
H	1.195315	3.948489	4.749530
H	0.609636	4.977860	2.537256
H	-0.242713	3.501971	0.728589
H	1.250280	0.538723	-0.451101
H	1.074702	1.106617	0.047938

Co(0)-H-BPY2H
E(UB3LYP) = -2793.96166718 Hartree
Solvent: acetonitrile

C	14.177509	5.032239	0.211693
N	13.156913	4.167500	0.283071
C	12.332411	4.217025	1.344756
C	12.508329	5.142291	2.369649
C	13.560500	6.049494	2.284850
C	14.414152	5.993543	1.186280
Co	12.455697	2.818807	-1.212645
N	9.270861	5.031140	-2.201036
C	8.053673	4.439249	-2.196137
C	6.966591	5.168560	-2.667941
C	7.155909	6.469976	-3.121026
C	8.427824	7.042313	-3.102393
C	9.482472	6.284090	-2.632099

C	8.009374	3.062098	-1.662641
N	9.089052	2.721308	-0.938822
C	9.181969	1.497638	-0.443899
C	8.168788	0.544373	-0.641471
C	7.050883	0.897370	-1.380333
C	6.959762	2.183745	-1.912602
C	10.387521	1.092259	0.379620
N	11.529153	2.036666	0.524217
C	11.184940	3.228378	1.343462
N	13.493102	2.974715	-2.869947
C	14.420570	1.986095	-3.046820
C	15.217812	1.929014	-4.185167
C	15.070343	2.901985	-5.168357
C	14.126511	3.907016	-4.985906
C	13.357943	3.904797	-3.828277
C	14.489166	1.029459	-1.927361
N	13.637993	1.354050	-0.933726
C	13.549023	0.631257	0.188399
C	14.323917	-0.510170	0.359484
C	15.205521	-0.870779	-0.660145
C	15.301317	-0.096387	-1.814668
C	12.626622	1.251002	1.204994
H	10.032934	0.811139	1.380377
H	10.793206	0.179061	-0.062622
H	8.262954	-0.451296	-0.222924
H	6.257845	0.179332	-1.552889
H	6.106937	2.469827	-2.514625
H	5.978254	4.730632	-2.662527
H	6.308602	7.040601	-3.481438
H	8.600325	8.053283	-3.444998
H	10.503752	6.636455	-2.585176
H	12.208846	0.512536	1.893206
H	13.216979	1.942782	1.807366
H	14.246601	-1.099954	1.264498
H	15.820308	-1.756774	-0.554892
H	15.987837	-0.373413	-2.604021
H	15.947568	1.138331	-4.302578
H	15.683989	2.873201	-6.060865
H	13.977971	4.683628	-5.725540
H	12.607589	4.660800	-3.645400
H	10.921208	2.943692	2.368665
H	10.310851	3.689831	0.883797
H	11.833594	5.149599	3.218051
H	13.715687	6.782474	3.068384
H	15.249929	6.675192	1.085407
H	14.816680	4.944427	-0.659979
H	10.096971	4.471765	-1.870283
H	11.474428	3.961452	-1.595760

TS [Co(0)-H-BPY2H → Co(0)-BPY2 + H_2]
E(UB3LYP) = -2793.95128913 Hartree
Solvent: acetonitrile

C	14.147447	5.035382	0.296984
N	13.124893	4.172210	0.363432
C	12.317853	4.192677	1.440135
C	12.513979	5.087232	2.487557
C	13.569025	5.991742	2.409636

