Supporting Information for

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

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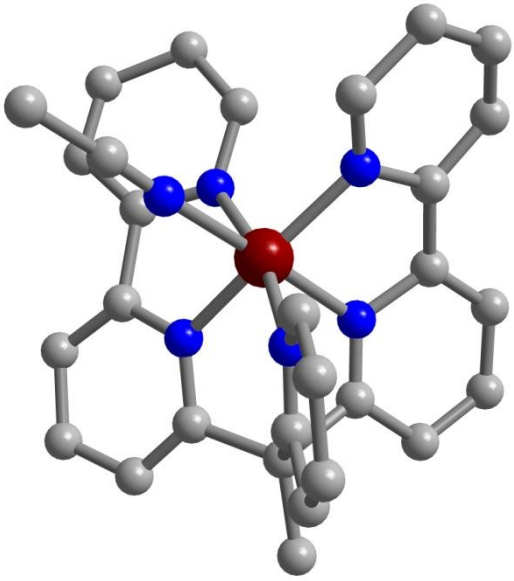


Fig. S1. Molecular structure of the dicationic Fe complex in the crystal structure of **1**. Red, blue, and grey spheres represent Fe, N, C atoms, respectively; hydrogen atoms have been omitted for clarity.

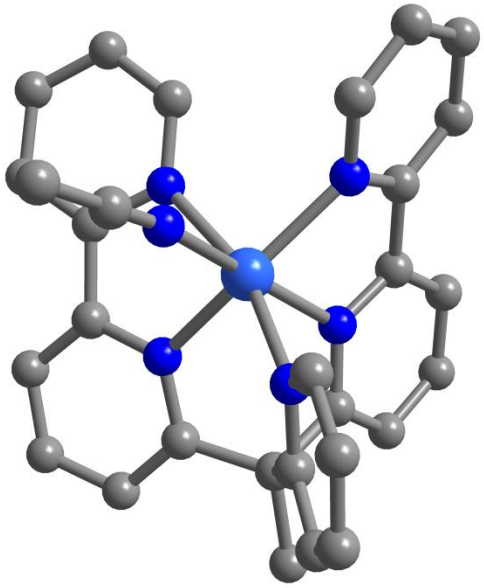


Fig. S2. Molecular structure of the dicationic Ni complex in the crystal structure of **3**. light blue, blue, and grey spheres represent Ni, N, C atoms, respectively; hydrogen atoms have been omitted for clarity.

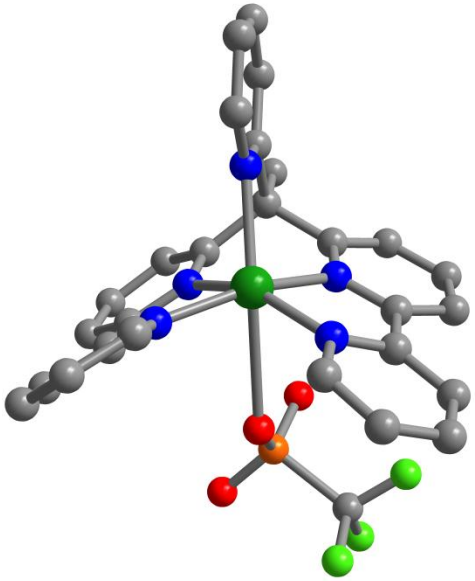


Fig. S3. Molecular structure of the monocationic Cu complex in the crystal structure of **4**. Green, blue, grey, red, orange, and light green spheres represent Cu, N, C, O, S, and F atoms, respectively; hydrogen atoms have been omitted for clarity.

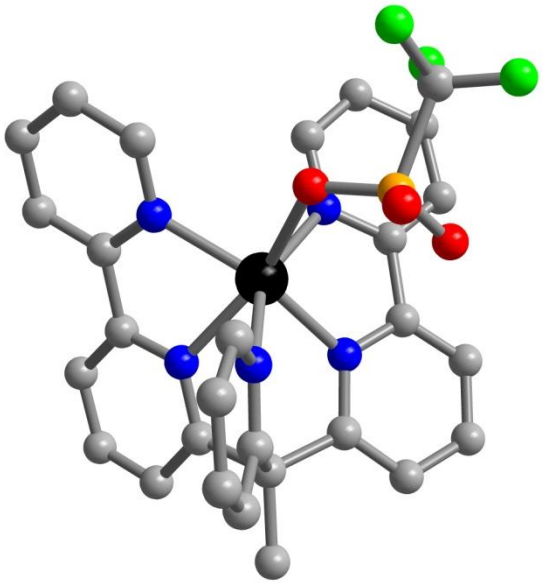


Fig. S4. Molecular structure of the monocationic Zn complex in the crystal structure of **5**. Black, blue, grey, red, orange, and light green spheres represent Zn, N, C, O, S, and F atoms, respectively; hydrogen atoms have been omitted for clarity.

