

Supporting Information for

**Catalytic Proton Reduction with Transition Metal Complexes of the Redox-Active Ligand
bpy2PYMe**

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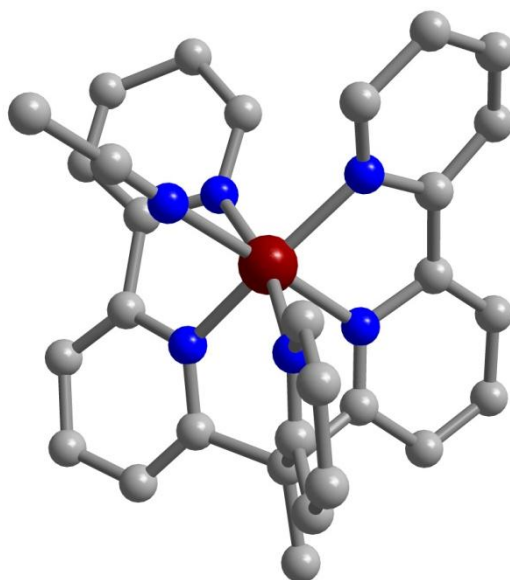


Fig. S1. Molecular structure of the dicationic Fe complex in the crystal structure of **1**. Red, blue, and grey spheres represent Fe, N, C atoms, respectively; hydrogen atoms have been omitted for clarity.

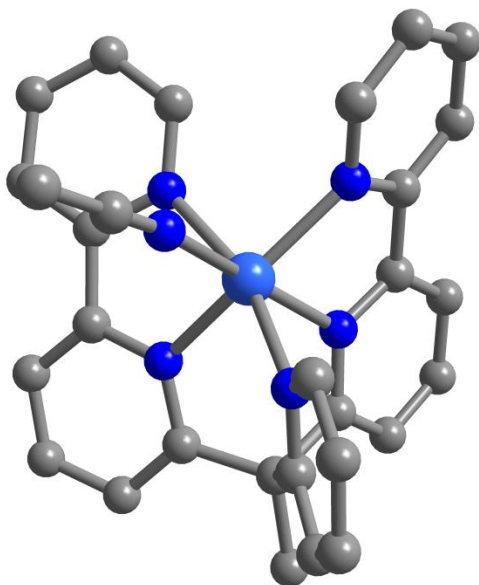


Fig. S2. Molecular structure of the dicationic Ni complex in the crystal structure of **3**. light blue, blue, and grey spheres represent Ni, N, C atoms, respectively; hydrogen atoms have been omitted for clarity.

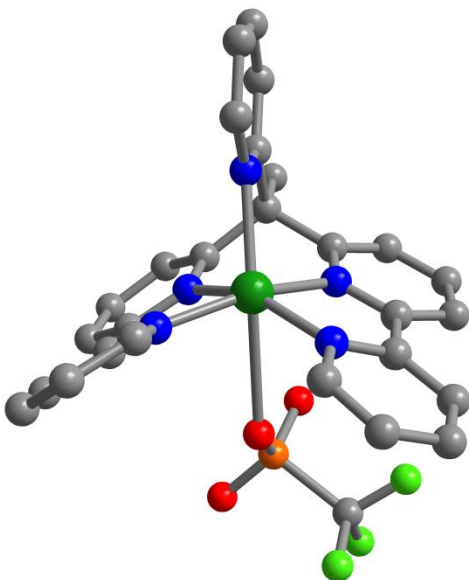


Fig. S3. Molecular structure of the monocationic Cu complex in the crystal structure of **4**. Green, blue, grey, red, orange, and light green spheres represent Cu, N, C, O, S, and F atoms, respectively; hydrogen atoms have been omitted for clarity.

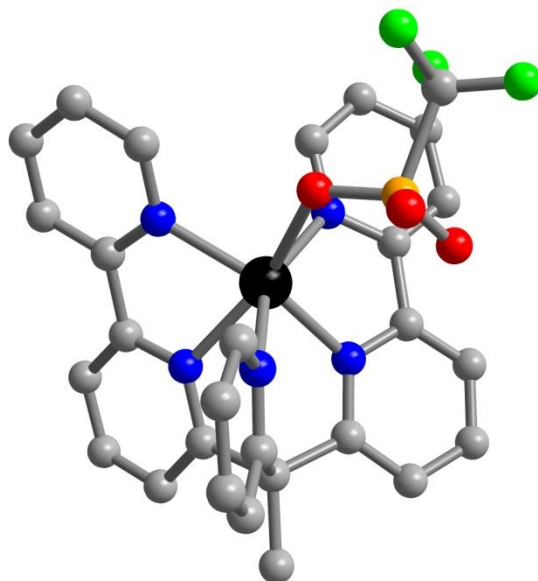


Fig. S4. Molecular structure of the monocationic Zn complex in the crystal structure of **5**. Black, blue, grey, red, orange, and light green spheres represent Zn, N, C, O, S, and F atoms, respectively; hydrogen atoms have been omitted for clarity.

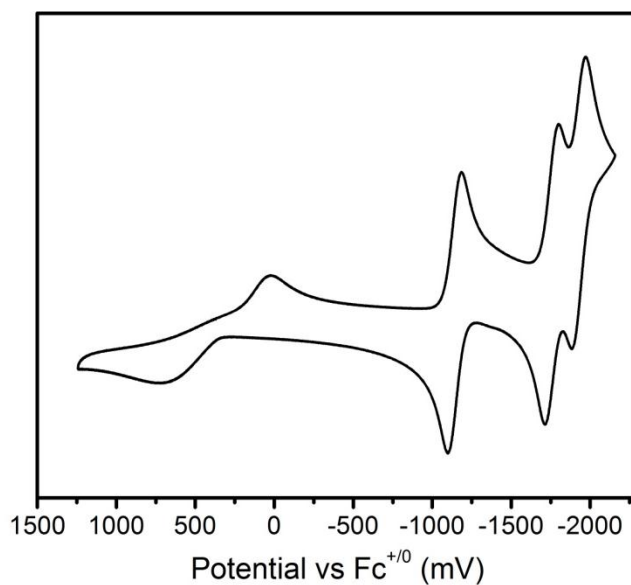


Fig. S5. Cyclic voltammogram of **6** measured in CH₃CN (0.1 M NBu₄PF₆, ν = 100 mV/s).

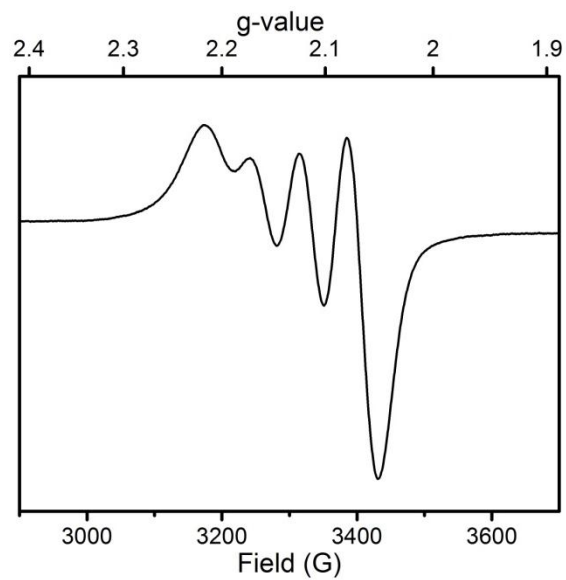


Fig. S6. X-band EPR spectrum of a CH_2Cl_2 solution of **4** (0.2 mM) at 298 K.