C	14.404606	5.965041	1.296287
Co	12.377195	2.825350	-1.143812
N	9.448182	4.942295	-2.313350
C	8.226806	4.373645	-2.323868
C	7.140821	5.059819	-2.872902
C	7.332432	6.329197	-3.407833
C	8.601799	6.899145	-3.382621
C	9.635745	6.162521	-2.819974
C	8.121866	3.027845	-1.705765
N	9.180500	2.662456	-0.961504
C	9.184534	1.478943	-0.368407
C	8.111120	0.583509	-0.475270
C	7.020512	0.952255	-1.247456
C	7.019265	2.193440	-1.882282
C	10.391597	1.062243	0.443375
N	11.523957	2.025152	0.583415
C	11.175330	3.197775	1.431916
N	13.376722	3.060548	-2.820391
C	14.272207	2.060116	-3.070298
C	15.018150	2.026823	-4.242069
C	14.850337	3.038645	-5.182582
C	13.941784	4.057814	-4.923192
C	13.223842	4.029948	-3.733596
C	14.375710	1.074489	-1.981327
N	13.552999	1.366855	-0.953487
C	13.525887	0.638668	0.168584
C	14.327112	-0.490349	0.295492
C	15.167832	-0.827654	-0.763980
C	15.207483	-0.038271	-1.912301
C	12.644857	1.241029	1.227073
H	10.058039	0.768833	1.446054
H	10.805645	0.160545	-0.014630
H	8.138953	-0.376322	0.028174
H	6.177105	0.281154	-1.362512
H	6.181443	2.482686	-2.503014
H	6.152312	4.620445	-2.868289
H	6.494300	6.870108	-3.831537
H	8.789675	7.887414	-3.782452
H	10.646260	6.553844	-2.763778
H	12.251072	0.495491	1.920454
H	13.255147	1.928915	1.813562
H	14.298617	-1.086122	1.198998
H	15.800547	-1.704199	-0.693872
H	15.871558	-0.290865	-2.728152
H	15.722929	1.225142	-4.419457
H	15.423656	3.028151	-6.101677
H	13.781710	4.865857	-5.625316
H	12.507011	4.801716	-3.494161
H	10.926043	2.885448	2.451345
H	10.289747	3.658273	0.992358
H	11.854603	5.072843	3.347544
H	13.740999	6.700747	3.211361
H	15.241352	6.646101	1.201985
H	14.771364	4.971389	-0.587404
H	10.627620	4.306642	-1.774501
H	11.443878	4.147952	-1.446415

Co(0)-BPY2 + H_2

E(UB3LYP) = -2793.95189524 Hartree
Solvent: acetonitrile

C	2.425142	2.034447	1.478806
N	1.402285	1.171347	1.545966
C	0.594817	1.191468	2.622641
C	0.791125	2.085758	3.669868
C	1.846212	2.990096	3.591597
C	2.682002	2.963484	2.478399
Co	0.656238	-0.180072	0.039958
N	-2.278905	1.941156	-1.135162
C	-3.498246	1.377455	-1.145114
C	-4.587623	2.060062	-1.692468
C	-4.394667	3.329737	-2.227625
C	-3.125719	3.900093	-2.202736
C	-2.093307	3.159731	-1.639745
C	-3.599976	0.029014	-0.525161
N	-2.540387	-0.338434	0.218862
C	-2.538595	-1.522257	0.812621
C	-3.611322	-2.418005	0.706948
C	-4.701746	-2.048817	-0.065640
C	-4.702145	-0.807402	-0.699620
C	-1.331010	-1.939449	1.623734
N	-0.197485	-0.975375	1.763698
C	-0.547530	0.196702	2.613639
N	1.654774	0.059575	-1.638389
C	2.549617	-0.941268	-1.888504
C	3.295337	-0.974333	-3.059994
C	3.127305	0.037885	-4.000215
C	2.218441	1.056606	-3.740969
C	1.500434	1.029031	-2.551150
C	2.652708	-1.926876	-0.800151
N	1.829140	-1.635825	0.227579
C	1.802762	-2.362564	1.350763
C	2.604526	-3.491254	1.477395
C	3.444849	-3.828521	0.417934
C	3.484703	-3.039014	-0.730411
C	0.922618	-1.760204	2.409004
H	-1.662145	-2.231015	2.627446
H	-0.916282	-2.841074	1.166477
H	-3.583138	-3.377933	1.210227
H	-5.545137	-2.719989	-0.181299
H	-5.540137	-0.517369	-1.319906
H	-5.577254	1.622337	-1.688506
H	-5.232876	3.870781	-2.651495
H	-2.939043	4.888871	-2.602900
H	-1.082714	3.554331	-1.585729
H	0.527122	-2.505248	3.101567
H	1.533155	-1.072992	2.996021
H	2.576105	-4.086624	2.381061
H	4.077729	-4.704891	0.487996
H	4.149378	-3.290893	-1.545898
H	4.000097	-1.775892	-3.237566
H	3.700864	0.027857	-4.919112
H	2.058139	1.864658	-4.442919
H	0.782895	1.801153	-2.313553
H	-0.796256	-0.117905	3.632173
H	-1.434460	0.656009	2.175387
H	0.131699	2.071434	4.529721
H	2.018045	3.699155	4.393244