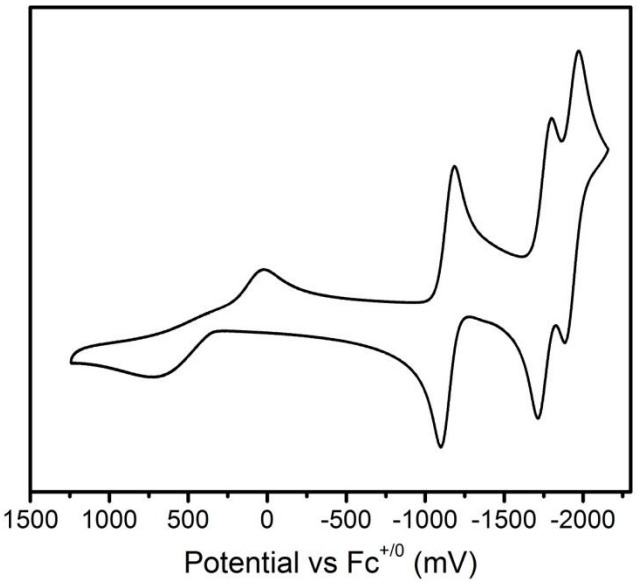


Fig. S5. Cyclic voltammogram of **6** measured in CH_3CN (0.1 M NBu_4PF_6, ν = 100 mV/s).

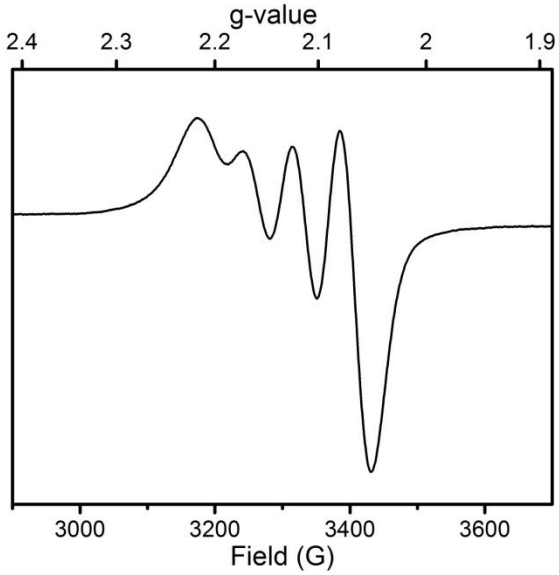


Fig. S6. X-band EPR spectrum of a CH_2Cl_2 solution of **4** (0.2 mM) at 298 K.

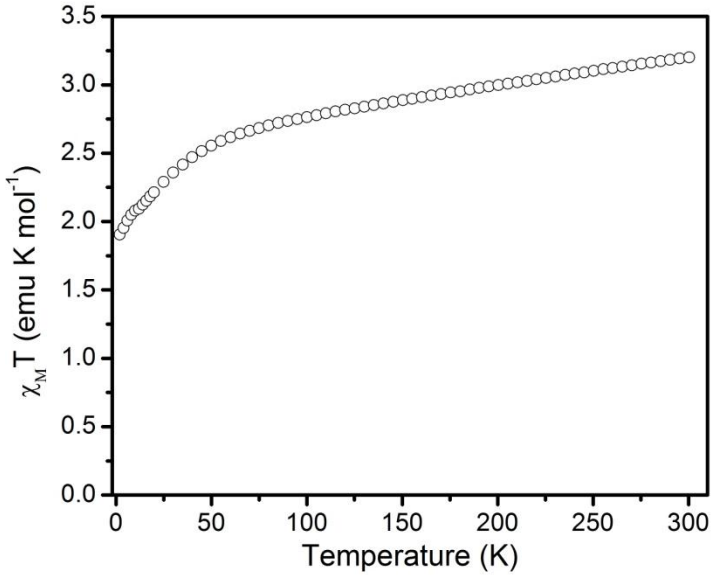


Fig. S7. Variable-temperature dc magnetic susceptibility data for a restrained polycrystalline sample of **2** collected under a 1 kOe applied dc field.