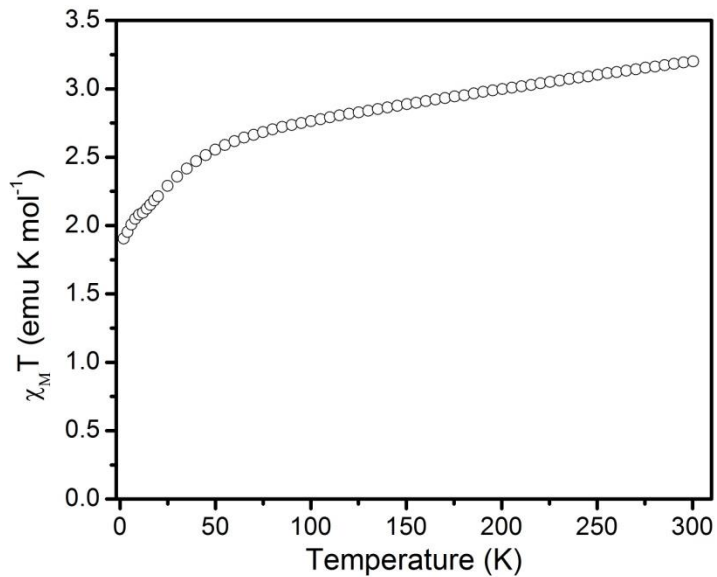


Fig. S7. Variable-temperature dc magnetic susceptibility data for a restrained polycrystalline sample of **2** collected under a 1 kOe applied dc field.

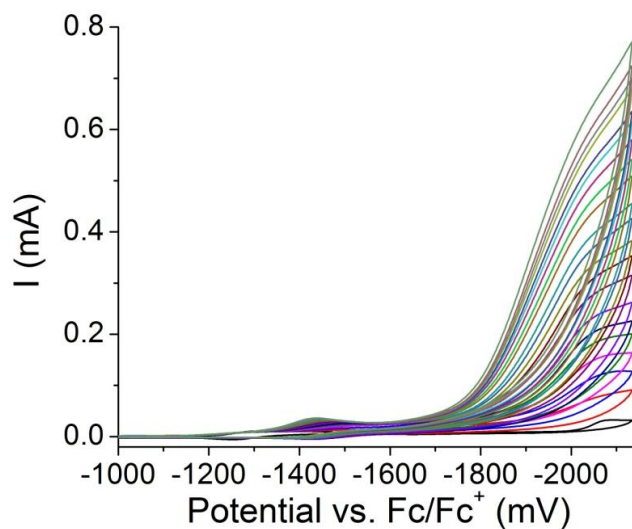


Fig. S8. Electrochemical response of $(\text{Co}(\text{CF}_3\text{-PY5Me}_2)(\text{CH}_3\text{CN}))^{2+}$ to addition of acetic acid (0-100 eq) in CH_3CN (0.1 M NBu_4PF_6).

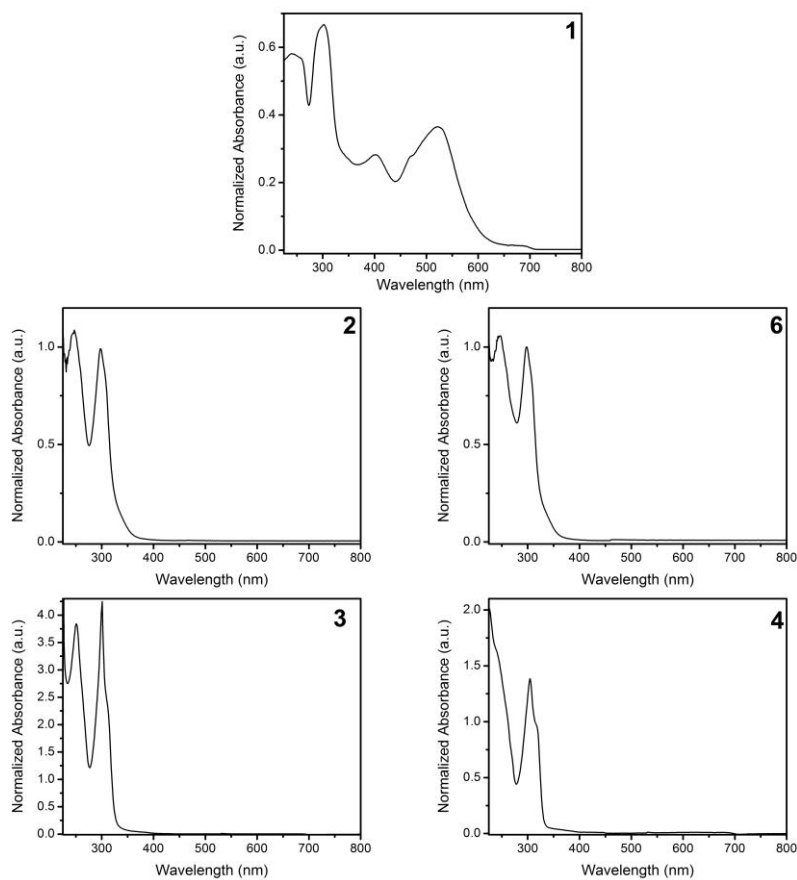


Fig. S9. Electronic absorption spectra of **1**, **2**, **3**, **4**, and **6** in CH_3CN .

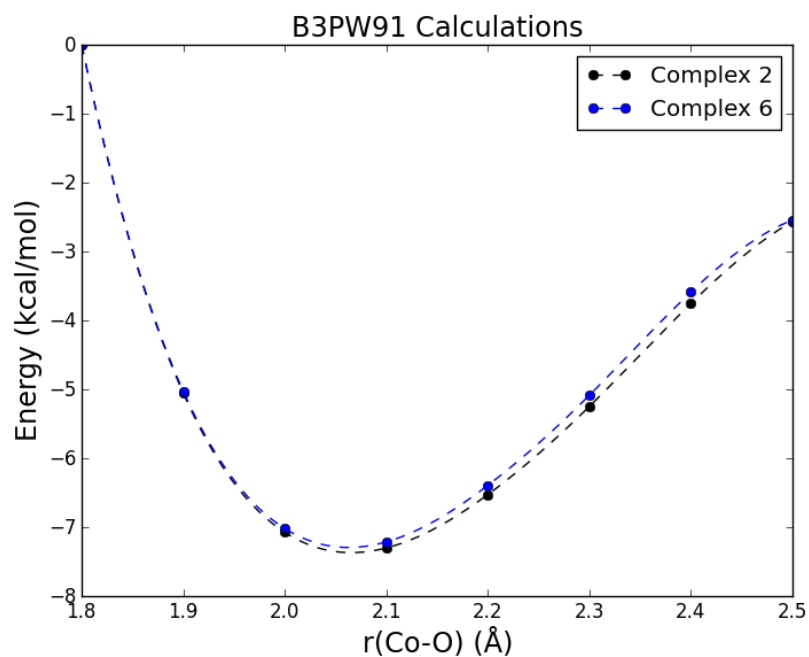


Fig. S10. Dependence of the potential energy surface on variation of Co–O bond distance in **6** (top) and **2** (bottom).

