Evaluation of the Coordination Preferences and Catalytic Pathways of Heteroaxial Cobalt Oximes towards Hydrogen Generation

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Figure S1. Synthetic schemes of complexes **1**, **2**, and **3**.

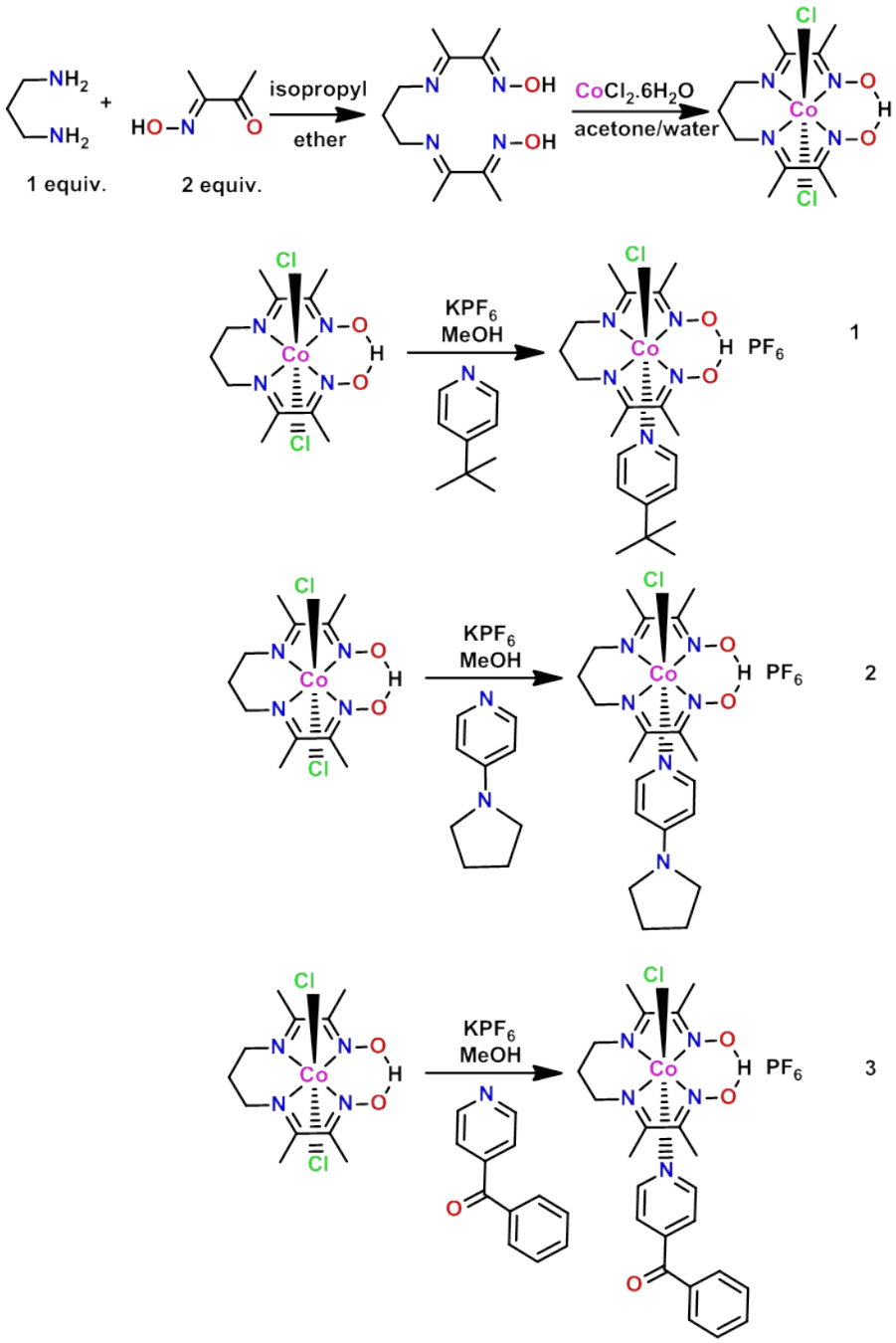


Figure S2. Experimental (bars) and simulated (line) isotopic distribution for the molecular ions of complexes **1**-**3** (left to right) [ESI-Mass spectra of **1**-**3** in CH_3OH: $[M^+]^+$].

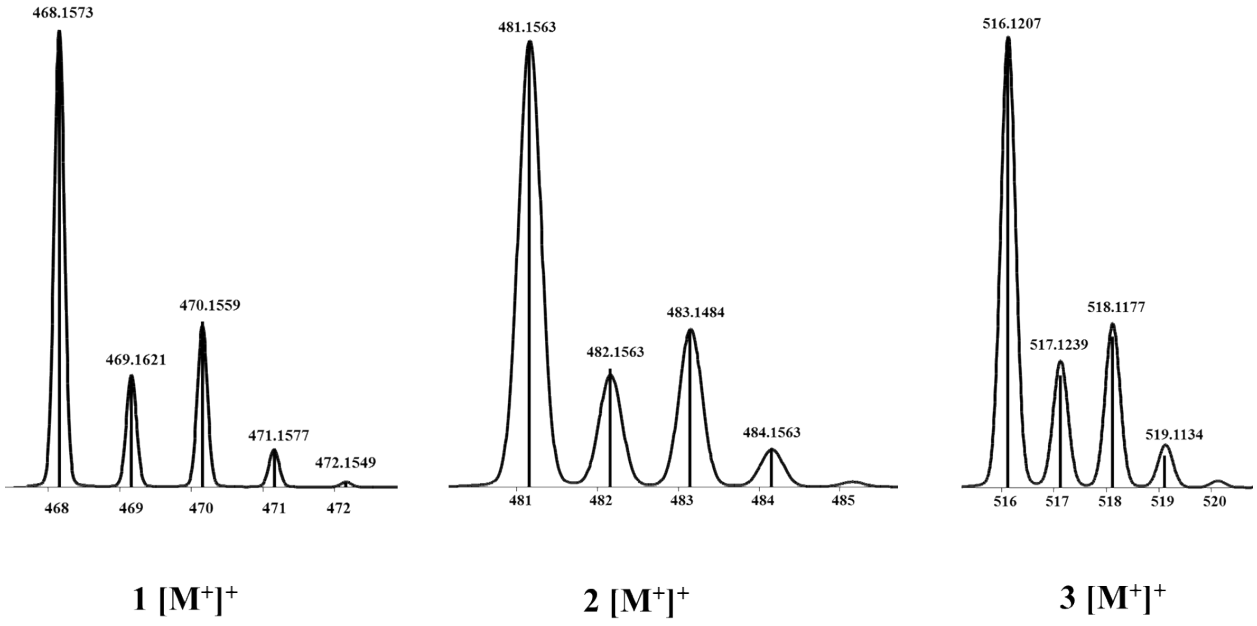


Figure S3. Cyclic voltammograms of **1** in coordinating (CH_3CN) *versus* in a non-coordinating (CH_2Cl_2) solvent. The redox processes undergo cathodic shift in CH_2Cl_2.

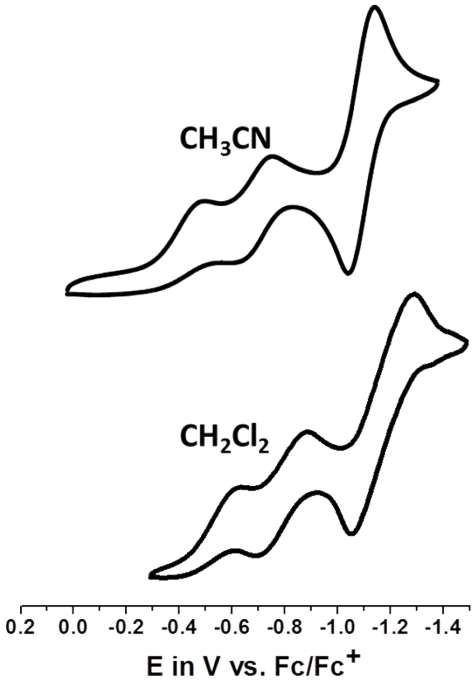


Figure S4. UV-Visible Spectra of **1**-**3** ([C] = 1.0 × 10^{-5} M) in acetonitrile.

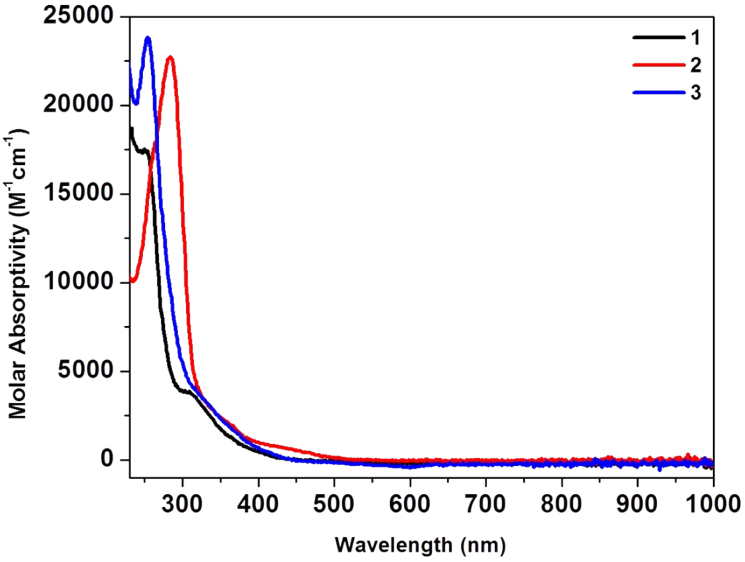


Table S1. Calculated electronic energy difference between high-spin and low-spin configurations of several [Co^{I}(L')(prdioxH)], [Co^{II}(L')(prdioxH)]$^{+}$ and [Co^{II}(L')(Cl)(prdioxH)] species (L'= $^{4\text{-}tBu}$py, $^{4\text{-}Pyr}$py, $^{4\text{-}Bz}$py)

Species	ΔE_{SCF}(Low spin - High spin) (kcal/mol)
$Co^{I}(^{4\text{-}tBu}py)(prdioxH)$	-6.5
$Co^{I}(^{4\text{-}Bz}py)(prdioxH)$	-3.4
$Co^{I}(^{4\text{-}Pyr}py)(prdioxH)$	-7.2
$Co^{II}(^{4\text{-}tBu}py)(prdioxH)$	-7.0
$Co^{II}(^{4\text{-}Bz}py)(prdioxH)$	-7.6
$Co^{II}(^{4\text{-}Pyr}py)(prdioxH)$	-5.3
$Co^{II}(Cl)(prdioxH)$	-5.8
$Co^{II}(^{4\text{-}tBu}py)(Cl)(prdioxH)$	-7.2
$Co^{II}(^{4\text{-}Bz}py)(Cl)(prdioxH)$	-7.4
$Co^{II}(^{4\text{-}Pyr}py)(Cl)(prdioxH)$	-6.2
$Co^{II}(Cl)_2(prdioxH)$	-7.3

Figure S5. Change of Cyclic voltammogram of **1** upon addition of 1 equivalent of Et_4NCl and $^{4\text{-tBu}}$pyridine in CH_3CN.