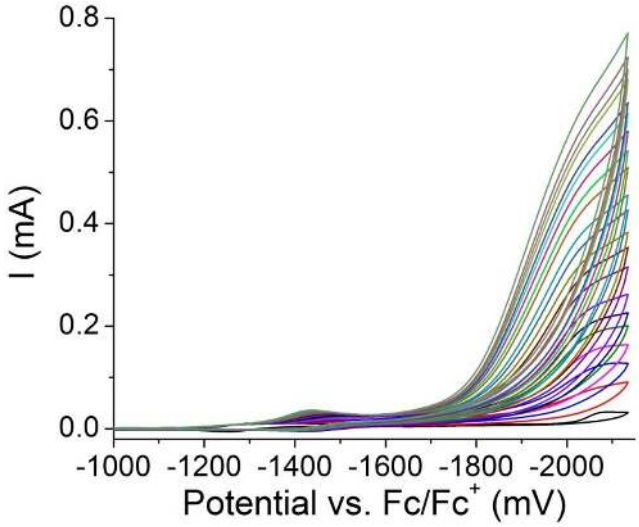


Fig. S8. Electrochemical response of $(Co(CF3\text{-}PY5Me_2)(CH_3CN)]^{2+}$ to addition of acetic acid (0-100 eq) in CH_3CN (0.1 M NBu_4PF_6).

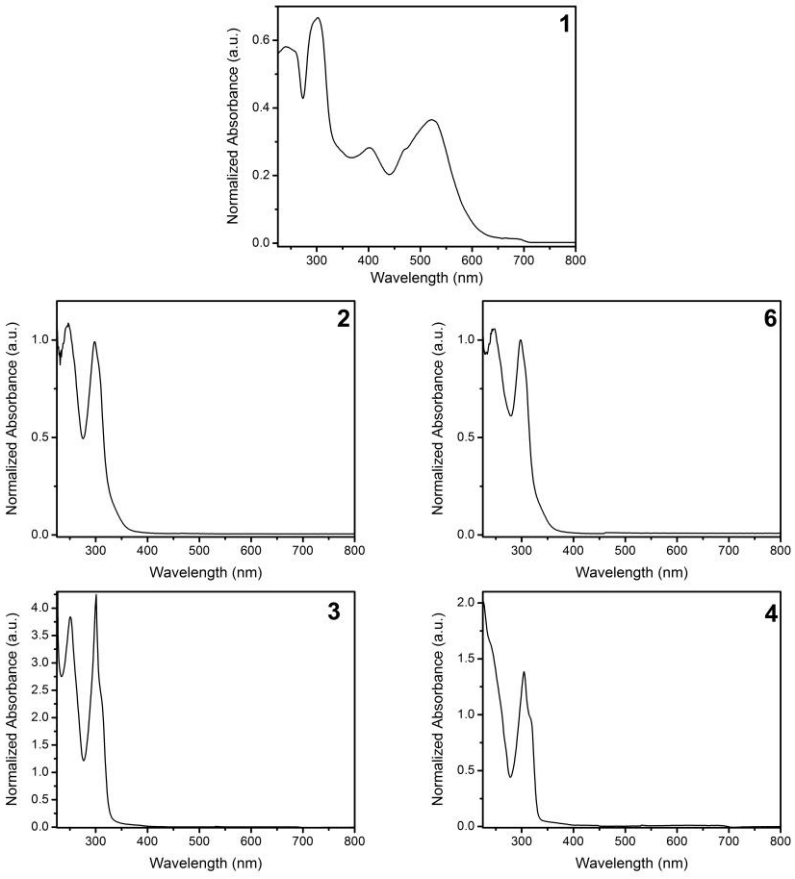


Fig. S9. Electronic absorption spectra of **1**, **2**, **3**, **4**, and **6** in CH_3CN.