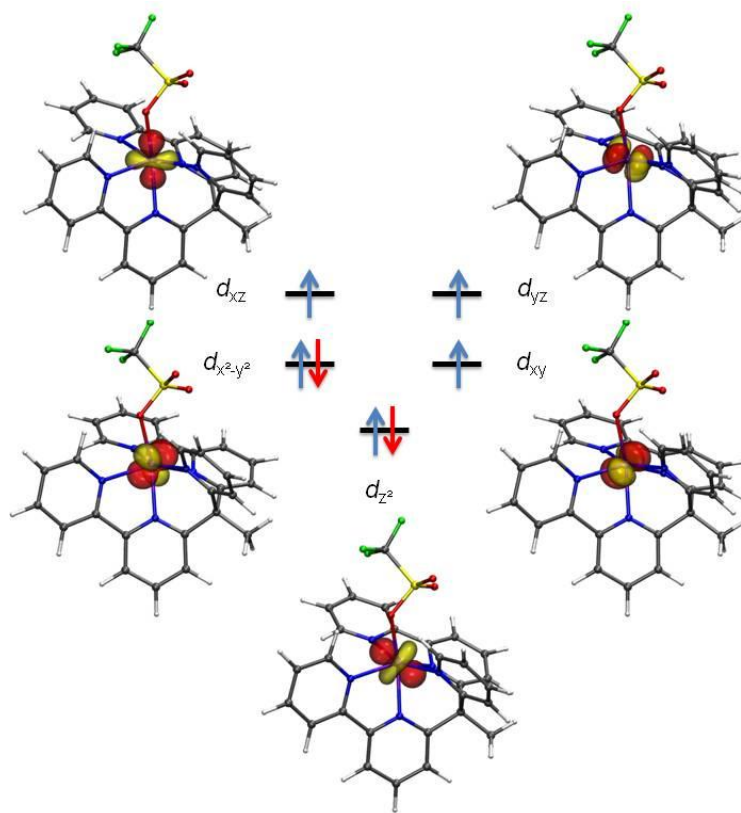


Fig. S11. Isosurface (0.07 au) plots of localized d orbitals in **2**.

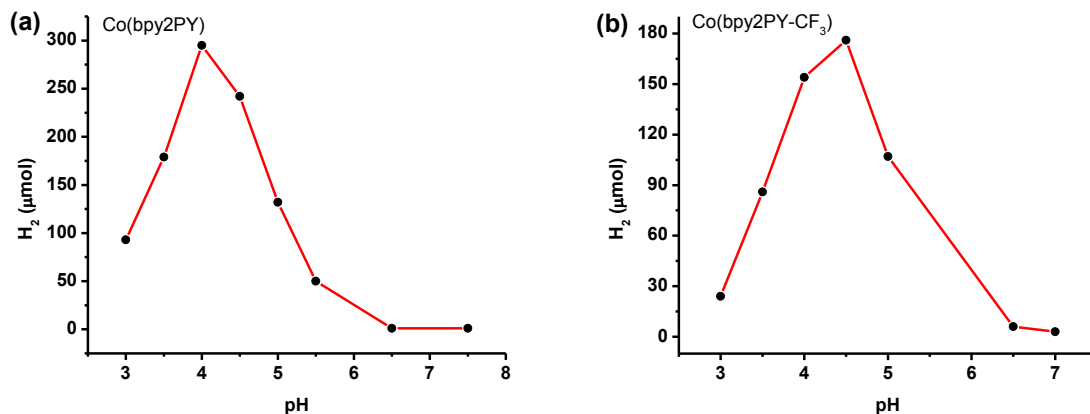


Fig. S12. The pH dependence of Co(bpy2PYMe) **(a)** and Co(bpy2PYMe-CF₃) **(b)** catalysts on H₂ production with the totals collected after hydrogen production ceased using 3.3×10^{-4} M Ru(bpy)₃²⁺ and 2.0×10^{-5} M catalyst in 0.1 M ascorbic acid/ascorbate (H₂A/HA⁻) in water.

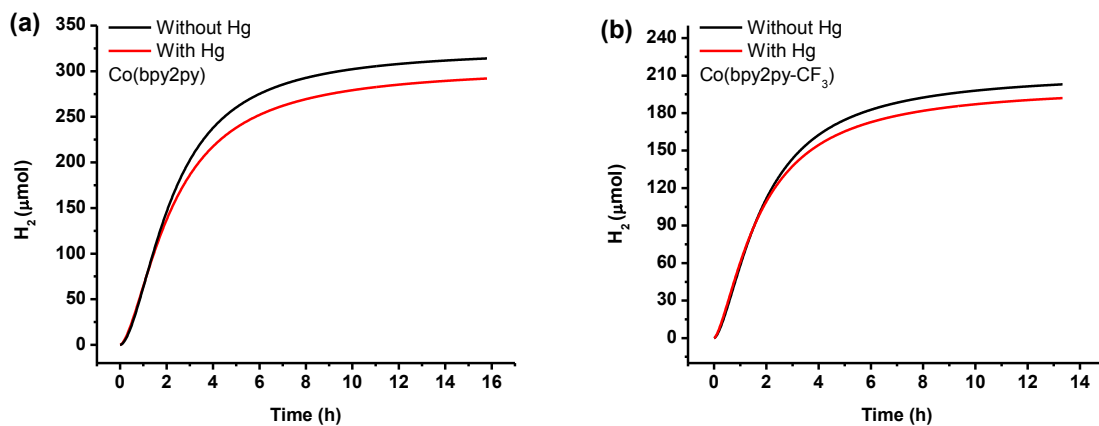


Fig. S13. Mercury poisoning test performed on Co(bpy2PYMe), pH 4 **(a)** and Co(bpy2PYMe-CF₃), pH 4.5 **(b)** at 2.0×10^{-5} M catalyst and 3.3×10^{-4} M Ru(bpy)₃²⁺ in 0.1 M ascorbic acid/ascorbate in water.