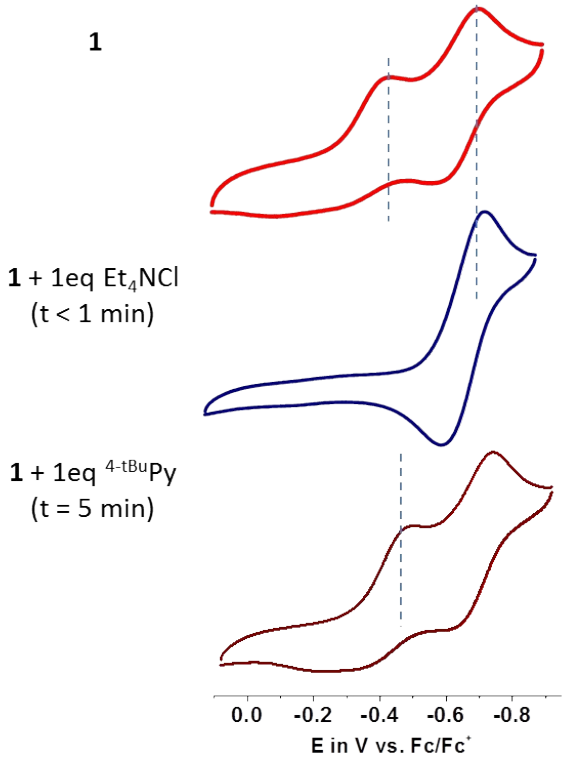


Figure S6. Cyclic voltammetric experiments for hydrogen generation with complex **2**.

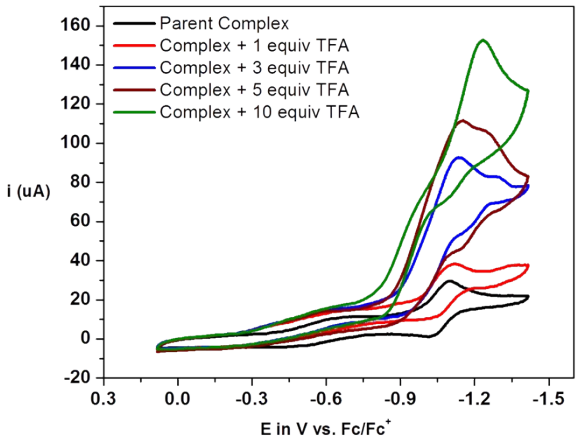


Figure S7. Cyclic voltammetric experiments for hydrogen generation with complex **3**.

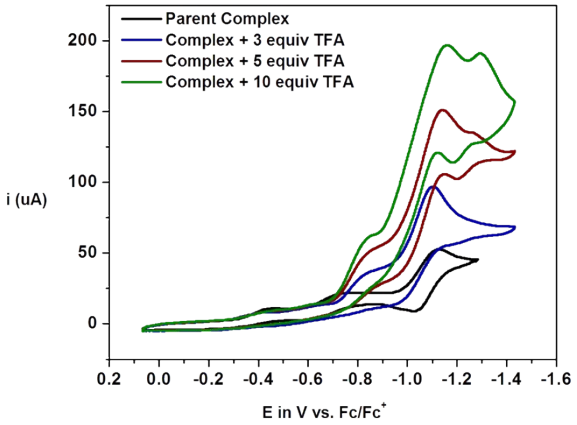


Figure S8. Cyclic voltammetric experiments for dihydrogen generation with the blank

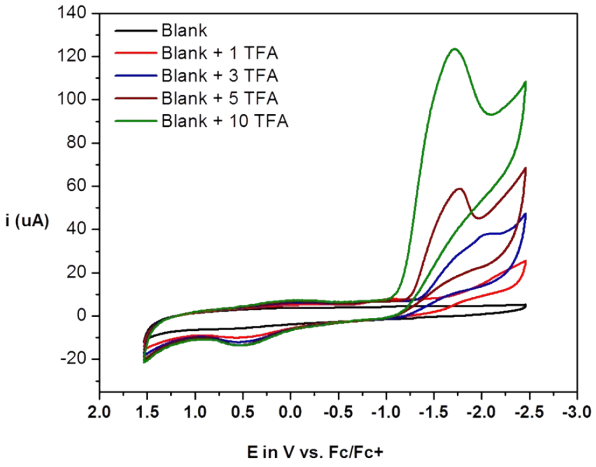


Figure S9. Plot of charge *versus* time during bulk-electrolysis experiment of **1** after 1h.

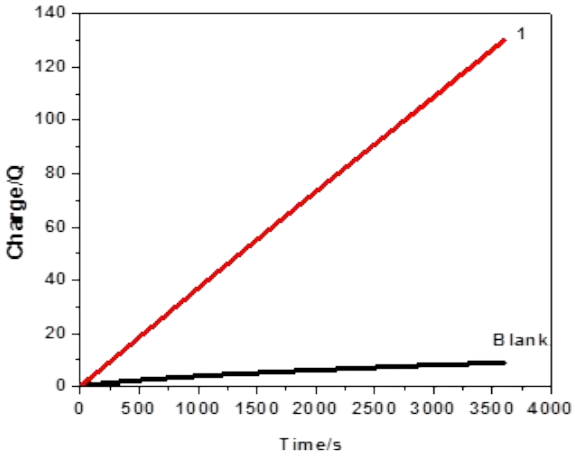


Figure S10. Plots of charge *versus* time during bulk-electrolysis experiments of **2** and **3** after 1h.

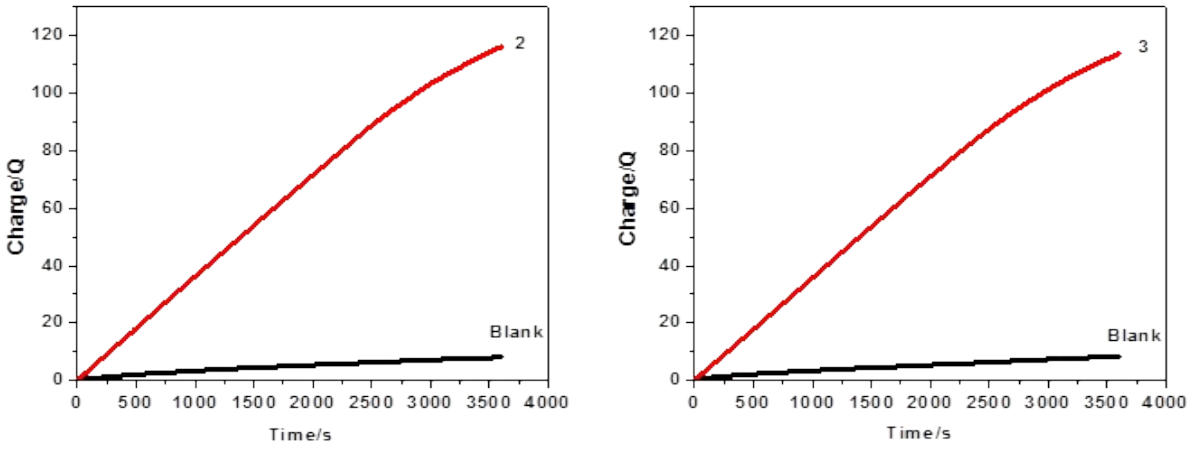
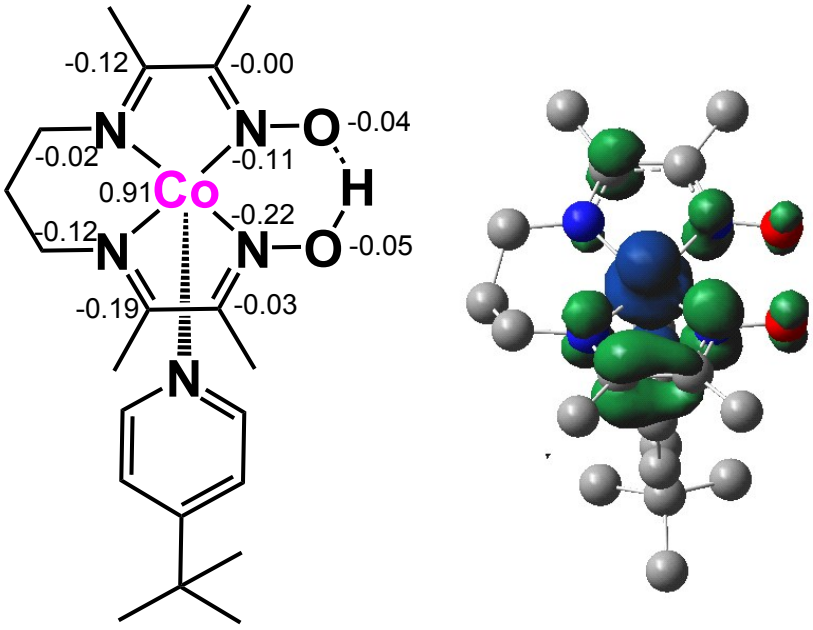


Figure S11. Redox non-innocence of the oxime ligand during the reduction of $[Co^{II}(^{4\text{-}tBu}py)(prdioxH)]^{+}$. Mulliken spin density analysis **i** and spin density plot **ii** for the complex. The hydrogen atoms are omitted for clarity in the spin density plot **ii**.



(i) **(ii)**

Calculations found that the reduction of $[Co^{II}(^{4\text{-}tBu}py)(prdioxH)]^{+}$ complex may have significant degree of redox non-innocence character displayed by the oxime ligand as the resulting metal-reduced, closed-shell (S=0), $3d^8$ Co^{I}-complex, $[Co^{I}(^{4\text{-}tBu}py)(prdioxH)]$, is 3.7 kcal/mol higher in energy than the ligand-

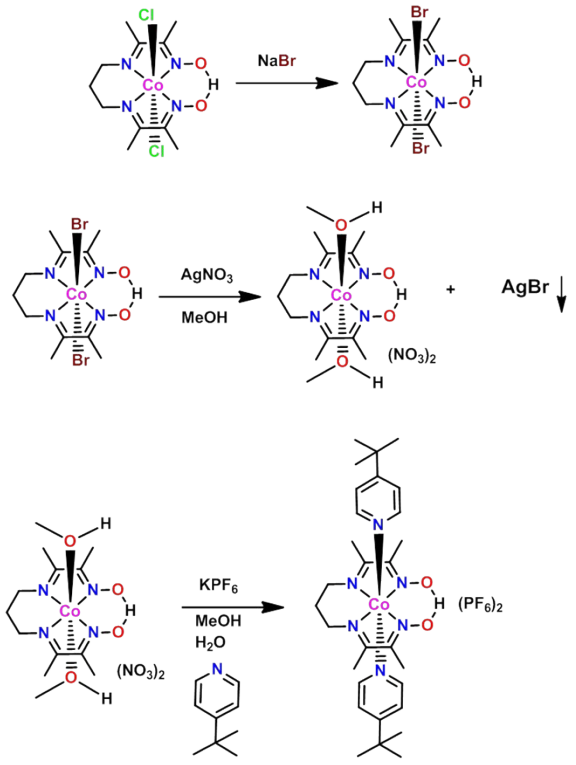
reduced, open-shell (S=0), $3d^7$ Co^{II}-complex, [Co^{II}($^{4\text{-}tBu}$py)(prdioxH$^{\bullet}$)]. As illustrated in **Figure S6**, spin density analysis of [Co^{II}($^{4\text{-}tBu}$py)(prdioxH$^{\bullet}$)] complex shows that the total spin on the cobalt center is +0.91 while it is -0.90 on the imine-oxime ligand framework confirming the electronic state of the complex as open-shell [Co^{II}($^{4\text{-}tBu}$py)(prdioxH$^{\bullet}$)]. The two unpaired electrons on the cobalt center and imine-oxime ligand HL are antiferromagnetically coupled as shown by the spin density plot (blue and green) in **ii** giving rise to an overall singlet (S=0) state. However, the EPR experiment (**Figure 8d**) demonstrated a silent spectrum that is characteristic of an overall singlet state (S=0) and failed to distinguish between the closed-shell and open-shell configurations of the species obtained from the reduction of [Co^{II}($^{4\text{-}tBu}$py)(prdioxH)]$^{+\cdot}$ When we reevaluated the energy difference of these two configurations with different functionals, it was found that the energy difference between the two electronic states is dependent on the functional used and hybrid functionals favor the open-shell configuration while the pure functionals predict the two configurations to be isoenergetic (**Table S2**).