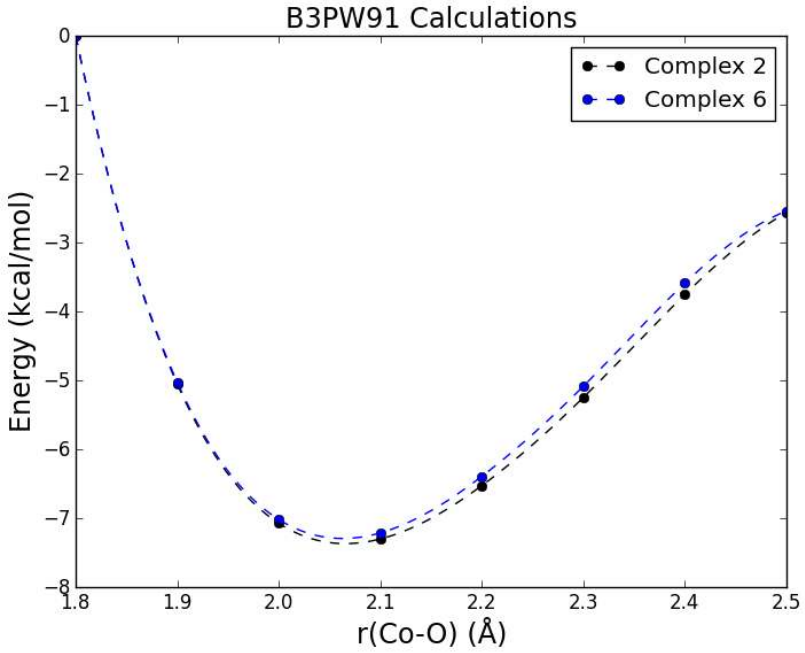


Fig. S10. Dependence of the potential energy surface on variation of Co−O bond distance in **6** (top) and **2** (bottom).

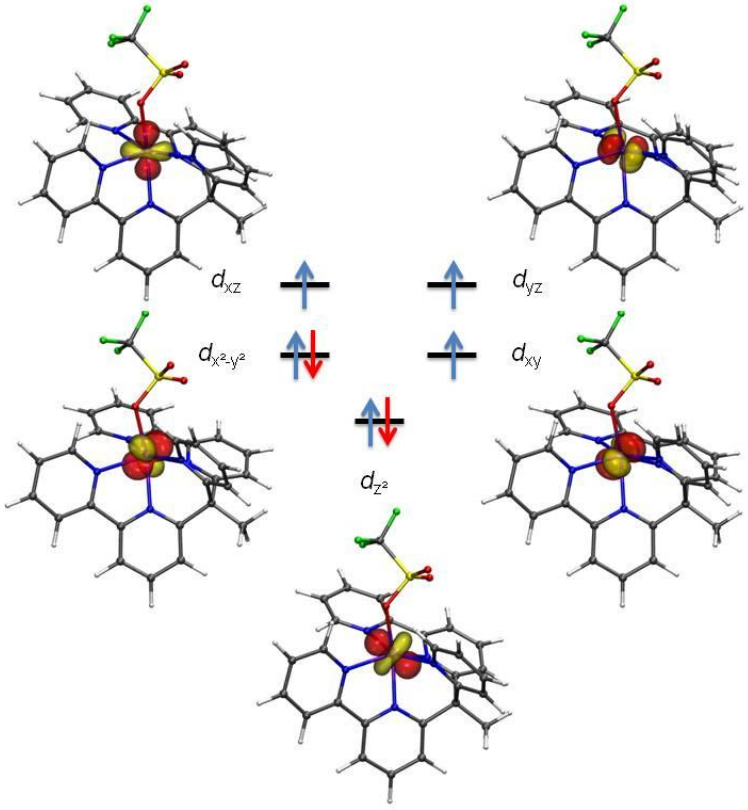


Fig. S11. Isosurface (0.07 au) plots of localized *d* orbitals in **2**.