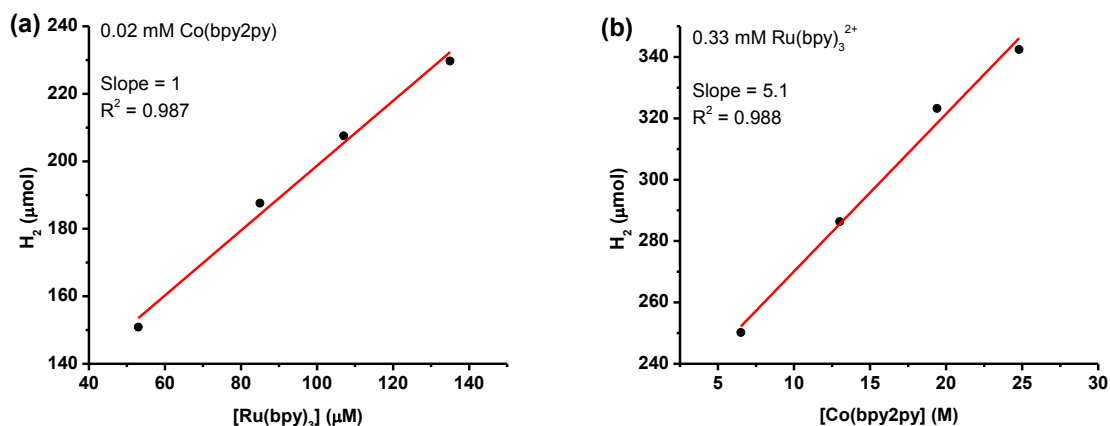


Fig. S14. Linear dependence of hydrogen produced as a function of $Ru(bpy)_3^{2+}$ concentration at $2.0 \times 10^{-5} \text{ M}$ $Co(bpy_2PYMe)$ (a), and as a function of $Co(bpy_2PYMe)$ concentration at $3.3 \times 10^{-4} \text{ M}$ $Ru(bpy)_3^{2+}$ (b). These experiments were performed in 0.1 M ascorbic acid/ascorbate at pH 4 in water.

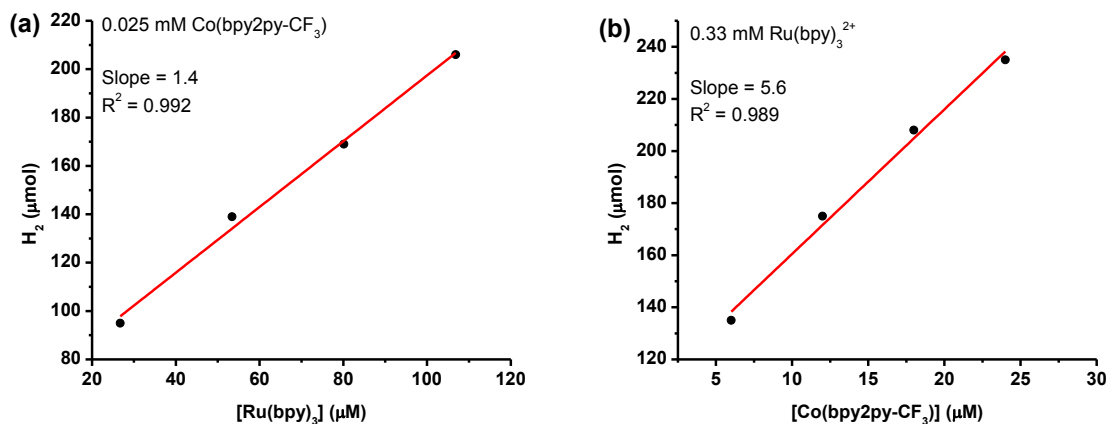


Fig. S15. Linear dependence of hydrogen produced as a function of $Ru(bpy)_3^{2+}$ concentration with $2.5 \times 10^{-5} \text{ M}$ $Co(bpy_2PYMe-CF_3)$ (a), and as a function of $Co(bpy_2PYMe-CF_3)$ concentration with $3.3 \times 10^{-4} \text{ M}$ $Ru(bpy)_3^{2+}$ (b). These experiments were performed in 0.1 M ascorbic acid/ascorbate at pH 4.5 in water.

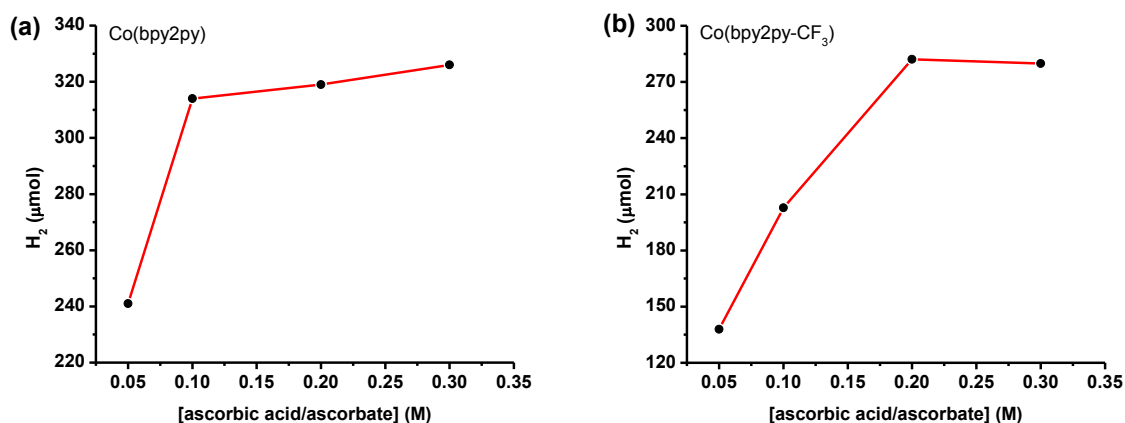


Fig. S16. Ascorbic acid/ascorbate concentration dependence of H_2 production collected after hydrogen production ceased utilizing 3.3×10^{-4} M $\text{Ru}(\text{bpy})_3^{2+}$ and 2.0×10^{-5} M $\text{Co}(\text{bpy}2\text{PYMe})$ at pH 4 (a), $\text{Co}(\text{bpy}2\text{PYMe}-\text{CF}_3)$, pH 4.5 (b).

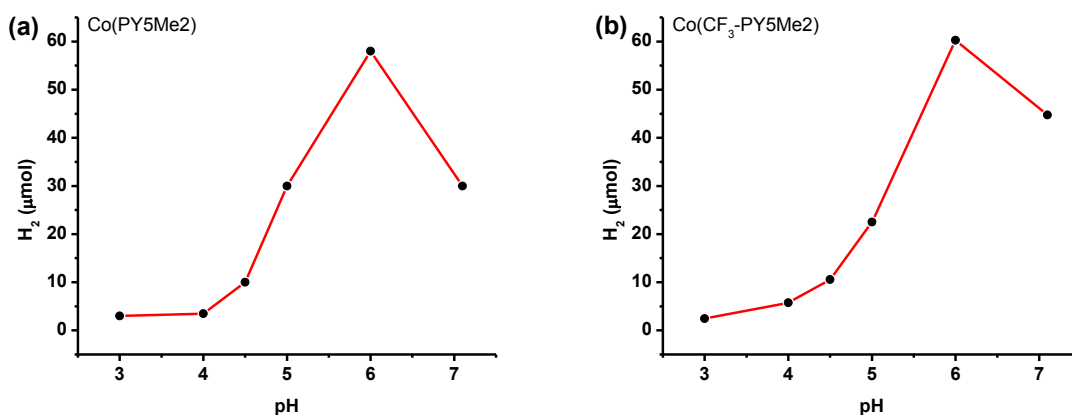


Fig. S17. The pH dependence of H_2 production with $\text{Co}(\text{PY}5\text{Me}_2)$ (a) and $\text{Co}(\text{CF}_3-\text{PY}5\text{Me}_2)$ (b) collected after hydrogen production ceased in a composition of 3.3×10^{-4} M $\text{Ru}(\text{bpy})_3^{2+}$ and 2.0×10^{-5} M catalyst in 0.3 M ascorbic acid/ascorbate in water.