Table S2. Dependence of the relative energy of the closed-shell and open-shell electronic states on the functional used

Functional used	[E(SCF)closed-shell - E(SCF)open-shell] (kcal/mol)
B3PW91	3.25
B3LYP	4.23
M06	3.71
BP86	-0.73
M06-L	0.09

Scheme S1. Synthesis and characterization of $[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2](PF_6)_2$

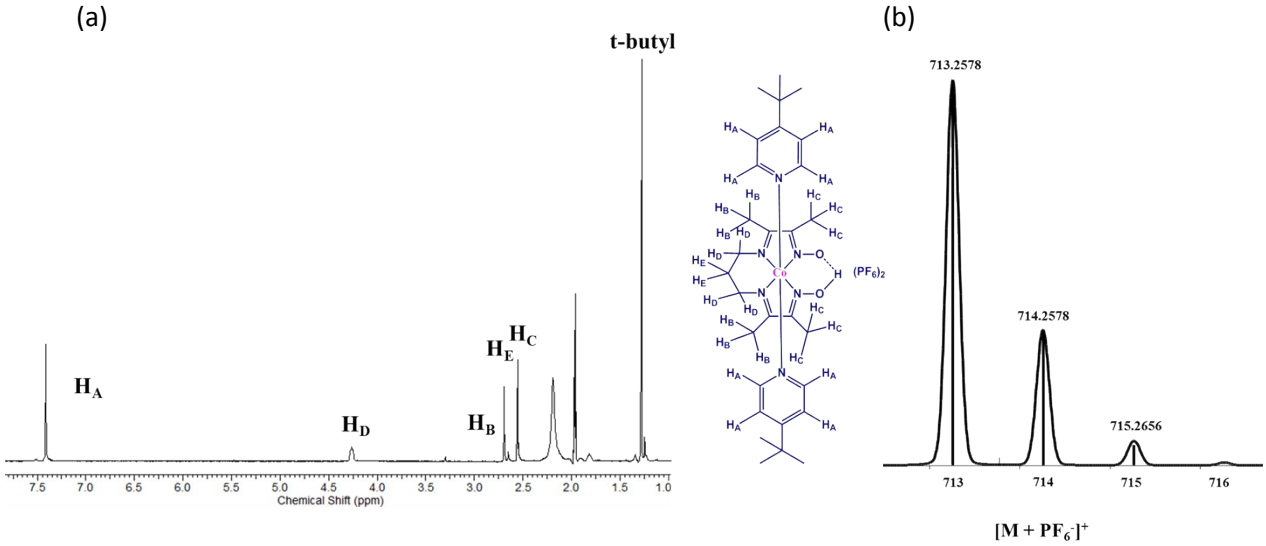
$[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2](PF_6)_2$: $[Co^{III}(prdioxH)Br_2]$ was synthesized from $[Co^{III}(prdioxH)Cl_2]$ by following literature procedure.[1,2] $[Co^{III}(prdioxH)Br_2]$ (1 mmol, 0.458 g) was dissolved in 20 mL methanol. $AgNO_3$ (2 mmol, 0.34 g) in 10 mL of methanol was added to the methanol solution of $[Co^{III}(prdioxH)Br_2]$. The solution was stirred for 2 hours and the greyish white precipitate of AgBr was removed upon filtration. $^{4\text{-}tBu}$pyridine (2 mmol, 0.27 g) in 5 mL of methanol was added to the solution followed by KPF_6 (3.4 mmol, 0.6256 g) in 10 mL of water. The reaction mixture was stirred for 2 hours and then, rotary-evaporated to 10 mL. This solution was kept for 3-4 days and brownish-yellow precipitate was generated. X-ray quality crystals were obtained after recrystalization from methanol/water (2:1) mixture. Yield: 80 %. IR (KBr, cm^{-1}) 3671 (w) (OH); 3246 (w), 3149 (w), 3106 (w) (Aromatic-CH); 2971 (s), 2911 (m), 2875 (w) (t-butyl and other aliphatic CH); 1621 (s), 1508 (m) (C=N); 1436 (m) (C=C); 822 (s) (PF_6^-). ^{1}H-NMR [400MHz, CD_3CN, 300K] δ/ppm = 1.278 [s, 18H (t-butyl)]; 2.458 [m, 2H (CH_2)]; 2.556 [s, 6H (CH_3)]; 2.692 [s, 6H (CH_3)]; 4.262 [t, 4H (CH_2)]; 7.411 [s, 8H (aryl)]. ESI pos. in MeOH: m/z = 713.2578 for $[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2]$ + PF_6^-. Anal. Calcd for $C_{29}H_{45}CoF_{12}N_6O_2P_2$: C: 40.57; H: 5.28; N: 9.79; Found: C: 40.49; H: 5.19; N: 9.91.



1. R. Hay and R. Bradshaw, *Trans. Met. Chem.*, 1996, **21**, 64.
2. P. A. Jacques, V. Artero, J. Pecaut and M. Fontecave, *Proc. Nat. Acad. Sci.*, 2009, **106**, 20627.

Associated files to Scheme S1

(a) ^{1}H-NMR spectrum of $[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2](PF_6)_2$ in CD_3CN, and (b) ESI-MS spectrum in CH_3OH



(c) Crystallographic description: An orange block crystal with dimensions 0.28 x 0.16 x 0.15 mm was mounted on a Nylon loop using very small amount of paratone oil.

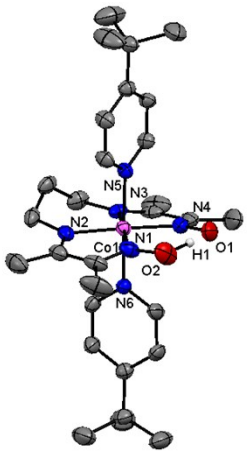
Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 0.5° per frame for 20 s. The total number of images was based on results from the program COSMO[3] where redundancy was expected to be 4.0 and completeness of 100% out to 0.83 Å. Cell parameters were retrieved using APEX II software[4] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[5] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[6] multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL- 97, which are incorporated in SHELXTL-PC V 6.10.[7]

The structure was solved in the space group $P2_1/n$ (# 14). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model except for the hydrogen located near atom O1 and atom O2 which was found and refined isotropically. The crystal used for the diffraction study showed no decomposition during data collection. All drawings are done at 50% ellipsoids.

3. COSMO V1.61, *Software for the CCD Detector Systems for Determining Data Collection Parameters.* Bruker Analytical X-ray Systems, Madison, WI (2009).
4. APEX2 V2010.11-3. Software *for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2010).

5. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).
6. SADABS V2.008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.
7. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

(d) ORTEP representation of $[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2](PF_6)_2$ (CCDC 1449138) with 50% ellipsoidal probability and selected bond-lengths (Å).



Co(1)-N(1) 1.901 Å
Co(1)-N(2) 1.915 Å
Co(1)-N(3) 1.912 Å
Co(1)-N(4) 1.886 Å
Co(1)-N(5) 1.973 Å
Co(1)-N(6) 1.977 Å

Scheme S2. Synthesis and characterization of $[Co^{III}(prdioxH)(Cl)_2]$

$[Co^{III}(prdioxH)(Cl)_2]$: This synthesis was performed by following a literature procedure of the reaction of ligand, $prdioxH_2$, with $CoCl_2.6H_2O$ in acetone/water (9:1) mixture.[8] The ligand H_2L^{oxime} (1 mmol, 0.24 g) was dissolved in 45 mL of acetone in a 100 mL round-bottom flask. A solution of $CoCl_2.6H_2O$ (1 mmol, 0.24 g) in 5 mL water was slowly added to the stirring solution of the ligand. The reaction was stirred for three hours in aerobic condition. A brown precipitate was obtained which was discarded to get a green colored filtrate. Green colored crystals were obtained from the filtrate after few days of slow evaporation. Yield: 70 %. IR (KBr, cm^{-1}) 3446 (w) (OH); 1618 (m) (C=N); 1143 (m) (N-O). ^{1}H-NMR [400 MHz, CD_3CN, 300K] δ/ppm = 2.55 [m, 2H (CH_2)]; 2.62 [s, 6H (CH_3)]; 2.68 [s, 6H (CH_3)]; 4.18 [t, 4H (CH_2)]. ESI pos. in MeOH: m/z = 333.0529 for $[Co^{III}(prdioxH)(Cl)]^+$. Anal. Calcd for $C_{11}H_{19}Cl_2CoN_4O_2$: C: 35.79; H: 5.19; N: 15.18; Found: C: 35.75; H: 5.07; N: 15.16.

8) G. Costa, G. Mestroni and E. D. Savorgnani, *Inorg. Chim. Acta,* 1969, 323.

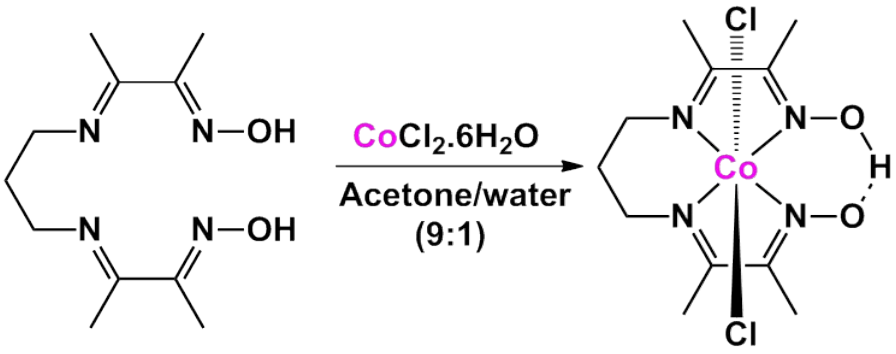


Figure S12. ^{1}H-NMR spectrum of the Co^{I}-complex, [Co^{I}(prdioxH)(^{4tBu}py)], in CD_3CN.