H	3.518557	3.644665	2.384248
H	3.048712	1.970962	0.594323
H	-0.957566	1.242143	-0.521729
H	-0.194959	1.224043	-0.219649

TS_1 [Co(I) → Co(I) decoordination of BPY1]
E(UB3LYP) = -2792.94571625 Hartree
Solvent: acetonitrile

C	7.167172	3.012470	3.945438
C	8.473879	2.609220	3.584337
N	8.719036	2.166992	2.302440
C	7.683666	1.941884	1.466561
C	6.382898	2.262489	1.788515
C	6.132825	2.858422	3.050450
C	9.597866	2.497984	4.468679
N	10.728927	1.930633	3.906006
C	11.760977	1.641970	4.727003
C	11.781060	1.920066	6.076458
C	10.655403	2.562663	6.643984
C	9.575268	2.843567	5.840096
Co	10.639638	1.675257	1.808044
N	11.406548	-0.317588	1.789285
C	10.515282	-1.262559	1.429782
C	10.831162	-2.616722	1.466824
C	12.103533	-3.005687	1.875662
C	13.032139	-2.026041	2.214556
C	12.640599	-0.695370	2.154654
C	9.163685	-0.755277	0.969505
N	9.330617	0.541601	0.298072
C	8.082419	1.316107	0.150462
N	11.246383	2.413367	-0.161386
C	11.998353	3.519932	-0.359020
C	12.347920	3.948225	-1.642092
C	11.902302	3.234888	-2.745557
C	11.127069	2.101121	-2.539993
C	10.830583	1.716161	-1.236334
C	12.480757	4.242843	0.841236
N	12.616465	3.511001	1.961528
C	13.119988	4.114900	3.044047
C	13.494258	5.454480	3.076969
C	13.314148	6.218925	1.928441
C	12.799826	5.605447	0.793493
C	10.058574	0.445567	-0.969148
H	7.269417	0.704237	-0.258500
H	8.277709	2.108846	-0.577123
H	5.576683	2.061360	1.092690
H	5.125157	3.151067	3.324445
H	6.972382	3.407669	4.935234
H	8.696177	3.317349	6.260804
H	10.638240	2.819160	7.697579
H	12.645377	1.656780	6.674109
H	12.614766	1.164544	4.259031
H	9.394541	0.212935	-1.809834
H	10.775136	-0.377030	-0.904861

H	10.758389	1.514704	-3.373111
H	12.162579	3.553985	-3.748199
H	12.980258	4.815590	-1.774649
H	12.631361	6.182640	-0.106567
H	13.565343	7.273487	1.915229
H	13.903227	5.882552	3.984385
H	13.225216	3.499633	3.929503
H	8.672771	-1.499335	0.329970
H	8.520690	-0.600456	1.840138
H	10.093922	-3.351905	1.166463
H	12.370391	-4.055789	1.910420
H	14.040827	-2.281330	2.514757
H	13.332447	0.104193	2.391785

TS_2 [Co(I) → Co(I) decoordination of BPY1]
E(UB3LYP) = -2792.94571625 Hartree
Solvent: acetonitrile

C	7.396473	2.997557	3.852373
C	8.685331	2.584001	3.449010
N	8.859774	2.046935	2.197427
C	7.805733	1.873273	1.370367
C	6.525856	2.234391	1.727615
C	6.326820	2.825974	3.000189
C	9.888566	2.624288	4.241649
N	11.031256	2.150788	3.611635
C	12.179256	2.118216	4.329950
C	12.280360	2.520654	5.642242
C	11.124565	3.019677	6.284148
C	9.942746	3.070920	5.578492
Co	10.689721	1.414540	1.725802
N	11.088558	-0.653396	1.965064
C	10.256599	-1.511272	1.340905
C	10.458346	-2.887116	1.378167
C	11.544060	-3.396189	2.083742
C	12.401035	-2.510111	2.729620
C	12.136886	-1.150663	2.642315
C	9.061262	-0.896591	0.648313
N	9.377448	0.441063	0.133581
C	8.181332	1.302554	0.016825
N	11.348318	2.326413	-0.092026
C	12.038701	3.481253	-0.183952
C	12.368597	4.046829	-1.414298
C	11.978212	3.407654	-2.584126
C	11.257852	2.223642	-2.489310
C	10.961924	1.710874	-1.231912
C	12.466117	4.184796	1.068476
N	13.604860	3.758347	1.631073
C	14.067770	4.441866	2.683729
C	13.432694	5.561170	3.216304
C	12.244688	5.987659	2.632023
C	11.751515	5.290182	1.532814
C	10.200537	0.413683	-1.078158
H	7.339888	0.770964	-0.442239
H	8.433730	2.131257	-0.650099
H	5.695949	2.074242	1.049039