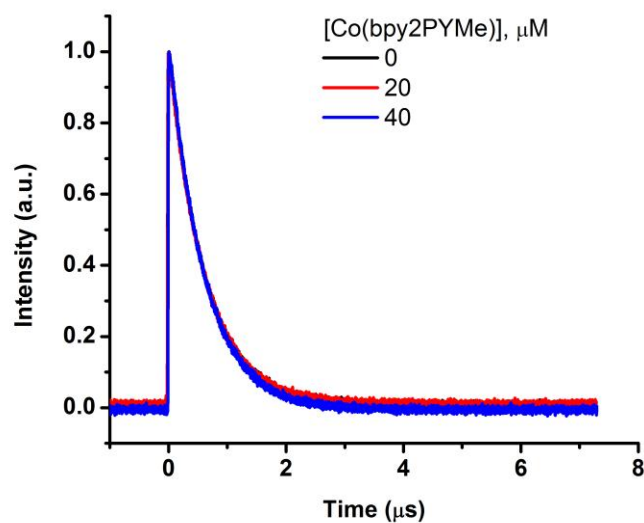


Fig. S18. Dynamic photoluminescence quenching of $[\text{Ru}(\text{bpy})_3]^{2+}$ measured at 610 ± 2 nm in H_2O as a function of added $\text{Co}(\text{bpy}_2\text{PYMe})$ from a stock solution indicating no oxidative quenching of the excited state of $[\text{Ru}(\text{bpy})_3]^{2+}$ by the $\text{Co}(\text{II})$ catalyst.

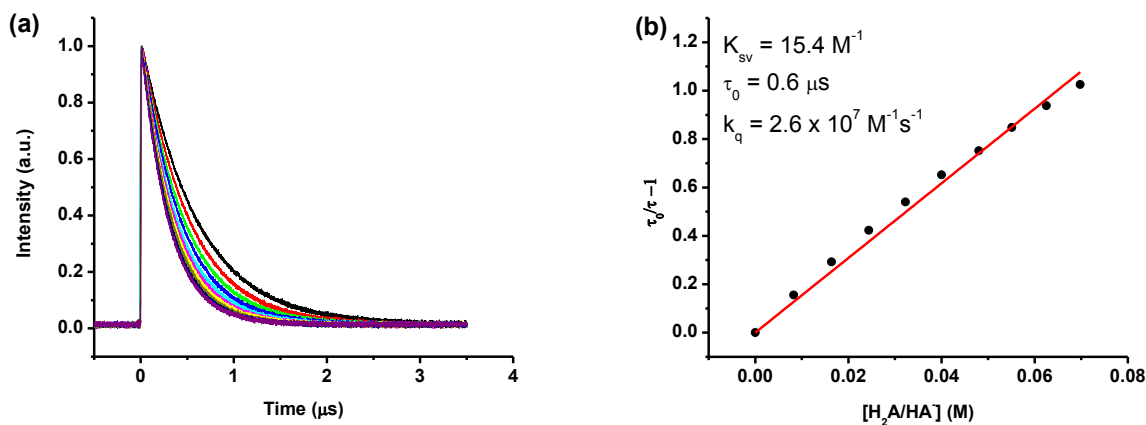


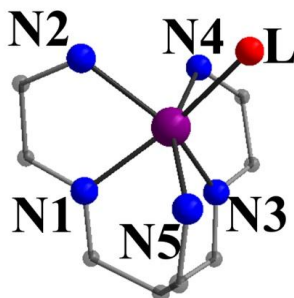
Fig. S19. Dynamic photoluminescence quenching of $[\text{Ru}(\text{bpy})_3]^{2+}$ measured at 610 ± 2 nm in H_2O as a function of added ascorbic acid/ascorbate $\text{H}_2\text{A}/\text{HA}^-$ from a stock solution at pH 4 **(a)**. Stern-Volmer plot of the lifetime data **(b)**.

Table S1. Crystallographic Data.

Compound	2	3	4	5	6
Formula	C _{30.50} H _{23.25} CoF ₆ N _{5.75} O ₆ S	C ₃₃ H _{30.50} B _{0.50} F ₁₁ N ₇ NiO _{0.50} P _{1.50}	C ₃₃ H ₂₇ CuF ₆ N ₇ O ₆ S ₂	C ₃₁ H ₂₄ F ₆ N ₆ O ₆ S ₂ Zn	C ₃₂ H ₂₃ CoF ₉ N ₆ O ₆ S ₂
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> -1	<i>P</i> 2(1)/ <i>n</i>	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
<i>a</i> , Å	9.8107(3)	11.605(3)	9.9247(6)	9.8290(3)	10.1178(2)
<i>b</i> , Å	12.2952(3)	26.456(6)	13.1783(8)	12.2969(3)	10.1848(2)
<i>c</i> , Å	13.4212(4)	12.584(3)	14.8490(9)	13.4196(4)	18.5692(4)
<i>α</i> , °	93.235(1)	90	66.577(2)	92.874(1)	93.060(1)
<i>β</i> , °	91.814(1)	114.443(3)	80.638(2)	91.805(1)	101.838(1)
<i>γ</i> , °	91.350(1)	90	81.873(2)	91.232(1)	106.548(1)
<i>V</i> , Å ³	1615.01(8)	3517.3(14)	1752.0(2)	1618.70(8)	1782.45(6)
<i>Z</i>	2	4	2	2	2
<i>ρ</i> , Mg m ⁻³	1.611	1.476	1.475	1.498	1.643
R1 ^a , wR2 ^b (<i>I</i> > 2σ(<i>I</i>))	0.0361, 0.0925	0.0515, 0.1394	0.0411, 0.1054	0.0284, 0.0786	0.0332, 0.0783
R1 ^a , wR2 ^b (all data)	0.0445, 0.0990	0.0550, 0.1423	0.0439, 0.1079	0.0303, 0.0798	0.0397, 0.0817

^aR1 = 3||*F*_o| - |*F*_c||/3|*F*_o|. ^bwR2 = [3[*w*(*F*_o² - *F*_c²)²]/3[*w*(*F*_o²)²]]^{1/2}, *w* = 1/σ²(*F*_o²) + (*aP*)² + *bP*, where *P* = [max(0 or *F*_o²) + 2(*F*_c²)]/3.

Table S2. Metal-ligand bond distances in compounds **2-6**.