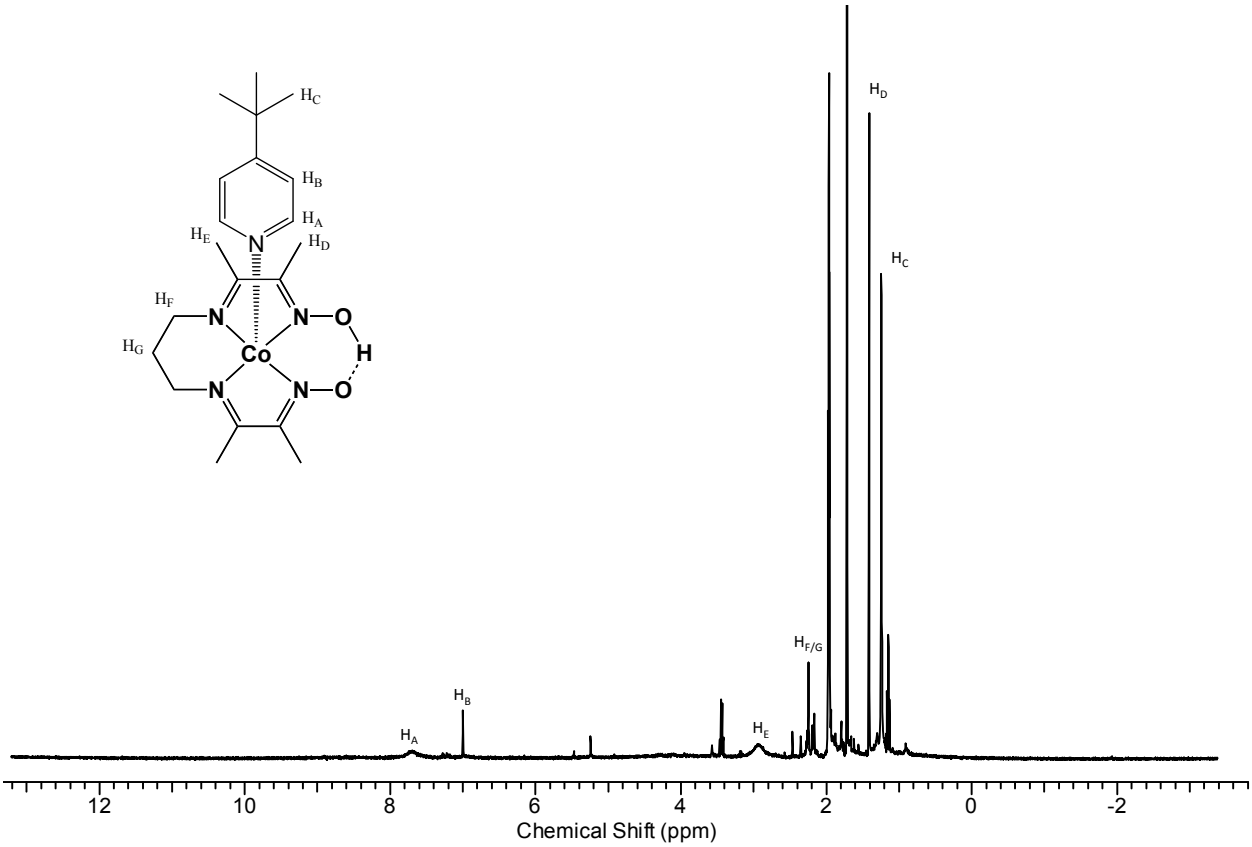
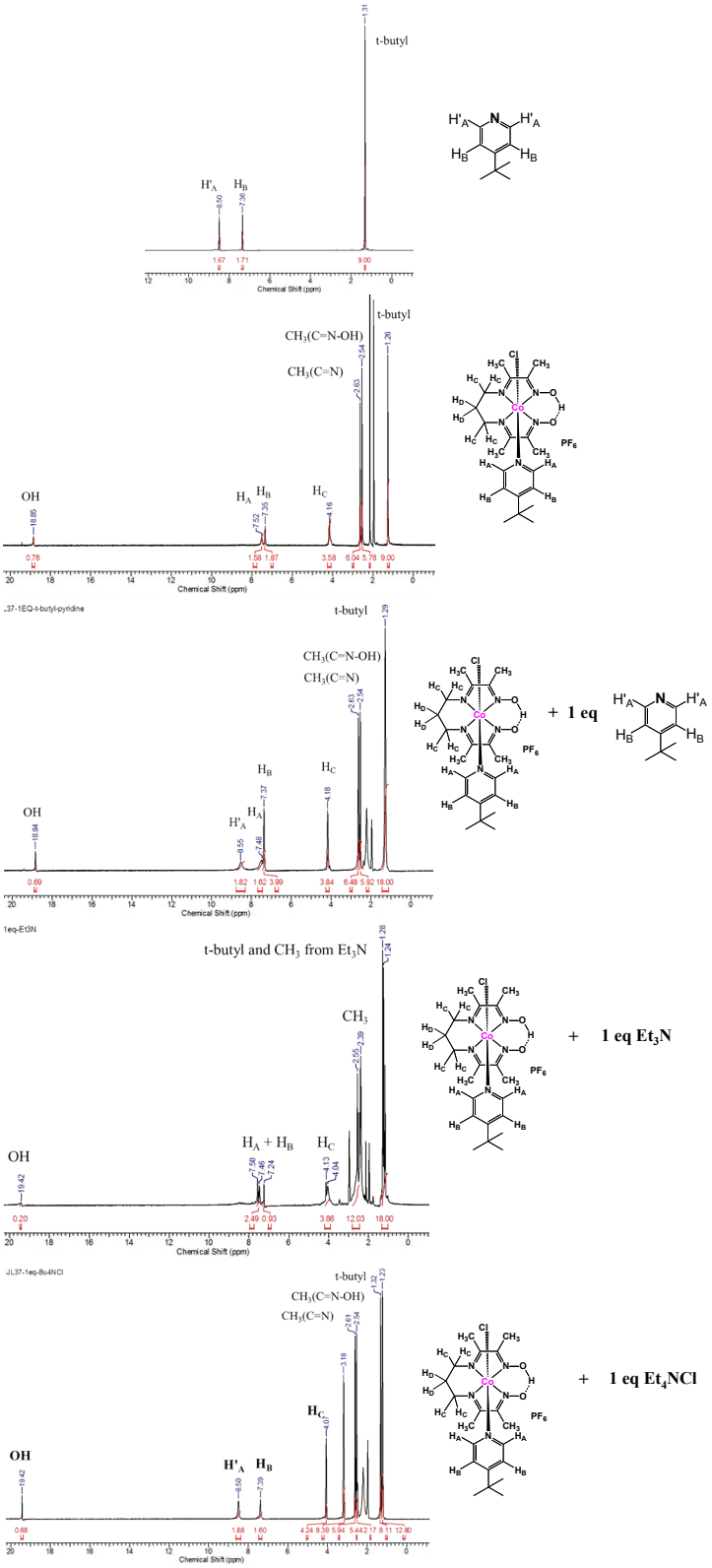


Figure S13. The full spectra for ^{1}H-NMR experiments of **1** in CD_3CN upon addition of ^{4tBu}pyridine, Et_3N, and Et_4NCl.



Energetics of addition of CH_3CN to $[Co^{II}(^{4\text{-}tBu}py)(prdioxH)]^+$

Coordination of CH_3CN to the five-coordinate $[Co^{II}(^{4tBu}py)(prdioxH)]^+$ species is calculated to be thermodynamically unfavorable by about 11 kcal/mol (ΔG), in good agreement with the literature,[9] however it may take place considering the large excess of CH_3CN as solvent. Addition of CH_3CN is calculated to be isoenergetic in terms of potential energy and there may be uncertainty in calculating the entropic contributions for association and dissociation reactions in solution.

9. A. Bhattacharjee, E. S. Andreiadis, M. C. Kerlidou, M. Fontecave, M. J. Field and V. Artero, *Chem. Eur. J.,* **2013**, *19*, 15166.

Table S3. Crystallographic information for complexes **1**, **3**, $\mathbf{4_{dimer}}$,and $\mathbf{[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2](PF_6)_2}$

	1	**3**	$\mathbf{4_{dimer}}$	$\mathbf{[Co^{III}(prdioxH)(^{4\text{-}tBu}py)_2](PF_6)_2}$
Empirical formula	$C_{21}H_{34}Cl_3CoF_6N_5O_2P$	$C_{23}H_{28}ClCoF_6N_5O_3P$	$C_{20}H_{30}CoN_5O_2$	$C_{30}H_{49}CoF_{12}N_6O_3P_2$
Formula weight	698.78	661.85	431.42	890.62
Temperature (K)	173(2)	173.15	100.1	173(2) K
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system, space group	Tetragonal, I -4	Monoclinic, P21/c	Monoclinic, C2/c	Monoclinic, P 21/n
a (Å)	28.715(4)	6.9686(4)	14.9757(13)	12.5242(14)
b (Å)	28.715(4)	22.9724(13)	10.6987(13)	16.7919(19)
c (Å)	7.0017(9)	17.7667(12)	24.941(3)	18.462(2)
α (º)	90	90	90	90
β (º)	90	96.4950(10)	98.286(8)	91.4660(10)
γ (º)	90	90	90	90
Volume ($Å^3$)	5773.5(13)	2825.9(3)	3954.3(7)	3881.4(8)
Z	8	4	8	4
Calculated density (Mg/m^3)	1.608	1.556	1.449	1.524
Absorption coefficient (mm^1)	0.996	0.833	0.895	0.622
F (000)	2864	1352	1824	1840
R(F) (%)	3.55	5.18	5.97	5.79
R_w(F) (%)	3.85	7.88	15.31	8.27
CCDC number	1434960	1434959	1448834	1449138

Table S4: Cartesian coordinates of the optimized structures

$Co^{I}(^{4\text{-}tBu}py)(prdioxH)$ (low-spin/open-shell)

Co	1.38651000	0.00629000	-0.13259900
N	1.72667400	1.43924200	1.08374800
N	1.76174000	-1.41358900	1.08293100
N	1.60092500	-1.37824000	-1.37840000
N	1.53874100	1.39724800	-1.40171300
C	1.84471300	1.29618300	2.54271900
C	1.86475800	-1.26975100	2.54215400
C	1.18874500	0.00846400	3.04452300
H	2.91034300	1.29509800	2.82712600
H	1.38247000	2.15413700	3.05022900
H	1.23251500	0.00972800	4.14182500
H	0.12984400	0.00084200	2.75768300
H	1.40403600	-2.12989500	3.04839200
H	2.92601400	-1.25720700	2.84608100
C	1.75671400	2.63300800	-0.92985500
C	1.87823800	2.63808400	0.50997500
C	1.82006300	-2.62568400	-0.91678100
C	1.93201900	-2.63219300	0.51272100
C	1.87289000	3.84161300	-1.81210000
H	2.88446600	4.26818400	-1.78300200
H	1.65119200	3.55864600	-2.84351400
H	1.17489500	4.63151000	-1.50854300
C	2.17320800	3.89712500	1.28149600
H	1.32840500	4.18163200	1.92378300
H	3.04549400	3.76778900	1.93421700
H	2.37629400	4.73280800	0.60922300
C	1.93425100	-3.79760400	-1.84704700
H	1.98757800	-4.74348900	-1.30356000
H	1.07196400	-3.83812500	-2.52348200
H	2.82807800	-3.71663000	-2.48023700
C	2.24224700	-3.86677100	1.31926500
H	3.10567600	-3.70397100	1.97714000
H	1.39837700	-4.15602800	1.96139500
H	2.47366700	-4.71797000	0.67608000
O	1.39554800	1.20766700	-2.75139700
O	1.45209300	-1.22694000	-2.76261800
H	1.40074600	-0.12539600	-2.87140000
C	-1.40010500	1.15560500	-0.05073200
C	-1.35718200	-1.16411500	-0.02099000
C	-2.79525400	1.16764000	-0.01045600
H	-0.83441300	2.08019300	-0.08035900
C	-2.75509700	-1.22678100	0.02107000
H	-0.75762500	-2.06800700	-0.02634200
C	-3.52214300	-0.04446400	0.02746200
H	-3.30228900	2.12698300	-0.01000800
H	-3.22575800	-2.20220100	0.04779500
N	-0.67650000	0.00664500	-0.05638300
C	-5.05664700	-0.03533200	0.07012600
C	-5.64780800	-1.45966600	0.11540800
H	-6.74189300	-1.39659700	0.14567500
H	-5.37330600	-2.04399800	-0.77159300
H	-5.32126300	-2.00811700	1.00772500
C	-5.52474600	0.73332000	1.33444800
H	-5.16156300	0.24506900	2.24720400
H	-5.16923600	1.77008400	1.33668800
H	-6.62095000	0.75439200	1.37000400
C	-5.59400600	0.68151500	-1.19720600
H	-5.28341200	0.15381800	-2.10733700
H	-6.69050900	0.70523500	-1.17196400
H	-5.23695300	1.71552600	-1.26311600

$Co^{I}(^{4\text{-}tBu}py)(prdioxH)$ (high-spin/open-shell)

Co	1.46012300	0.00965400	-0.13312300
N	1.73052000	1.44843200	1.10438700
N	1.71982600	-1.43772900	1.09723100
N	1.55617600	-1.40193700	-1.38203900
N	1.54085600	1.42300500	-1.39963700
C	1.84509200	1.28497200	2.56106900
C	1.83640100	-1.28610600	2.55058500
C	1.16748000	0.00052700	3.04680600
H	2.91070700	1.26200800	2.84655600
H	1.39723300	2.14588400	3.07611700
H	1.19461900	0.00028400	4.14480200
H	0.11367300	0.00578200	2.74195900
H	1.37331600	-2.14011800	3.06687300