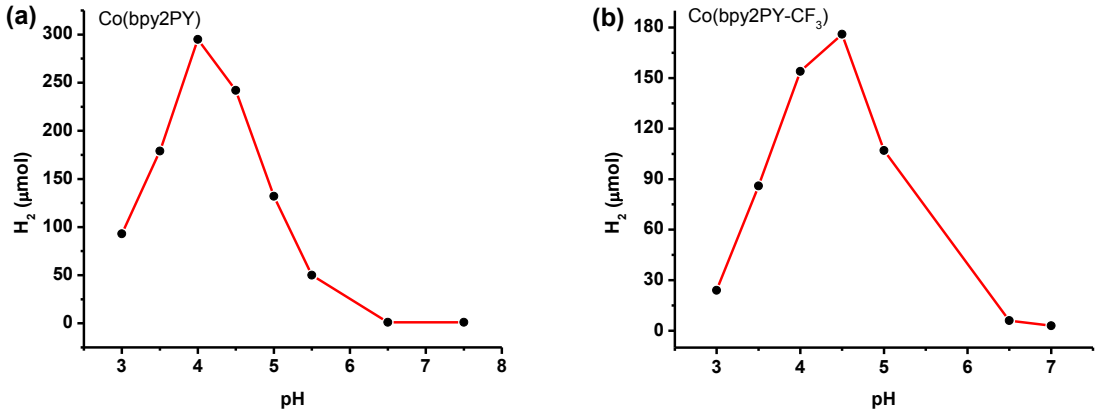


Fig. S12. The pH dependence of Co(bpy2PYMe) **(a)** and Co(bpy2PYMe-CF_3) **(b)** catalysts on H_2 production with the totals collected after hydrogen production ceased using 3.3 x 10^{-4}M $Ru(bpy)_3^{2+}$ and 2.0 x 10^{-5} M catalyst in 0.1 M ascorbic acid/ascorbate (H_2A/HA^-) in water.

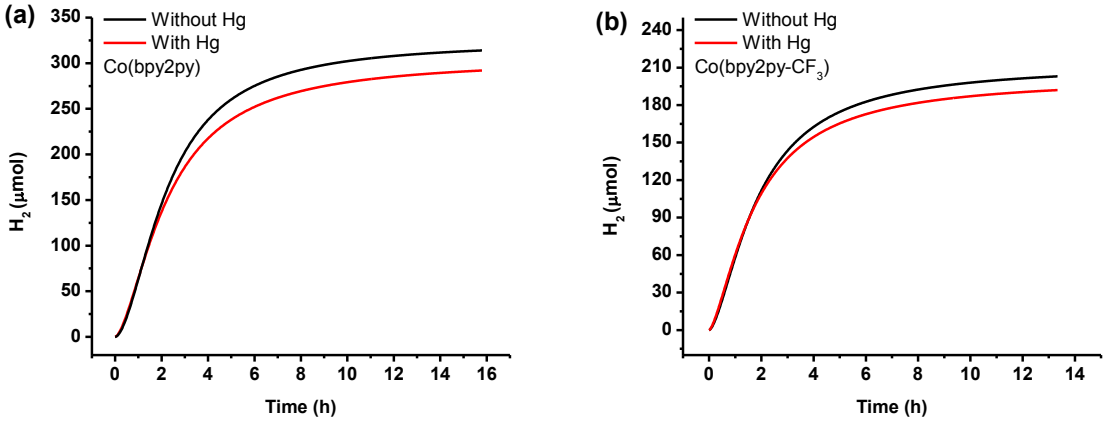


Fig. S13. Mercury poisoning test performed on Co(bpy2PYMe), pH 4 **(a)** and Co(bpy2PYMe-CF_3), pH 4.5 **(b)** at 2.0 x 10^{-5} M catalyst and 3.3 x 10^{-4} M $Ru(bpy)_3^{2+}$ in 0.1 M ascorbic acid/ascorbate in water.