	2	3	4	5	6
M–N1, Å	2.098(2)	2.029(3)	1.985(2)	2.136(2)	2.087(2)
M–N2, Å	2.111(2)	2.149(3)	2.042(2)	2.124(2)	2.198(2)
M–N3, Å	2.071(2)	2.015(3)	1.994(2)	2.103(2)	2.078(2)
M–N4, Å	2.183(2)	2.086(3)	2.024(2)	2.167(2)	2.105(2)
M–N5, Å	2.112(2)	2.061(3)	2.258(2)	2.150(2)	2.134(2)
M–L ^a , Å	2.175(2)	2.149(3)	2.776(2)	2.222(1)	2.127(2)

^a L = SO₃CF₃[−] for **2,4,5,6**; L = CH₃CN for **3**

Table S3. Redox potentials^a observed in CH₃CN (0.1 M NBu₄PF₆) for complexes **1-6**.

complex	E ^{1/2} (red1)	E ^{1/2} (red2)	E ^{1/2} (red3)	E ^{1/2} (red4)	E ^{1/2} (ox)
1	-1546	-1664	-2349	-	686
2	-1197	-1786	-1941	-	235
3	-1199	-1759	-2186	-2581	1392
4	-837	-	-	-	-
5	-1629	-1763	-	-	-
6	-1136	-1703	-1860	-	310

^a Potentials in mV; referenced to internal ferrocene (Fc).

Table S4. Overview of calculated energies and bond lengths in **2**, **6**, **2+e⁻**, and **6+e⁻**. (^a = Co–O distance was fixed to the crystallographically determined value). Energies in parenthesis include a solvent correction computed *via* the SWIG C-PCM approach (acetonitrile, $\epsilon = 35.688$).

Co(II) - R = H	Multiplicity	<S ² >	q(Co)	ρ (Co)	Co-O, Å	Co-N _{bpy(s)} , Å	Co-N _{bpy(l)} , Å	Co-N _(py) , Å	$\Delta E(S=1/2-S=3/2)$, kcal/mol
Experimental	S = 3/2				2.175	2.085	2.147	2.112	
	S = 1/2	0.774	0.842	0.930	1.996	1.927	2.128	2.179	0.0 (0.0)
Calculated	S = 3/2	3.761	1.078	2.717	2.065	2.120	2.188	2.152	-10.2 (-10.3)
	S = 3/2	3.761	1.129	2.720	2.175 ^a	2.113	2.178	2.142	-9.6 (-10.3)

Co(II) - R = CF ₃	Multiplicity	<S ² >	q(Co)	ρ (Co)	Co-O, Å	Co-N _{bpy(s)} , Å	Co-N _{bpy(l)} , Å	Co-N _(py) , Å	$\Delta E(S=1/2-S=3/2)$, kcal/mol
Experimental					2.127	2.083	2.152	2.134	
	S = 1/2	0.776	0.848	0.932	1.999	1.928	2.117	2.187	0.0 (0.0)
Calculated	S = 3/2	3.761	1.080	2.717	2.064	2.119	2.184	2.160	-9.8 (-9.8)
	S = 3/2	3.761	1.111	2.720	2.127 ^a	2.116	2.178	2.154	-9.6 (-9.8)

Co(I) - R = H	Multiplicity	<S ² >	q(Co)	ρ (Co)	Co-N _(CH₃CN) , Å	Co-N _{bpy(s)} , Å	Co-N _{bpy(l)} , Å	Co-N _(py) , Å
Calculated	S = 1	2.404	0.987	2.284	2.212	2.066	2.161	2.157

Co(I) - R = CF ₃	Multiplicity	<S ² >	q(Co)	ρ (Co)	Co-N _(CH₃CN) , Å	Co-N _{bpy(s)} , Å	Co-N _{bpy(l)} , Å	Co-N _(py) , Å
Calculated	S = 1	2.373	0.979	2.263	2.218	2.070	2.163	2.135

COMPUTED STRUCTURES AND ENERGIES

2 (S=1/2)

Energy = -3659.016422
Enthalpy 0K = -3658.560276
Enthalpy 298K = -3658.525757
Free Energy 298K = -3658.625777

Co 0.01524 8.50626 3.18760
S -2.60281 9.05407 5.00792
F -3.69802 11.23681 3.98482
O -1.86791 8.94859 3.67797
F -4.91546 10.22411 5.46147
O -1.90068 9.89239 5.97292
F -4.72282 9.40097 3.46610
N 1.64504 7.77884 2.54334
N -0.14624 6.57562 4.18493
N -0.54342 8.18697 1.33562
O -3.13773 7.77878 5.45884
N 0.97094 9.19945 4.74721
C 0.76841 10.48703 5.09013
N 0.03188 10.77510 2.85178
C 0.09779 11.32435 4.07567
C -1.25935 5.83955 4.16681
H -2.09677 6.25599 3.62233
C -1.36240 4.62283 4.82553
H -2.29056 4.06471 4.79158
C 2.56908 7.25163 3.35979
C -4.08401 10.04523 4.44624
C 1.80709 8.42608 5.45230
C 0.92436 6.14362 4.86362
C 0.50455 7.98758 0.49842
C 1.76404 7.70286 1.20002
C 0.89935 4.93503 5.55215
H 1.75799 4.58097 6.10621
C 3.32677 6.42717 5.61263
H 3.60591 5.46417 5.18285
H 3.05476 6.24652 6.65261
H 4.20798 7.07154 5.60787
C -0.93278 12.79814 2.01714
H -1.32419 13.34948 1.16965
C 1.28972 10.99759 6.27325
H 1.12009 12.02994 6.55002
C -1.76851 8.35604 0.82914
H -2.55122 8.52425 1.55948
C -0.26154 4.16725 5.53113
H -0.29707 3.22488 6.06824
C 2.17107 7.06444 4.83937
C -2.00844 8.33362 -0.53894
H -3.01924 8.46369 -0.90792
C 2.05246 10.17126 7.07807
H 2.45495 10.53808 8.01635
C -0.90044 13.35284 3.28967
H -1.28442 14.35154 3.46907
C 3.77539 6.80509 2.82207
H 4.55324 6.40751 3.45882
C -0.46725 11.49955 1.85351
H -0.49870 11.01907 0.87990
C -0.93844 8.15327 -1.40641
H -1.09178 8.14438 -2.48033
C 0.33631 7.97839 -0.88154
H 1.18411 7.83241 -1.54052

C 2.35004 8.88446 6.64850
H 3.00420 8.26216 7.24240
C 3.97627 6.85505 1.44739
H 4.91924 6.52388 1.02563
C -0.37770 12.60693 4.33643
H -0.36856 13.00972 5.34169
C 2.94493 7.26483 0.61530
H 3.05341 7.22190 -0.46163

2 (S=3/2)

Energy = -3659.032616
Enthalpy 0K = -3658.577039
Enthalpy 298K = -3658.541996
Free Energy 298K = -3658.644032