H	2.89849300	-1.27349600	2.86005200
C	1.79673100	2.64325600	-0.91669800
C	1.92201000	2.63481700	0.53130900
C	1.85686500	-2.63633500	-0.91952900
C	1.95908600	-2.64483700	0.50862900
C	1.93720900	3.85880200	-1.78444600
H	2.95476300	4.26955500	-1.74407000
H	1.71825700	3.58878900	-2.82003700
H	1.24872600	4.65597400	-1.47789600
C	2.24949800	3.88459300	1.30336600
H	1.40357300	4.19447000	1.93223400
H	3.10548200	3.72442700	1.97004500
H	2.48984100	4.71311700	0.63514100
C	2.04440200	-3.79390800	-1.85683500
H	2.33922500	-4.70288500	-1.32794900
H	1.12014900	-4.00839700	-2.41011800
H	2.81303800	-3.56702200	-2.60658400
C	2.29716700	-3.87125000	1.31663600
H	3.15170100	-3.68776600	1.98136500
H	1.45587900	-4.17858900	1.95474800
H	2.55074300	-4.71949800	0.67764400
O	1.39674700	1.23457100	-2.73900000
O	1.46087000	-1.24230100	-2.77915700
H	1.39305000	-0.17731900	-2.87984900
C	-1.48187500	1.17356100	-0.10567800
C	-1.42455600	-1.13981000	-0.00857100
C	-2.87810400	1.18160900	-0.05031000
H	-0.92265800	2.10087700	-0.17043900
C	-2.82302000	-1.21166600	0.05044100
H	-0.81696200	-2.03802900	0.00697300
C	-3.59654600	-0.03342600	0.03238700
H	-3.39222700	2.13712500	-0.07264700
H	-3.28859400	-2.18828700	0.11041900
N	-0.74980900	0.03144300	-0.08385900
C	-5.13089300	-0.03062200	0.09657700
C	-5.71424300	-1.45593500	0.18777500
H	-6.80822400	-1.39786000	0.23212400
H	-5.44898300	-2.06209800	-0.68730900
H	-5.37189800	-1.97879100	1.08947100
C	-5.58435800	0.76849600	1.34733200
H	-5.20430500	0.30632100	2.26684200
H	-5.23426400	1.80671700	1.31676200
H	-6.68003900	0.78492700	1.39952800
C	-5.69100700	0.65041400	-1.18049800
H	-5.39046400	0.10111400	-2.08123900
H	-6.78722500	0.66876700	-1.13996300
H	-5.34080400	1.68429200	-1.27813100

$Co^{I}(^{4\text{-}tBu}py)(prdioxH)$ (low-spin/closed-shell)

Co	1.34572110	0.00469700	-0.13237301
N	1.72582112	1.42167310	1.07499608
N	1.75662712	-1.40054510	1.07458808
N	1.60369812	-1.35283610	-1.37288610
N	1.55661311	1.37307010	-1.38604210
C	1.81675013	1.29269309	2.53869218
C	1.83548613	-1.26864409	2.53928318
C	1.15997008	0.00733300	3.04139822
H	2.87688121	1.30283410	2.84037820
H	1.33898410	2.15064515	3.03126022
H	1.20239809	0.00743100	4.13851030
H	0.10138101	-0.00036200	2.75443820
H	1.36391510	-2.13133215	3.02951322
H	2.89330821	-1.26638609	2.84967220
C	1.73258913	2.62256819	-0.92295107
C	1.84349613	2.63372119	0.50980604
C	1.80106613	-2.60421019	-0.91767006
C	1.90662414	-2.61671619	0.51390204
C	1.81899413	3.82750528	-1.81421813
H	2.82882420	4.25977831	-1.81331313
H	1.57304911	3.54051525	-2.83883520
H	1.12506808	4.61472033	-1.49583211
C	2.10060715	3.89801928	1.28725609
H	1.24573709	4.16586330	1.92332814
H	2.97198622	3.79098627	1.94538414
H	2.28930317	4.73803834	0.61556904
C	1.89797214	-3.77240927	-1.85355814
H	1.96022514	-4.72090434	-1.31561210
H	1.02505507	-3.80911628	-2.51653618

H	2.78063420	-3.68696526	-2.50119718
C	2.19211216	-3.85940828	1.31676009
H	3.03552622	-3.70375026	2.00081115
H	1.32928109	-4.15566530	1.92914814
H	2.44217718	-4.70243634	0.67019305
O	1.40283010	1.19782309	-2.75002720
O	1.44671710	-1.20179109	-2.74460020
H	1.40646510	-0.02594100	-2.86030920
C	-1.33630310	1.14153208	-0.02625900
C	-1.30487810	-1.18250408	-0.01202300
C	-2.73033820	1.15713308	0.00736200
H	-0.76664206	2.06423315	-0.04664200
C	-2.70217219	-1.23652009	0.02283600
H	-0.71188505	-2.09087415	-0.02072700
C	-3.46410425	-0.05104200	0.03177900
H	-3.23203823	2.11912415	0.01217300
H	-3.17642723	-2.21036416	0.04031400
N	-0.62010305	-0.01322100	-0.03840300
C	-4.99834636	-0.03447600	0.05786200
C	-5.59610942	-1.45594510	0.09976401
H	-6.69018248	-1.38854910	0.11903201
H	-5.31504036	-2.04260915	-0.78349606
H	-5.28139538	-2.00397914	0.99655007
C	-5.47950140	0.73992305	1.31366910
H	-5.12947437	0.25366602	2.23259616
H	-5.12207237	1.77598913	1.31710010
H	-6.57607546	0.76316506	1.33501509
C	-5.51445440	0.68209205	-1.21867009
H	-5.18975837	0.15315001	-2.12310415
H	-6.61110747	0.70766605	-1.21091009
H	-5.15428737	1.71551912	-1.27928709

$Co^{II}(^{4\text{-}tBu}py)(prdioxH)$ (low-spin)

Co	-1.42790400	0.01164500	-0.13577100
N	-1.77200800	-1.43299100	1.09195300
N	-1.72603600	1.47107800	1.08576400
N	-1.50316400	1.42340800	-1.41365700
N	-1.55302600	-1.40164100	-1.40882600
C	-1.86699300	-1.26559100	2.55293200
C	-1.82925400	1.31131800	2.54711400
C	-1.17394500	0.01389500	3.02945100
H	-2.92978500	-1.24225200	2.83807900
H	-1.41642400	-2.12861900	3.05835400
H	-1.19910800	0.01650700	4.12562300
H	-0.11980800	-0.00259600	2.73066500
H	-1.35570900	2.16245400	3.05154800
H	-2.89309900	1.31945400	2.82906900
C	-1.84011700	-2.60365500	-0.95074200
C	-1.98550300	-2.59841500	0.51914300
C	-1.74646300	2.63682500	-0.96026300
C	-1.89548000	2.64195600	0.50915300
C	-1.99064700	-3.81679000	-1.81150000
H	-3.01509700	-4.20661200	-1.76505200
H	-1.76278400	-3.56708000	-2.84896800
H	-1.31799700	-4.61888900	-1.48622300
C	-2.33962200	-3.84760800	1.27069000
H	-1.48095100	-4.20374500	1.85544900
H	-3.15807800	-3.66266100	1.97492200
H	-2.64061500	-4.64968100	0.59642200
C	-1.84786500	3.85155700	-1.82567100
H	-1.13562100	4.62276800	-1.50990300
H	-1.64013700	3.58674300	-2.86359500
H	-2.85235700	4.28924200	-1.77286900
C	-2.20324100	3.90615900	1.25619400
H	-3.03902300	3.75849200	1.94887200
H	-1.33760800	4.22248600	1.85345800
H	-2.45786700	4.72151500	0.57875600
O	-1.36077700	-1.20061500	-2.74314500
O	-1.31411700	1.21127100	-2.74664800
H	-1.29485400	0.00450000	-2.84802700
C	1.37408600	-1.18811500	-0.03720800
C	1.40861000	1.12917200	-0.01298500
C	2.77121600	-1.24798200	0.00775600
H	0.78995100	-2.10012000	-0.06617600
C	2.80252400	1.14527200	0.03243700
H	0.84976900	2.05698500	-0.02224300
C	3.53432300	-0.06399000	0.04263700
H	3.24358200	-2.22260300	0.01221700

H	3.30513200	2.10613000	0.05709900
N	0.68554300	-0.02088000	-0.04940500
C	5.06781200	-0.04927100	0.08267700
C	5.59482400	0.69802500	-1.17174100
H	6.69129900	0.71852800	-1.15489000
H	5.27507500	0.19371700	-2.09181300
H	5.23984700	1.73432000	-1.20835900
C	5.53549700	0.69587800	1.36138500
H	5.17701100	0.18820300	2.26524400
H	6.63164800	0.71831100	1.39334900
H	5.17809100	1.73168100	1.38549600
C	5.66462800	-1.47151100	0.09623300
H	5.34217800	-2.04071500	0.97687600
H	5.39206400	-2.03685500	-0.80342100
H	6.75834300	-1.40485200	0.12725000

$Co^{II}(^{4\text{-}tBu}py)(Cl)(prdioxH)$ (low-spin)

Co	-0.00244800	-0.44467900	-0.11240500
N	1.48297500	-0.59738100	1.10575200
N	-1.45669100	-0.59309500	1.14419400
N	-1.44225300	-0.42455500	-1.35739900
N	1.40483700	-0.42424900	-1.39427100
C	1.32190900	-0.72895900	2.56057900
C	-1.26047100	-0.71888900	2.59538000
C	0.03975100	-0.05372300	3.06178400
H	1.29505200	-1.80044300	2.81043700
H	2.18370300	-0.29628000	3.08370400
H	0.05421200	-0.08858800	4.15834100
H	0.03996000	1.00302600	2.77035800
H	-2.10490700	-0.27496200	3.13716100
H	-1.23799200	-1.78916400	2.85095500
C	2.63563300	-0.55136300	-0.94316600
C	2.65991400	-0.67511500	0.52703700
C	-2.66127200	-0.55159800	-0.87499000
C	-2.64813400	-0.66966200	0.59568700
C	3.85107800	-0.58367600	-1.81612200
H	4.35105300	-1.55890100	-1.75981100
H	3.56539600	-0.40309600	-2.85396800
H	4.57951800	0.17803100	-1.51379400
C	3.95043800	-0.88888600	1.26831000
H	4.18886200	-0.02241200	1.89907300
H	3.88233000	-1.76254200	1.92640900
H	4.78460100	-1.04309000	0.58303600
C	-3.89794700	-0.58812400	-1.71749600
H	-4.61566100	0.18038900	-1.40660600
H	-3.63670000	-0.42060200	-2.76397500
H	-4.40059900	-1.56028800	-1.63779000
C	-3.92003200	-0.87531600	1.37063300
H	-3.83832900	-1.74552600	2.03174200
H	-4.13942500	-0.00444800	2.00223500
H	-4.77194500	-1.03032100	0.70777600
O	1.17227300	-0.29736800	-2.73408100
O	-1.24398500	-0.30009600	-2.70255900
H	-0.03564100	-0.28226600	-2.81373700
C	1.15847300	2.54527300	0.02407000
C	-1.15291700	2.55530400	-0.01212600
C	1.20479400	3.94445900	0.07617600
H	2.07765200	1.97115700	0.01799200
C	-1.18765800	3.95066900	0.03737000
H	-2.07481300	1.98691500	-0.04795200
C	0.01279000	4.69530500	0.08490300
H	2.17395600	4.42744700	0.10934900
H	-2.15466300	4.44302600	0.03805100
Cl	0.00200100	-3.18437200	-0.28454300
N	0.00232200	1.84152000	-0.01936700
C	-0.01759700	6.22896100	0.13980300
C	-0.73406800	6.76591600	-1.12786700
C	-0.80077100	6.67562100	1.40295900
C	1.39826700	6.83878900	0.19908400
H	-0.77404100	7.86165300	-1.09375300
H	-0.19594500	6.47076100	-2.03701500
H	-1.76222400	6.39418400	-1.20332000
H	-0.31308500	6.31221700	2.31591300
H	-0.83750400	7.77102800	1.44690400
H	-1.83239200	6.30553100	1.39582000
H	1.94559700	6.51154900	1.09184500
H	1.99169900	6.58052400	-0.68675600
H	1.32034900	7.93158200	0.23878200