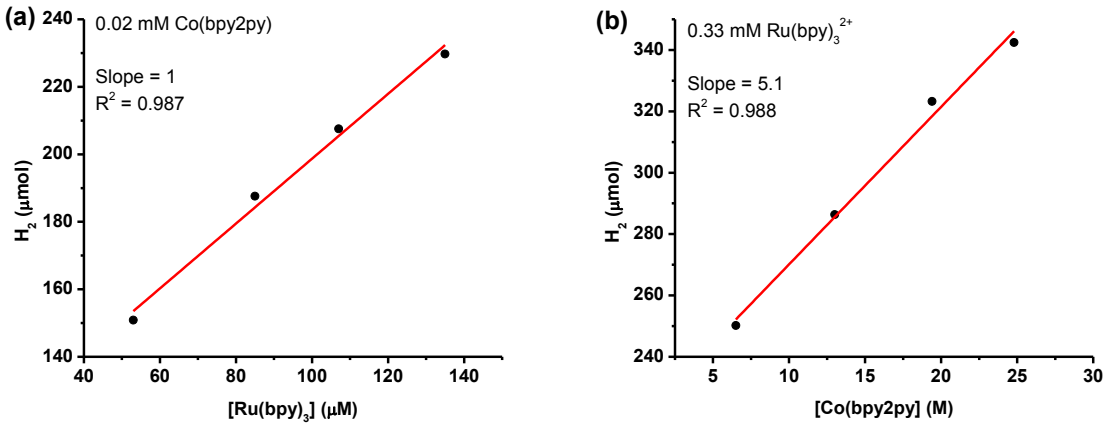


Fig. S14. Linear dependence of hydrogen produced as a function of $Ru(bpy)_3^{2+}$ concentration at 2.0 x 10^{-5} M Co(bpy2PYMe) **(a)**, and as a function of Co(bpy2PYMe) concentration at 3.3 x 10^{-4} M $Ru(bpy)_3^{2+}$ **(b)**. These experiments were performed in 0.1 M ascorbic acid/ascorbate at pH 4 in water.

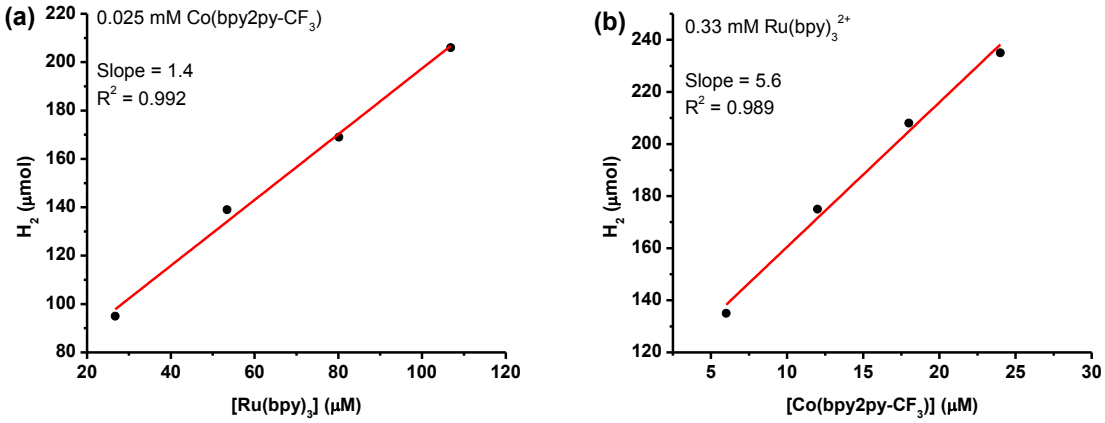


Fig. S15. Linear dependence of hydrogen produced as a function of $Ru(bpy)_3^{2+}$ concentration with 2.5 x 10^{-5} M Co(bpy2PYMe-CF_3) **(a)**, and as a function of Co(bpy2PYMe-CF_3) concentration with 3.3 x 10^{-4} M $Ru(bpy)_3^{2+}$ **(b)**. These experiments were performed in 0.1 M ascorbic acid/ascorbate at pH 4.5 in water.

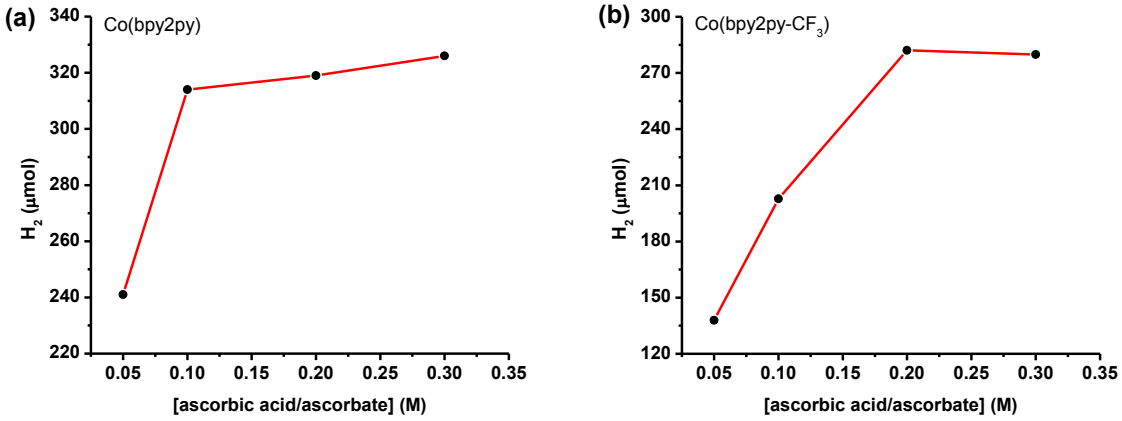


Fig. S16. Ascorbic acid/ascorbate concentration dependence of H_2 production collected after hydrogen production ceased utilizing 3.3 x 10^{-4} M $Ru(bpy)_3^{2+}$ and 2.0 x 10^{-5} M Co(bpy2PYMe) at pH 4 **(a)**, Co(bpy2PYMe-CF_3), pH 4.5 **(b)**.