Co 0.21865 0.31560 -0.07386
S -2.39279 -1.38725 -0.92212
F -4.33260 -0.04603 0.27735
O -1.62342 -0.07406 -0.92189
F -5.00001 -1.75814 -0.86916
O -2.18525 -2.13450 0.31481
F -4.38569 0.05530 -1.88432
N 2.17951 1.12485 0.08343
N 1.19576 -0.79417 -1.63728
N -0.01588 2.39197 -0.50527
O -2.28991 -2.09509 -2.18823
N 0.99266 -1.09722 1.29244
C 0.16649 -1.48438 2.27683
N -0.96664 0.56257 1.81295
C -0.92705 -0.53783 2.58417
C 0.60532 -0.90817 -2.83360
H -0.38945 -0.49015 -2.91157
C 1.20545 -1.54413 -3.90980
H 0.67902 -1.61971 -4.85379
C 3.24701 0.34014 0.24425
C -4.14575 -0.74630 -0.84669
C 2.11038 -1.77435 1.01567
C 2.42020 -1.31628 -1.44702
C 1.03886 3.18082 -0.22651
C 2.26973 2.45971 0.17038
C 3.08140 -1.96591 -2.48480
H 4.06615 -2.38908 -2.34503
C 4.41042 -1.87671 0.00869
H 5.12465 -1.41856 -0.67702
H 4.31962 -2.92670 -0.26945
H 4.83585 -1.83936 1.01305
C -2.80351 1.38240 3.10975
H -3.52752 2.17094 3.27957
C 0.39351 -2.66602 2.97580
H -0.28506 -3.00153 3.74902
C -1.13993 2.93599 -0.98077
H -1.93801 2.23485 -1.20167
C 2.46799 -2.08035 -3.72859
H 2.97839 -2.59078 -4.53900
C 3.05435 -1.16551 -0.04277
C -1.27593 4.30375 -1.18174
H -2.20265 4.70379 -1.57677
C 1.51110 -3.41667 2.65512
H 1.70742 -4.35067 3.17128
C -2.77693 0.23941 3.89549
H -3.48762 0.10343 4.70383
C 4.47250 0.89724 0.61103

H	5.34898	0.28287	0.76312
C	-1.88329	1.49220	2.07641
H	-1.88426	2.36256	1.43045
C	-0.20462	5.12941	-0.86575
H	-0.27429	6.20350	-1.00268
C	0.96952	4.56271	-0.38633
H	1.82118	5.19299	-0.16082
C	2.39783	-2.95993	1.68738
H	3.28925	-3.53220	1.47257
C	4.56617	2.27357	0.78039
H	5.50915	2.71907	1.07977
C	-1.82370	-0.73294	3.63143
H	-1.78887	-1.63140	4.23428
C	3.46249	3.07638	0.53744
H	3.53736	4.15261	0.63238

2+e (S=1)

Energy	=	-2830.377706
Enthalpy 0K	=	-2829.906928
Enthalpy 298K	=	-2829.876195
Free Energy 298K	=	-2829.967642

C	0.57835	3.01845	-2.84659
N	0.83161	2.34566	-1.71096
C	0.24382	1.15957	-1.51261
C	-0.60272	0.56171	-2.43009
C	-0.84793	1.23265	-3.61913
C	-0.25587	2.47127	-3.82407
Co	2.09813	3.24006	-0.21191
N	2.79826	1.18048	0.18954
C	3.37215	0.18316	0.26211
C	4.09972	-1.06777	0.34263
H	-1.49810	0.80764	-4.37711
C	1.20616	4.42204	-3.00957
C	0.77703	5.03398	-4.34712
N	0.90365	4.84858	-0.60012
C	0.31758	5.44685	0.46191
C	-0.38653	6.64105	0.31433
C	-0.51860	7.18262	-0.95177
C	-0.00317	6.49238	-2.05104
C	0.69301	5.30810	-1.84634
C	0.42079	4.69033	1.71417
N	1.04276	3.48799	1.61178
C	1.06929	2.69497	2.69398
C	0.52772	3.04868	3.91655
C	-0.07411	4.30225	4.03711
C	-0.12924	5.12318	2.92505
N	4.05746	3.65286	0.69656
C	5.05375	3.81462	-0.19956
C	6.39657	3.81110	0.18884
C	6.71885	3.66745	1.52794
C	5.68640	3.53321	2.45362
C	4.38189	3.52569	1.98852
C	4.61402	4.04877	-1.58399
N	3.28460	3.94008	-1.78531
C	2.74481	4.34573	-2.94353
C	3.55529	4.74411	-4.00444
C	4.93681	4.75772	-3.84181
C	5.47473	4.44104	-2.60729
H	3.58724	-1.76473	1.00949
H	5.10738	-0.89277	0.72593

H	4.17551	-1.52218	-0.64774
H	0.46837	0.67956	-0.56705
H	-1.05546	-0.39920	-2.21232
H	-0.45768	2.99902	-4.74533
H	-0.30721	5.13764	-4.40339
H	1.09475	4.41714	-5.18913
H	1.21164	6.02511	-4.48357
H	5.88663	3.43841	3.51518
H	6.54212	4.52111	-2.44250
H	1.55394	1.73317	2.55547
H	0.57649	2.36164	4.75414
H	5.58019	5.05440	-4.66351
H	7.75612	3.66842	1.84649
H	-0.16408	6.88985	-3.04360
H	3.54971	3.41990	2.67657
H	-0.50073	4.62604	4.98060
H	-0.60444	6.09440	2.99595
H	3.13387	5.05207	-4.95075
H	-1.05201	8.11585	-1.09758
H	7.18536	3.92159	-0.54568
H	-0.83855	7.13460	1.16630

6 (S=1/2)

Energy	=	-3996.023093
Enthalpy 0K	=	-3995.562477
Enthalpy 298K	=	-3995.524187
Free Energy 298K	=	-3995.634566

Co	-0.34935	-0.76400	-0.19035
S	-1.60390	2.20706	0.06799
F	6.08672	1.92408	-0.86649
F	5.01608	3.77603	-1.21094
F	5.41665	3.11127	0.81351
F	-3.03984	2.77979	-2.07573
F	-3.50717	3.97916	-0.33229
F	-4.18363	1.92519	-0.44740
O	-1.44633	0.85328	-0.61245
O	-1.90226	2.08962	1.49044
O	-0.59143	3.16546	-0.34913
N	-0.23095	-0.63417	1.75552
N	-2.38720	-1.49060	0.51080
N	0.88945	-2.20546	-0.14603
N	-0.66293	-1.44808	-1.99866
N	1.47329	0.43590	-0.34303
C	0.95069	-0.62815	2.38677
C	1.01773	-0.37841	3.75351
H	1.96561	-0.34352	4.27137
C	-0.15934	-0.18186	4.46466
H	-0.12322	0.03047	5.52788
C	-1.37458	-0.31640	3.81869
H	-2.30190	-0.25134	4.37273
C	-1.38383	-0.56265	2.45056
C	-2.60751	-0.89973	1.69678
C	-3.89276	-0.68592	2.18818
H	-4.05094	-0.15521	3.11879
C	-4.97631	-1.13357	1.44589
H	-5.98775	-0.97231	1.80360
C	-4.74525	-1.77998	0.23873
H	-5.56233	-2.15433	-0.36760
C	-3.43232	-1.92071	-0.19199
H	-3.20981	-2.39589	-1.14278