$Co^{II}(Cl)(prdioxH)$ (low-spin)

Co	-0.00005400	-0.11754400	-0.10954700
N	-1.45928400	1.12583600	-0.28141600
N	1.45919500	1.12591600	-0.28148800
N	1.41741800	-1.38323800	-0.22854200
N	-1.41750900	-1.38329700	-0.22834300
C	-1.29042400	2.58903100	-0.28830500
C	1.29031700	2.58912100	-0.28817900
C	-0.00009800	3.01945400	0.41680900
H	-1.27875700	2.93597000	-1.33311600
H	-2.14332200	3.07167600	0.20377600
H	-0.00012600	4.11515000	0.46931000
H	-0.00014400	2.63549100	1.44314200
H	2.14314300	3.07169500	0.20409200
H	1.27877300	2.93622000	-1.33293000
C	-2.63941700	-0.90891000	-0.35325000
C	-2.64318800	0.56620000	-0.39706400
C	2.63931000	-0.90885100	-0.35343000
C	2.64308200	0.56627300	-0.39719100
C	-3.86712500	-1.76079700	-0.42217500
H	-4.37175900	-1.65231200	-1.39036900
H	-3.59774500	-2.80983500	-0.28866900
H	-4.58534400	-1.48010500	0.35715400
C	-3.92557200	1.33363900	-0.54789300
H	-4.19271000	1.82652200	0.39649000
H	-3.83221500	2.11423400	-1.31016800
H	-4.75202700	0.67877300	-0.82635500
C	3.86701000	-1.76075500	-0.42234700
H	4.58560800	-1.47944000	0.35639400
H	3.59771100	-2.80970200	-0.28793000
H	4.37114900	-1.65301000	-1.39088500
C	3.92554200	1.33358800	-0.54797900
H	3.83172800	2.11560800	-1.30870600
H	4.19389100	1.82454200	0.39706900
H	4.75144500	0.67889500	-0.82853000
O	-1.20622900	-2.72926600	-0.15968200
O	1.20619000	-2.72924700	-0.16001700
H	0.00013800	-2.83140700	-0.13550900
Cl	0.00041200	-0.16421400	2.40386300

$Co^{II}(Cl_2)(prdioxH)$ (low-spin)

Co	0.11441800	-0.00968300	-0.00444800
N	-1.35113400	1.11690200	-0.54104900
N	1.57651100	1.21553400	-0.27831900
N	1.53474000	-1.15900700	0.52239400
N	-1.30018600	-1.24952200	0.27976300
C	-1.17146200	2.49467100	-1.01737900
C	1.39797100	2.58831000	-0.77079100
C	0.03934600	3.16958800	-0.36100100
H	-1.03561000	2.46898000	-2.10935200
H	-2.06720000	3.09434000	-0.81522600
H	0.02881200	4.22861800	-0.64861700
H	-0.06383800	3.11198100	0.72868500
H	2.19413700	3.24092800	-0.39189200
H	1.48113100	2.57799500	-1.86854100
C	-2.52267500	-0.84297300	0.01076800
C	-2.53189300	0.54632300	-0.48191800
C	2.75746500	-0.67671800	0.45997200
C	2.76334600	0.71642300	-0.02209100
C	-3.74580200	-1.68857900	0.18770800
H	-4.24221600	-1.87698200	-0.77270100
H	-3.46890100	-2.64895800	0.62653800
H	-4.47458000	-1.19955500	0.84526600
C	-3.81838700	1.21915100	-0.87874500
H	-4.06461300	2.03254800	-0.18357600
H	-3.74323500	1.65512200	-1.88114600
H	-4.65231100	0.51605700	-0.87612400
C	3.98464500	-1.44875800	0.83510500
H	4.55529100	-0.93210100	1.61634700
H	3.70068800	-2.43562300	1.20534500
H	4.65044400	-1.58009100	-0.02720200
C	4.05318000	1.47160200	-0.19687400
H	4.12074700	1.90801000	-1.19973300
H	4.12537200	2.29545200	0.52527800
H	4.91775500	0.82317600	-0.04952000
O	-1.08352100	-2.51553600	0.74764500
O	1.32242600	-2.44028000	0.94955700
H	0.12140500	-2.56650800	0.88317400
Cl	-0.13250500	0.81677400	2.57691800

Cl	0.36079400	-0.88427400	-2.56370500

$Co^{II}(H)(^{4\text{-}tBu}py)(prdioxH)$ (low-spin)

Co	-0.01190400	-0.54354800	0.31092200
N	-1.41738800	-1.04030000	-0.88652800
N	1.47758800	-1.08738400	-0.76296000
N	1.35587700	-0.21112200	1.58696400
N	-1.47447100	-0.18371800	1.43832300
C	-1.19556600	-1.62855300	-2.20759100
C	1.36763600	-1.62426200	-2.12736600
C	0.10765700	-1.13680000	-2.84466500
H	-1.16297600	-2.73294900	-2.14533000
H	-2.02698500	-1.37934600	-2.88215600
H	0.14899100	-1.50702100	-3.87763100
H	0.10573200	-0.04079000	-2.88698100
H	2.25159300	-1.34125200	-2.71378900
H	1.35343900	-2.72575200	-2.07920300
C	-2.70603900	-0.55297000	1.00939300
C	-2.66209900	-1.05311900	-0.32260100
C	2.59282500	-0.55045700	1.22841500
C	2.63962800	-1.07301200	-0.13009400
C	-3.90764000	-0.41109700	1.89868200
H	-3.78292200	-0.99065000	2.82256700
H	-4.05382500	0.63427700	2.20116800
H	-4.82072900	-0.75030400	1.40439700
C	-3.86980500	-1.55479000	-1.07270200
H	-4.09158000	-0.93248800	-1.95189100
H	-3.71878000	-2.58017600	-1.43578300
H	-4.76048400	-1.55696900	-0.44097400
C	3.77948700	-0.40652600	2.13289200
H	4.56069100	0.21516500	1.67853900
H	3.46527700	0.05887200	3.06962800
H	4.22747300	-1.38130900	2.36538000
C	3.92456500	-1.56640700	-0.73808300
H	3.81071600	-2.58647100	-1.12368700
H	4.23320500	-0.93342600	-1.58058400
H	4.73447000	-1.56758200	-0.00732900
O	-1.36691000	0.27241400	2.76868100
O	1.11666500	0.30312200	2.81303700
H	-0.31724700	0.35518400	2.89590100
C	-1.11639400	2.09341100	-0.68860200
C	1.19529800	2.15361200	-0.53989700
C	-1.15714400	3.41142500	-1.14691500
H	-2.02327300	1.51594600	-0.55872000
C	1.23092400	3.47754400	-0.99528000
H	2.11308800	1.63332400	-0.29186900
C	0.03570700	4.15108400	-1.31578200
H	-2.12471800	3.84946800	-1.36916100
H	2.19450500	3.96299700	-1.09185100
N	0.04483900	1.45861500	-0.38429600
H	-0.05096800	-1.92297300	0.79398100
C	-0.00674700	5.59915300	-1.82352300
C	1.39987600	6.22445200	-1.92303300
H	2.04121000	5.67653200	-2.62457800
H	1.31383900	7.25477100	-2.28799500
H	1.90037400	6.25755700	-0.94740900
C	-0.85968800	6.45454100	-0.84921700
H	-0.90449500	7.48990200	-1.20905900
H	-1.88731200	6.08143000	-0.77166800
H	-0.42055000	6.45965400	0.15596100
C	-0.65837400	5.62049800	-3.23208000
H	-0.70112200	6.65155700	-3.60449300
H	-0.07457900	5.02298700	-3.94317600
H	-1.68101900	5.22691200	-3.21301700

$Co^{III}(Cl)(^{4\text{-}tBu}py)(prdioxH)$ (low-spin)

Co	-1.24783000	0.01105900	-0.13994700
N	-1.47592600	-1.36886400	1.18635500
N	-1.39971200	1.55028600	1.00587700
N	-1.09057000	1.35637500	-1.48227200
N	-1.26447300	-1.48633500	-1.31711200
C	-1.81411200	-1.11300900	2.59782800
C	-1.80136500	1.46388100	2.42294600
C	-1.28112600	0.21302400	3.13743000
H	-2.91085300	-1.12626500	2.67735900
H	-1.43183800	-1.92645300	3.22409600
H	-1.61049200	0.28558000	4.18055500
H	-0.18772100	0.19745500	3.16608200

H	-1.45589000	2.35178600	2.96333800
H	-2.90015700	1.47039500	2.44980000
C	-1.36587400	-2.67457900	-0.76853600
C	-1.51678900	-2.58490000	0.69569800
C	-1.09836400	2.60372600	-1.07830900
C	-1.33515300	2.70016400	0.37628500
C	-1.38124600	-3.94932400	-1.54618200
H	-2.35854200	-4.44183200	-1.47126400
H	-1.17634200	-3.74739800	-2.59835900
H	-0.62774200	-4.64768900	-1.16531500
C	-1.77270400	-3.81183900	1.51986800
H	-1.00346000	-3.93067000	2.29233900
H	-2.74037200	-3.74045000	2.03026400
H	-1.77801700	-4.71195100	0.90610300
C	-0.93729500	3.77626200	-1.98969400
H	-0.16123600	4.45437800	-1.61811800
H	-0.66238000	3.43875700	-2.98984200
H	-1.87115600	4.34726000	-2.06254900
C	-1.54622300	4.03032400	1.03549300
H	-2.53909700	4.07849100	1.49753700
H	-0.80679100	4.19603800	1.82821000
H	-1.46408200	4.84845500	0.32087100
O	-1.15873100	-1.34320600	-2.66063200
O	-0.94069100	1.05178200	-2.79545800
H	-1.05568900	-0.11709100	-2.84457200
C	1.47373300	-0.67073200	-0.99825200
C	1.42386800	0.60385300	0.94247100
C	2.86906500	-0.71246700	-0.96940600
H	0.94709600	-1.14624300	-1.81254000
C	2.81285900	0.59360600	1.02528100
H	0.84851900	1.14562200	1.67459600
C	3.59172700	-0.08181100	0.06049400
H	3.37161400	-1.24320200	-1.76813400
H	3.27162200	1.12413400	1.85196500
Cl	-3.54048400	0.08756900	-0.35000400
N	0.73740600	-0.03327300	-0.04757100
C	5.12027200	-0.09718000	0.15338400
C	5.76513900	-0.89448400	-0.99855700
H	5.52634900	-0.46236900	-1.97808800
H	6.85494900	-0.87456900	-0.88514200
H	5.45053300	-1.94538800	-0.99387300
C	5.53557500	-0.74518200	1.50153900
H	6.62917600	-0.75363700	1.58124700
H	5.14141900	-0.19132100	2.36104900
H	5.17919100	-1.78033900	1.56677200
C	5.64164700	1.36451400	0.10023700
H	5.24809700	1.97042400	0.92430900
H	6.73547700	1.36482900	0.17625800
H	5.36394800	1.84700800	-0.84462900

$Co^{III}(Cl)(^{4\text{-}Pyr}py)$(prdioxH) (low-spin)