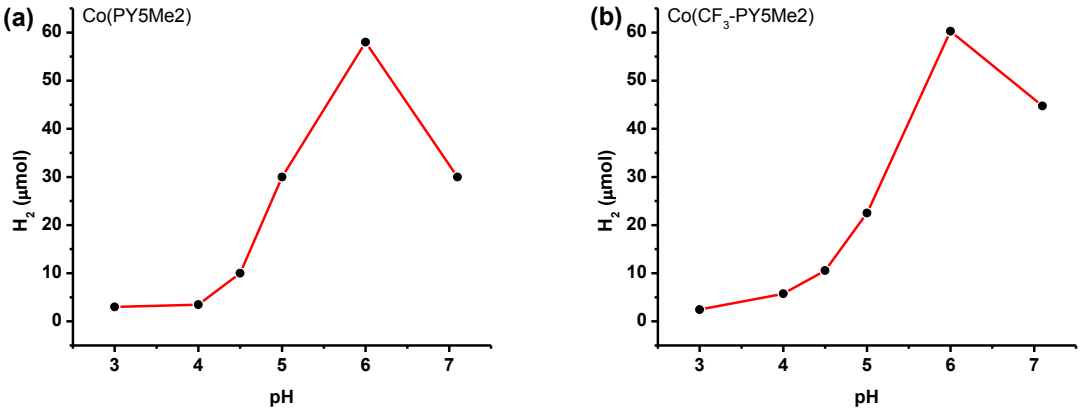


Fig. S17. The pH dependence of H_2 production with Co($PY5Me_2$) **(a)** and Co(CF_3-$PY5Me_2$) **(b)** collected after hydrogen production ceased in a composition of 3.3 x 10^{-4} M $Ru(bpy)_3^{2+}$ and 2.0 x 10^{-5} M catalyst in 0.3 M ascorbic acid/ascorbate in water.

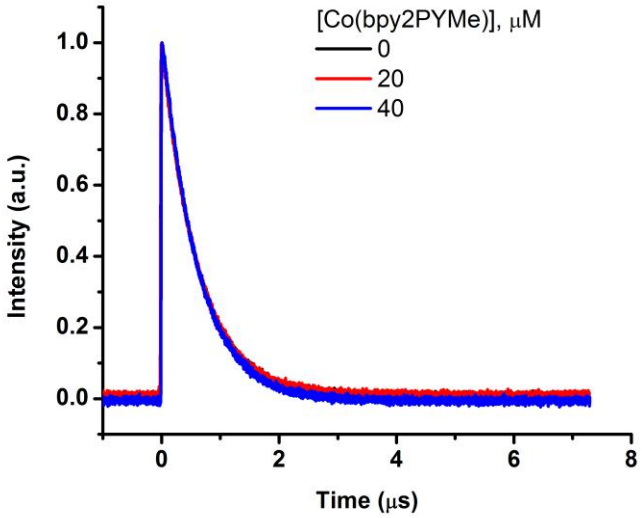


Fig. S18. Dynamic photoluminescence quenching of $[Ru(bpy)_3]^{2+}$ measured at 610 ± 2 nm in H_2O as a function of added Co(bpy2PYMe) from a stock solution indicating no oxidative quenching of the excited state of $[Ru(bpy)_3]^{2+}$ by the Co(II) catalyst.