C 1.91612 -2.24793 0.71554
C 2.73763 -3.37380 0.74017
H 3.55292 -3.45201 1.44582
C 2.51841 -4.40456 -0.16674
H 3.14437 -5.29008 -0.14113
C 1.54455 -4.26579 -1.14450
H 1.42402 -5.01811 -1.91457
C 0.75180 -3.12580 -1.12498
C -0.18495 -2.70486 -2.17624
C -0.50909 -3.44859 -3.30504
H -0.13230 -4.45704 -3.42910
C -1.31947 -2.87762 -4.27891
H -1.57943 -3.43948 -5.16975
C -1.78444 -1.58119 -4.09772
H -2.41015 -1.09670 -4.83833
C -1.44308 -0.90071 -2.93577
H -1.79577 0.10038 -2.71670
C 2.45189 0.17458 0.53459
C 3.63123 0.90731 0.53205
H 4.42554 0.71147 1.23891
C 3.78909 1.92875 -0.40225
C 2.77401 2.19474 -1.30232
H 2.85257 2.99109 -2.03142
C 1.62536 1.41704 -1.23086
H 0.78945 1.59756 -1.89357
C 2.18833 -0.97211 1.54219
C 3.40523 -1.18566 2.44427
H 3.22617 -1.98613 3.16438
H 3.64523 -0.28306 3.00651
H 4.28985 -1.44443 1.86060
C 5.08550 2.70271 -0.42067
C -3.18996 2.76331 -0.74885

6 (S=3/2)

Energy = -3996.038778
Enthalpy 0K = -3995.578791
Enthalpy 298K = -3995.539979
Free Energy 298K = -3995.652181

Co 0.49879 0.50979 -0.15395
S 1.49154 -2.54892 -0.18871
F -6.21852 -1.00387 -1.25647
F -5.43421 -2.95456 -1.78323
F -5.84550 -2.47058 0.28953
F 3.01910 -3.22475 -2.23399
F 3.40272 -4.34402 -0.41824
F 4.09186 -2.29841 -0.59756
O 1.35099 -1.21308 -0.90679
O 1.72794 -2.36852 1.24058
O 0.49012 -3.51552 -0.61140
N 0.16357 0.61326 1.92760
N 2.50714 0.83219 0.77356
N -0.70465 2.26385 -0.15723
N 1.10650 1.57813 -1.89603
N -1.46325 -0.37679 -0.33182
C -1.07517 0.67969 2.42246
C -1.32144 0.34240 3.75070
H -2.31732 0.37553 4.16917
C -0.25585 -0.05020 4.55237
H -0.43215 -0.33924 5.58320
C 1.03010 -0.04701 4.04063
H 1.86680 -0.32324 4.66863

C 1.21243 0.30956 2.70801
C 2.53518 0.45094 2.06253
C 3.73372 0.26096 2.74532
H 3.74137 -0.06181 3.77860
C 4.93207 0.48454 2.08330
H 5.87634 0.33767 2.59684
C 4.89928 0.89680 0.75901
H 5.80902 1.08731 0.20142
C 3.66258 1.04758 0.14703
H 3.59638 1.35134 -0.89128
C -1.70226 2.42869 0.71394
C -2.28653 3.68501 0.87590
H -3.08494 3.84982 1.58596
C -1.83202 4.74635 0.10190
H -2.26731 5.73233 0.22683
C -0.84514 4.53598 -0.84848
H -0.51168 5.35003 -1.48016
C -0.30446 3.25836 -0.96282
C 0.67574 2.84995 -1.99457
C 1.07947 3.67033 -3.04528
H 0.72910 4.69259 -3.12021
C 1.92379 3.15355 -4.01980
H 2.24321 3.77591 -4.84917
C 2.33655 1.83064 -3.92668
H 2.97906 1.38335 -4.67635
C 1.90668 1.07710 -2.84188
H 2.19428 0.03977 -2.70611
C -2.48527 0.06752 0.42239
C -3.76274 -0.45016 0.25492
H -4.59491 -0.10371 0.85112
C -3.98284 -1.43996 -0.70022
C -2.92647 -1.89500 -1.46501
H -3.04952 -2.67352 -2.20699
C -1.67776 -1.32960 -1.24340
H -0.81072 -1.66148 -1.79839
C -2.18506 1.16838 1.46685
C -3.44736 1.50010 2.26935
H -3.23173 2.22466 3.05634
H -3.86225 0.61280 2.74790
H -4.22560 1.92023 1.63029
C -5.38230 -1.98238 -0.87087
C 3.10811 -3.14925 -0.90684

6+e (S=1)

Energy = -3167.385885
Enthalpy 0K = -3166.910504
Enthalpy 298K = -3166.876011
Free Energy 298K = -3166.977643

C 0.61494 3.13740 -2.70560
C 0.85674 2.39811 -1.54876
N 0.28158 1.18836 -1.36417
C -0.65563 0.73896 -2.21668
C -0.93856 1.43690 -3.38398
C -0.26630 2.63231 -3.64518
Co 0.86772 0.12823 0.27923
N 2.86961 -0.81056 0.18345
C 2.85235 -2.08166 -0.26453
C 3.95833 -2.92378 -0.12507
C 5.11597 -2.43563 0.45968

C	5.14146	-1.11217	0.88909
C	3.99538	-0.34762	0.73540
C	1.61418	-2.48191	-0.95765
N	0.62252	-1.57093	-0.92421
C	-0.45885	-1.72372	-1.69911
C	-0.64401	-2.89134	-2.43866
C	0.32723	-3.88471	-2.39875
C	1.48877	-3.66732	-1.67841
C	-1.43301	-0.53103	-1.78592
C	-2.52999	-0.83369	-2.81151
C	1.65250	2.86830	-0.40947
N	1.63915	2.05411	0.67738
C	2.25467	2.47734	1.79306
C	2.92754	3.68199	1.88624
C	2.97837	4.50223	0.75819
C	2.33199	4.09015	-0.39364
N	1.04793	-0.66577	2.34288
C	1.15800	-1.30352	3.29718
C	1.29182	-2.11501	4.49066
H	1.15374	-1.50322	5.38492
N	-1.24072	0.07876	0.60906
C	-1.77097	0.41206	1.79362
C	-3.12847	0.41866	2.05201
C	-3.98336	0.05661	1.01876
C	-3.44648	-0.26684	-0.21903
C	-2.06396	-0.24005	-0.40626
C	-5.47018	-0.02301	1.24975
F	-5.80753	-1.21781	1.76484
H	2.28403	-2.57002	4.52727
H	0.54170	-2.90903	4.49049
F	-5.88206	0.91678	2.11189
F	-6.15956	0.13163	0.10938
H	-1.06011	0.69028	2.56252
H	-3.50428	0.70705	3.02645
H	-4.11733	-0.52513	-1.02499
H	-3.21412	0.00879	-2.91893
H	-3.12046	-1.70434	-2.52195
H	-2.10198	-1.03817	-3.79372
H	6.03022	-0.67816	1.33367
H	2.28673	-4.39911	-1.69993
H	2.19511	1.80360	2.64254
H	3.40085	3.97165	2.81791
H	0.19152	-4.80293	-2.96057
H	5.98614	-3.07425	0.57085
H	-1.67376	1.08178	-4.09300
H	3.97195	0.68658	1.06242
H	3.50529	5.45020	0.78306
H	2.35056	4.71928	-1.27571
H	-1.52275	-3.03889	-3.05017
H	-0.46669	3.17923	-4.56025
H	3.92131	-3.95008	-0.47016
H	1.08933	4.09797	-2.86699