Co	-1.44734400	0.00093600	-0.10763400
N	-1.58609200	-1.47167200	1.12134800
N	-1.59217900	1.45788900	1.13872900
N	-1.46697400	1.43268300	-1.36865700
N	-1.47427200	-1.41488900	-1.38641900
C	-1.67899500	-1.30073700	2.57964200
C	-1.69257900	1.26637300	2.59398100
C	-1.00277600	-0.01645500	3.06144000
H	-2.74342700	-1.28836400	2.85622300
H	-1.22048300	-2.16095500	3.08047900
H	-1.02772900	-0.02284300	4.15718200
H	0.05142800	-0.00972300	2.76458800
H	-1.24828300	2.12516600	3.10974200
H	-2.75852900	1.23641400	2.86309700
C	-1.65830600	-2.63086400	-0.92362400
C	-1.74634900	-2.64132800	0.54975000
C	-1.64889200	2.64321000	-0.89134000
C	-1.75066600	2.63454000	0.58108700
C	-1.76909800	-3.84428500	-1.78748600
H	-2.76736900	-4.29113800	-1.70271300
H	-1.59740200	-3.57758400	-2.83120800
H	-1.03907900	-4.60669100	-1.49285100
C	-2.00862000	-3.90963900	1.30479800
H	-1.13250700	-4.19512500	1.90128500
H	-2.84818200	-3.78288900	1.99697900
H	-2.24042700	-4.73528600	0.63240300
C	-1.74559200	3.86894400	-1.73935000

H	-1.02923500	4.63132300	-1.41342300
H	-1.54478900	3.61941400	-2.78209400
H	-2.74894000	4.30778300	-1.67469400
C	-2.02270500	3.89310300	1.34885600
H	-2.85672300	3.75156400	2.04459600
H	-1.14610000	4.18403500	1.94215700
H	-2.26763000	4.72130200	0.68416000
O	-1.35557700	-1.18486300	-2.71387000
O	-1.34118200	1.21934900	-2.69849700
H	-1.31866800	0.01864200	-2.81512800
C	1.24526800	-1.16049500	-0.07916600
C	1.24471800	1.16111500	0.00476300
C	2.62749700	-1.20728500	-0.05992200
H	0.69282300	-2.08669500	-0.12256400
C	2.62690400	1.20677200	0.03016100
H	0.69197000	2.08755900	0.03454800
C	3.39061400	-0.00040900	-0.00628500
H	3.10889400	-2.17646700	-0.09696300
H	3.10754000	2.17550200	0.08478400
N	0.52396100	0.00064000	-0.05154000
N	4.74327100	-0.00076200	0.00892200
C	5.57018700	-1.23006100	0.03019800
C	5.57171100	1.22766700	-0.00117400
C	6.98659400	-0.71034500	0.32871400
H	5.21309800	-1.92575100	0.79766300
C	6.99152100	0.70625600	-0.28054400
H	5.22580700	1.92347300	-0.77359700
H	7.14642100	-0.65839600	1.41185000
H	7.75609000	1.35377200	0.15683200
H	5.51106600	1.73458400	0.97181700
H	5.52200500	-1.73668500	-0.94364200
H	7.75608200	-1.35873400	-0.09862200
H	7.16548100	0.65395500	-1.36146000
Cl	-3.76338000	0.00141200	-0.19294500

$Co^{III}(Cl)(^{4\text{-}Bz}py)(prdioxH)$ (low-spin)

Co	-1.86761300	0.14036400	-0.07099200
N	-2.13875100	-1.08737700	1.38469200
N	-1.51782300	1.74179900	0.93810700
N	-1.76964100	1.36251700	-1.53347300
N	-2.37998100	-1.38573600	-1.09741800
C	-1.97933800	-0.71177300	2.79909600
C	-1.43569100	1.76828600	2.40829800
C	-0.98059500	0.43004400	2.99294800
H	-2.96384500	-0.41667400	3.18985500
H	-1.64680500	-1.58399400	3.37312100
H	-0.85150100	0.57209400	4.07188100
H	-0.00059900	0.15146600	2.59113400
H	-0.73959500	2.55437300	2.72156600
H	-2.42762600	2.02851100	2.80496500
C	-2.76453400	-2.44964100	-0.42845600
C	-2.64140700	-2.24614400	1.02878400
C	-1.63286000	2.63517800	-1.23557800
C	-1.51854100	2.84135400	0.22207100
C	-3.26765100	-3.70059600	-1.06966900
H	-4.32263900	-3.86661600	-0.81862500
H	-3.17819000	-3.62819100	-2.15436100
H	-2.70371200	-4.57473800	-0.72555300
C	-3.07337200	-3.30098700	2.00155900
H	-2.20775300	-3.71765500	2.53269600
H	-3.74776900	-2.87994000	2.75522300
H	-3.58644600	-4.12153300	1.50056800
C	-1.60011300	3.72969400	-2.25076400
H	-0.74122000	4.39010400	-2.09062500
H	-1.54045000	3.30795700	-3.25513500
H	-2.50748200	4.34364700	-2.18824200
C	-1.41166500	4.21910200	0.80151000
H	-2.06509700	4.33188000	1.67186900
H	-0.38364900	4.42038800	1.13095700
H	-1.68119300	4.97940400	0.06810100
O	-2.40319700	-1.36459300	-2.44890500
O	-1.88317200	0.95406500	-2.81678500
H	-2.12871300	-0.22830100	-2.74509200
C	0.48478300	-1.59862500	-0.13451400
C	0.98923900	0.65293200	-0.46713400
C	1.82673900	-1.95425400	-0.25442600
H	-0.25883700	-2.35796400	0.04488400
C	2.35183100	0.36974000	-0.58288700

H	0.64472700	1.67033100	-0.56098100
C	2.79369900	-0.95875700	-0.47171300
H	2.11233800	-2.99676600	-0.17771600
H	3.03895100	1.18449500	-0.77772200
N	0.05903100	-0.31028300	-0.23751000
Cl	-4.10861300	0.65862700	0.09660100
C	4.23264400	-1.35959800	-0.66605700
O	4.46984400	-2.42792700	-1.28592000
C	5.32723300	-0.50411000	-0.14352200
C	6.60541100	-0.61054700	-0.73847900
C	5.14173100	0.36231700	0.95746500
C	7.67510800	0.14989100	-0.25307000
H	6.74154500	-1.28358600	-1.57962500
C	6.21980000	1.11168500	1.45130800
H	4.17588900	0.43099800	1.44924800
C	7.48423200	1.01249800	0.84417000
H	8.65179700	0.07397200	-0.72129700
H	6.07630000	1.76579900	2.30585700
H	8.31578800	1.59911700	1.22407900

$Co^{III}(Cl_2)$(prdioxH) (low-spin)

Co	0.11389000	-0.01008400	0.00335000
N	-1.34860600	1.12085100	-0.51737700
N	1.56934800	1.21551200	-0.26140900
N	1.53670800	-1.17047900	0.51708300
N	-1.29958700	-1.26005500	0.27379700
C	-1.16680900	2.49306800	-1.01263100
C	1.39152200	2.58044600	-0.77801400
C	0.04309100	3.18540600	-0.38112600
H	-1.04085700	2.44483600	-2.10423300
H	-2.06489000	3.08650000	-0.81062600
H	0.03869700	4.22891100	-0.71775300
H	-0.05741300	3.18887700	0.70910500
H	2.19595100	3.22696700	-0.41073800
H	1.47447100	2.54213900	-1.87417400
C	-2.51760300	-0.84512500	0.01616700
C	-2.52555500	0.54822700	-0.46415000
C	2.75237700	-0.67974600	0.46545500
C	2.75374700	0.71595900	-0.00848800
C	-3.73913500	-1.68946500	0.18934600
H	-4.22636300	-1.87851200	-0.77509100
H	-3.46904500	-2.64860400	0.63355300
H	-4.46985100	-1.19339600	0.83823000
C	-3.80726700	1.22162700	-0.86371300
H	-4.05516400	2.02901900	-0.16282300
H	-3.72480300	1.66416800	-1.86202900
H	-4.64018200	0.51844100	-0.87051700
C	3.97827500	-1.44945300	0.83977300
H	4.54254500	-0.93160300	1.62400700
H	3.69991900	-2.43937600	1.20412200
H	4.64448200	-1.57067200	-0.02297400
C	4.03897100	1.47197600	-0.18703900
H	4.10727400	1.89640400	-1.19441500
H	4.10246200	2.30329800	0.52651600
H	4.90448200	0.82873600	-0.02845800
O	-1.07500800	-2.51827700	0.72262400
O	1.31875100	-2.44369400	0.92626200
H	0.12388200	-2.58183400	0.86115800
Cl	-0.09795200	0.65885400	2.19778500
Cl	0.32580000	-0.70651100	-2.18004200

$Co^{III}(^{4\text{-}tBu}py)_2$(prdioxH) (low-spin)

Co	-0.05183900	-0.01241500	-0.06974900
N	-0.04564700	1.45350100	1.18517900
N	-0.04125800	-1.46603000	1.18622200
N	0.02722200	-1.43660600	-1.32926300
N	0.03971200	1.41781500	-1.32865600
C	-0.25908700	1.29457600	2.63963000
C	-0.22843800	-1.29750300	2.64144700
C	-0.98245800	-0.00985600	2.98641200
H	0.70760200	1.34712300	3.15972100
H	-0.86022400	2.13446300	3.00486700
H	-1.14078900	-0.00966900	4.07067400
H	-1.97340100	-0.02267900	2.52359700
H	-0.79712200	-2.14959800	3.02931500
H	0.75037300	-1.31610000	3.14119800
C	0.23806800	2.62047800	-0.84442900
C	0.19771200	2.62121700	0.63854000

C	0.21999400	-2.64226500	-0.83855700
C	0.18760800	-2.63834000	0.63969600
C	0.41856200	3.84369100	-1.67841900
H	1.43986200	4.23077000	-1.57438200
H	0.24193600	3.61488100	-2.72998400
H	-0.26795800	4.63761700	-1.36583600
C	0.36008800	3.89862600	1.40020500
H	-0.61702600	4.37755000	1.55248200
H	0.80761600	3.73020500	2.38198400
H	0.98632300	4.60323800	0.84936300
C	0.38685200	-3.86597100	-1.67605600
H	-0.33214200	-4.64150200	-1.39020400
H	0.24288400	-3.62167100	-2.72938600
H	1.39279400	-4.28525600	-1.55077600
C	0.34395400	-3.91006500	1.41338800
H	0.89702200	-3.74821100	2.34210100
H	-0.64095800	-4.31918700	1.67755300
H	0.86662100	-4.66566100	0.82517000
O	-0.03857500	1.20563500	-2.66827800
O	-0.05721600	-1.21057600	-2.65531500
H	-0.11178600	0.05550900	-2.77883300
C	-2.75034900	1.15155300	-0.22833600
C	-2.74927500	-1.16981400	-0.23968300
C	-4.13724900	1.18371100	-0.32835900
H	-2.19885600	2.07737200	-0.18438200
C	-4.13994300	-1.20290700	-0.34184800
H	-2.19880000	-2.09685100	-0.20449700
C	-4.88749200	-0.01115600	-0.39138200
H	-4.61821800	2.15471100	-0.35773200
H	-4.61989100	-2.17217500	-0.38374200
N	-2.04106400	-0.01124500	-0.18235800
C	2.63461300	-0.06848400	-1.22289300
C	2.63767600	0.02932900	1.10093000
C	4.02902200	-0.07336000	-1.25430800
H	2.07711600	-0.10971500	-2.14833500
C	4.02823400	0.02719000	1.13306200
H	2.07950700	0.06964200	2.02249800
C	4.77835100	-0.02547500	-0.06299400
H	4.51144600	-0.11655900	-2.22228500
H	4.51156400	0.06678300	2.10258500
N	1.93039900	-0.01744000	-0.06061200
C	-6.41388600	0.02373500	-0.50594000
C	-7.02497900	-1.39019600	-0.58408500
C	-6.80364000	0.80616100	-1.78916800
C	-6.99259700	0.74977100	0.73868400
H	-6.80659800	-1.98149900	0.31373000
H	-8.11445100	-1.30747200	-0.66749300
H	-6.66602600	-1.94142200	-1.46192000
H	-7.89596600	0.84126000	-1.87600600
H	-6.43620700	1.83834900	-1.76868000
H	-6.40382900	0.31665500	-2.68531500
H	-6.61809400	1.77590000	0.82511900
H	-8.08504100	0.79660100	0.65773000
H	-6.74004900	0.21241600	1.66072900
C	6.30956500	-0.03241000	-0.03028800
C	6.92206400	-0.08662600	-1.44477300
C	6.78679200	-1.27595100	0.76784600
C	6.80371200	1.25840000	0.67678600
H	6.63593900	0.78378900	-2.04800300
H	8.01479200	-0.08802100	-1.36371000
H	6.62883400	-0.99651400	-1.98272000
H	7.88235600	-1.28476000	0.80842000
H	6.41333800	-1.27019000	1.79811500
H	6.45442600	-2.20370100	0.28674000
H	6.43292700	1.33084600	1.70527800
H	7.89940700	1.25605100	0.71526900
H	6.48222900	2.15369300	0.13108900