H	5.332702	3.132796	3.305910
H	7.243142	3.437798	4.830372
H	9.044635	3.445682	6.054973
H	11.164841	3.355315	7.314420
H	13.232777	2.464241	6.155491
H	13.052919	1.761611	3.795738
H	9.614235	0.204155	-1.981235
H	10.924143	-0.400600	-0.975696
H	10.918719	1.702666	-3.376598
H	12.221877	3.830783	-3.551909
H	12.922450	4.976828	-1.443637
H	10.835409	5.596440	1.041251
H	11.713628	6.850633	3.018399
H	13.860488	6.078266	4.067251
H	14.993874	4.076281	3.118563
H	8.681140	-1.563558	-0.135048
H	8.261395	-0.786566	1.386243
H	9.773182	-3.546591	0.858533
H	11.720051	-4.465081	2.123477
H	13.260554	-2.859081	3.288295
H	12.778739	-0.428509	3.131139

TS [Co(I) → Co(I) decoordination of BPY2]
E(UB3LYP) = -2792.94571625 Hartree
Solvent: acetonitrile

C	7.235607	1.934239	4.300208
C	8.499806	2.117787	3.737034
N	8.737095	1.904996	2.426774
C	7.699569	1.528113	1.642265
C	6.414491	1.348983	2.136774
C	6.176673	1.549740	3.491773
C	9.595353	2.594014	4.642214
N	10.099969	1.685758	5.489413
C	10.982611	2.111763	6.401755
C	11.379707	3.440746	6.525900
C	10.852465	4.374130	5.638448
C	9.948608	3.944198	4.671530
Co	10.679334	1.763462	1.423185
N	11.386645	-0.207852	1.553824
C	10.634920	-1.183249	1.004747
C	11.065953	-2.506037	0.970388
C	12.296854	-2.835094	1.528684
C	13.070419	-1.826380	2.096285
C	12.580530	-0.528719	2.079867
C	9.277217	-0.772119	0.473228
N	9.292491	0.626105	0.019358
C	8.007153	1.314593	0.180309
N	11.136962	2.536945	-0.351747
C	11.947821	3.644337	-0.353685
C	12.113042	4.382567	-1.545394
C	11.477216	3.969025	-2.696917
C	10.682058	2.795835	-2.681297
C	10.552634	2.112240	-1.493334
C	12.585320	3.897712	0.914716
N	12.205777	3.050382	1.945228
C	12.870367	3.149819	3.119887

C	13.871601	4.063558	3.363470
C	14.219633	4.970223	2.338088
C	13.574967	4.879839	1.123697
C	9.840298	0.784203	-1.344985
H	7.183797	0.782926	-0.311844
H	8.096833	2.290562	-0.306430
H	5.618415	1.042848	1.468938
H	5.186239	1.405670	3.907942
H	7.097890	2.102662	5.360794
H	9.510604	4.640929	3.966502
H	11.136390	5.418784	5.697911
H	12.082969	3.731045	7.297671
H	11.379473	1.352375	7.069754
H	9.065655	0.650469	-2.108760
H	10.576366	-0.010048	-1.497216
H	10.196229	2.437714	-3.581566
H	11.591210	4.534619	-3.614972
H	12.731149	5.272324	-1.558313
H	13.844766	5.550321	0.316417
H	14.988997	5.717457	2.497699
H	14.362433	4.085688	4.328832
H	12.556698	2.458037	3.893611
H	8.944214	-1.459781	-0.312513
H	8.554888	-0.860681	1.289573
H	10.443276	-3.264555	0.510447
H	12.649600	-3.860013	1.512715
H	14.038811	-2.033904	2.534348
H	13.156171	0.292517	2.489468

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