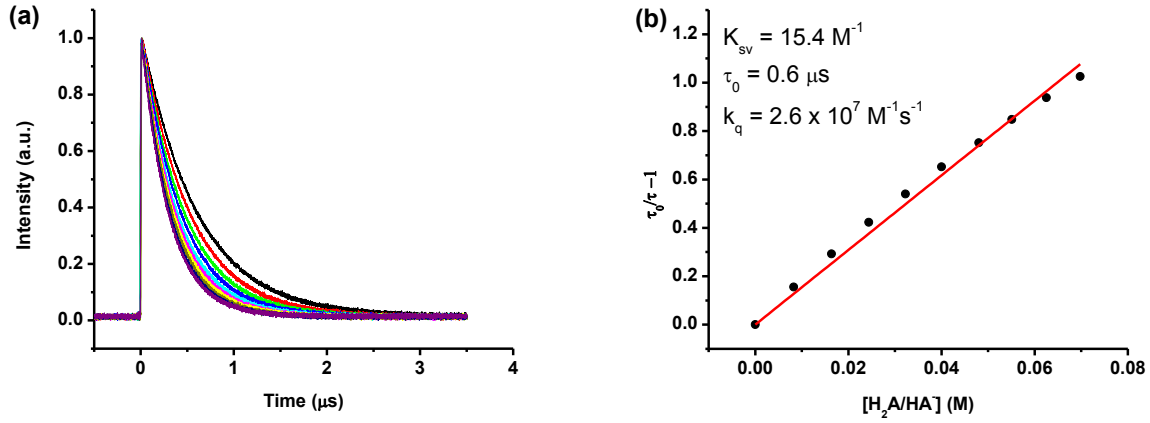


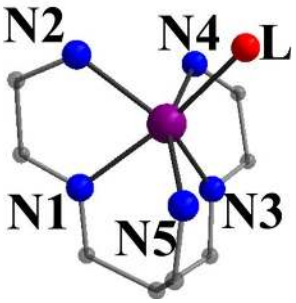
Fig. S19. Dynamic photoluminescence quenching of $[Ru(bpy)_3]^{2+}$ measured at 610 ± 2 nm in H_2O as a function of added ascorbic acid/ascorbate H_2A/HA^- from a stock solution at pH 4 **(a)**. Stern-Volmer plot of the lifetime data **(b)**.

Table S1. Crystallographic Data.

Compound	**2**	**3**	**4**	**5**	**6**
Formula	$C_{30.50}H_{23.25}CoF_6N_{5.75}O_6S$	$C_{33}H_{30.50}B_{0.50}F_{11}N_7NiO_{0.50}P_{1.50}$	$C_{33}H_{27}CuF_6N_7O_6S_2$	$C_{31}H_{24}F_6N_6O_6S_2Zn$	$C_{32}H_{23}CoF_9N_6O_6S_2$
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	*P-1*	*P2(1)/n*	*P-1*	*P-1*	*P-1*
a, Å	9.8107(3)	11.605(3)	9.9247(6)	9.8290(3)	10.1178(2)
b, Å	12.2952(3)	26.456(6)	13.1783(8)	12.2969(3)	10.1848(2)
c, Å	13.4212(4)	12.584(3)	14.8490(9)	13.4196(4)	18.5692(4)
a, °	93.235(1)	90	66.577(2)	92.874(1)	93.060(1)
β, °	91.814(1)	114.443(3)	80.638(2)	91.805(1)	101.838(1)
g, °	91.350(1)	90	81.873(2)	91.232(1)	106.548(1)
V, Å^3	1615.01(8)	3517.3(14)	1752.0(2)	1618.70(8)	1782.45(6)
Z	2	4	2	2	2
ρ, Mg m^{-3}	1.611	1.476	1.475	1.498	1.643
R1[a], *w*R2[b] ($I > 2\sigma(I)$)	0.0361, 0.0925	0.0515, 0.1394	0.0411, 0.1054	0.0284, 0.0786	0.0332, 0.0783
R1[a], *w*R2[b] (all data)	0.0445, 0.0990	0.0550, 0.1423	0.0439, 0.1079	0.0303, 0.0798	0.0397, 0.0817

[a]$R1 = 3||F_o| - |F_c||/3|F_o|$. [b]$wR2 = [3[w(F_o^2 - F_c^2)^2]/3[w(F_o^2)^2]]^{½}$, $w = 1/\sigma^2(F_o^2) + (aP)^2 + bP$, where $P = [\max(0 \text{ or } F_o^2) + 2(F_c^2)]/3$.

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 = $SO_3CF_3^-$ for **2**,**4**,**5**,**6**; L = CH_3CN for **3**

Table S3. Redox potentials[a] observed in CH_3CN (0.1 M NBu_4PF_6) 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, $\varepsilon = 35.688$).

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	ΔE(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	ΔE(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
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2 (S=3/2)

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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
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C -2.80351  1.38240  3.10975
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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