Co^{III}(Cl)(prdioxH) (low-spin)

Co	0.00042900	-0.11458400	-0.11743000
N	-1.45436000	1.12693700	-0.25856100
N	1.45584000	1.12700600	-0.25303200
N	1.42311700	-1.39498200	-0.19655800
N	-1.42272000	-1.39459500	-0.20167700
C	-1.28270300	2.59254700	-0.26011300
C	1.28733400	2.59316700	-0.24727300
C	-0.00120200	3.02504800	0.45370200
H	-1.27127800	2.93812900	-1.30366300

H	-2.14006100	3.06024600	0.23473200
H	-0.00139400	4.11989100	0.49403700
H	-0.00657400	2.65950600	1.48571400
H	2.14030300	3.05510900	0.26056200
H	1.28910100	2.94600800	-1.28839800
C	-2.63945900	-0.91236400	-0.31935800
C	-2.63678200	0.56487300	-0.37121900
C	2.63971100	-0.91309600	-0.31838100
C	2.63758100	0.56400500	-0.36911700
C	-3.86773500	-1.75669600	-0.37204000
H	-4.35390700	-1.67707200	-1.35204800
H	-3.61367900	-2.80244500	-0.19582200
H	-4.59237300	-1.43420200	0.38379700
C	-3.91441400	1.32967800	-0.52185100
H	-4.20887300	1.76368900	0.44359400
H	-3.80545200	2.15222100	-1.23437800
H	-4.72714800	0.68545800	-0.85741600
C	3.86739500	-1.75795600	-0.37695900
H	4.59744400	-1.43403300	0.37295700
H	3.61407800	-2.80323000	-0.19682800
H	4.34673800	-1.68080000	-1.36059400
C	3.91522900	1.32820600	-0.52166200
H	3.80284300	2.15690000	-1.22640700
H	4.21682400	1.75349900	0.44548500
H	4.72465900	0.68547600	-0.86806500
O	-1.20146400	-2.72346600	-0.12145100
O	1.20108300	-2.72343800	-0.11671000
H	-0.00163000	-2.84184000	-0.09357400
Cl	-0.00359000	-0.16638600	2.15568400

$Co^{III}(H)(^{4\text{-}tBu}py)(prdioxH)$ (low-spin)

Co	-0.011259000	-0.511904000	0.293394000
N	-1.417276000	-1.105035000	-0.863049000
N	1.482656000	-1.077915000	-0.761300000
N	1.350804000	-0.201350000	1.573927000
N	-1.466444000	-0.212232000	1.469029000
C	-1.193559000	-1.637047000	-2.218472000
C	1.372306000	-1.592954000	-2.137223000
C	0.101766000	-1.110946000	-2.838030000
H	-1.161246000	-2.735308000	-2.161641000
H	-2.036929000	-1.369221000	-2.865444000
H	0.141705000	-1.463459000	-3.875333000
H	0.083348000	-0.015973000	-2.870975000
H	2.246185000	-1.278154000	-2.719774000
H	1.384604000	-2.692586000	-2.100980000
C	-2.667031000	-0.548964000	1.042504000
C	-2.615994000	-1.096413000	-0.321240000
C	2.582389000	-0.527769000	1.236690000
C	2.638675000	-1.057645000	-0.133655000
C	-3.914304000	-0.395038000	1.851956000
H	-4.328592000	-1.374400000	2.122750000
H	-3.696998000	0.151665000	2.770823000
H	-4.684613000	0.146186000	1.291575000
C	-3.851662000	-1.603300000	-1.005447000
H	-4.156156000	-0.925119000	-1.813466000
H	-3.679091000	-2.588280000	-1.451582000
H	-4.685696000	-1.685527000	-0.307887000
C	3.763996000	-0.377594000	2.139896000
H	4.546335000	0.229347000	1.670033000
H	3.461931000	0.100842000	3.072703000
H	4.201823000	-1.355174000	2.376781000
C	3.926916000	-1.535710000	-0.736381000
H	3.811747000	-2.539205000	-1.160486000
H	4.247428000	-0.871912000	-1.549854000
H	4.726316000	-1.566575000	0.004167000
O	-1.307092000	0.322244000	2.708687000
O	1.094703000	0.323814000	2.801111000
H	-0.110397000	0.387409000	2.848975000
C	-1.150998000	2.074021000	-0.684264000
C	1.163568000	2.100770000	-0.552576000
C	-1.175998000	3.390405000	-1.140541000
H	-2.074618000	1.526128000	-0.553550000
C	1.211089000	3.422371000	-1.004788000
H	2.080436000	1.576325000	-0.317587000
C	0.024613000	4.114628000	-1.316100000
H	-2.139946000	3.838297000	-1.355413000
H	2.181176000	3.892441000	-1.106492000
N	0.003090000	1.419539000	-0.387666000

H	-0.021462000	-1.891192000	0.784450000
C	-0.000164000	5.562709000	-1.819909000
C	1.414863000	6.167006000	-1.926717000
H	2.043790000	5.612153000	-2.633938000
H	1.340825000	7.198865000	-2.289062000
H	1.921788000	6.191846000	-0.954240000
C	-0.835682000	6.426142000	-0.837133000
H	-0.866333000	7.462522000	-1.194559000
H	-1.868697000	6.069255000	-0.755598000
H	-0.391080000	6.422406000	0.165474000
C	-0.661347000	5.594188000	-3.224158000
H	-0.690529000	6.626596000	-3.593192000
H	-0.091266000	4.990031000	-3.940473000
H	-1.689987000	5.217066000	-3.199238000

Co^{II}(prdioxH)(CH_3CN) (low-spin)

Co	-1.147462000	0.013597000	-0.136526000
N	-1.548200000	-1.360099000	1.157649000
N	-1.440108000	1.555712000	0.983905000
N	-1.070316000	1.353744000	-1.495909000
N	-1.168471000	-1.479801000	-1.326104000
C	-1.756391000	-1.094567000	2.591614000
C	-1.652441000	1.480712000	2.440017000
C	-1.069092000	0.198420000	3.042342000
H	-2.838412000	-1.025788000	2.781042000
H	-1.374922000	-1.930257000	3.190057000
H	-1.177560000	0.267232000	4.131366000
H	0.004355000	0.142379000	2.828444000
H	-1.195277000	2.346883000	2.932768000
H	-2.733927000	1.525817000	2.638988000
C	-1.414885000	-2.661495000	-0.802300000
C	-1.654383000	-2.569123000	0.653842000
C	-1.226949000	2.603692000	-1.115795000
C	-1.462539000	2.701276000	0.340443000
C	-1.443725000	-3.935276000	-1.585033000
H	-2.445957000	-4.381302000	-1.576258000
H	-1.161951000	-3.740699000	-2.621097000
H	-0.750916000	-4.672751000	-1.163333000
C	-1.985084000	-3.789740000	1.462718000
H	-1.134054000	-4.071881000	2.096968000
H	-2.839325000	-3.607472000	2.122759000
H	-2.220438000	-4.641189000	0.823717000
C	-1.166858000	3.775574000	-2.042420000
H	-0.444247000	4.520042000	-1.689107000
H	-0.873170000	3.445726000	-3.040269000
H	-2.142893000	4.271576000	-2.115218000
C	-1.699139000	4.029271000	0.998840000
H	-2.555746000	3.985281000	1.679222000
H	-0.823722000	4.325591000	1.592220000
H	-1.883739000	4.812942000	0.263544000
O	-0.915503000	-1.353623000	-2.658877000
O	-0.836018000	1.053291000	-2.804068000
H	-0.841834000	-0.156978000	-2.831872000
C	2.075739000	-0.087496000	0.180926000
C	3.524842000	-0.136434000	0.299013000
H	3.832338000	-1.056997000	0.804329000
H	3.984895000	-0.110103000	-0.693507000
H	3.886800000	0.719437000	0.876790000
N	0.912676000	-0.048573000	0.083854000

Co^{II}(prdioxH)(CH_3CN)$_2$ (low-spin)

Co	-1.365300000	0.024563000	-0.121281000
N	-1.569439000	-1.370253000	1.203295000
N	-1.458459000	1.576611000	1.029507000
N	-1.175050000	1.371599000	-1.463466000
N	-1.276930000	-1.481293000	-1.294145000
C	-1.765410000	-1.093439000	2.634010000
C	-1.655555000	1.489359000	2.484358000
C	-1.066823000	0.200324000	3.071990000
H	-2.846401000	-1.011607000	2.824733000
H	-1.391209000	-1.924826000	3.242847000
H	-1.155702000	0.267920000	4.163284000
H	0.002010000	0.140886000	2.837256000
H	-1.199014000	2.350265000	2.986574000
H	-2.736007000	1.527880000	2.691034000
C	-1.387350000	-2.673666000	-0.750221000
C	-1.575570000	-2.588144000	0.714474000
C	-1.195930000	2.624538000	-1.063850000

C	-1.380292000	2.725629000	0.400211000
C	-1.331387000	-3.954910000	-1.521422000
H	-2.290249000	-4.486412000	-1.476403000
H	-1.102175000	-3.746611000	-2.567966000
H	-0.563205000	-4.625599000	-1.119127000
C	-1.762809000	-3.829569000	1.541546000
H	-0.887790000	-4.005268000	2.180888000
H	-2.635733000	-3.739135000	2.196700000
H	-1.897927000	-4.710903000	0.913883000
C	-1.049310000	3.799144000	-1.979336000
H	-0.250309000	4.468082000	-1.639331000
H	-0.813924000	3.455427000	-2.988139000
H	-1.975377000	4.386485000	-2.022172000
C	-1.469098000	4.066013000	1.075403000
H	-2.329426000	4.111055000	1.751485000
H	-0.569067000	4.258688000	1.674131000
H	-1.563719000	4.873239000	0.348396000
O	-1.100976000	-1.346057000	-2.640340000
O	-1.017451000	1.066269000	-2.783745000
H	-1.044903000	-0.146651000	-2.807782000
C	2.041683000	-0.089788000	0.129975000
C	3.495495000	-0.147059000	0.193714000
H	3.815796000	-1.041801000	0.736130000
H	3.916882000	-0.179228000	-0.815585000
H	3.887357000	0.734938000	0.709338000
N	0.874646000	-0.044574000	0.077901000
C	-4.757822000	0.114764000	-0.533371000
C	-6.200799000	0.147627000	-0.727114000
H	-6.465871000	-0.329534000	-1.675462000
H	-6.704382000	-0.384115000	0.085945000
H	-6.557305000	1.181966000	-0.743506000
N	-3.599450000	0.087225000	-0.378381000

Co^{II}(prdioxH) ($^{4\text{-}tBu}$py)(CH_3CN) (low-spin)

Co	-1.282876000	0.063769000	-0.150772000
N	-1.541100000	-1.476475000	0.983355000
N	-1.459048000	1.457410000	1.174126000
N	-1.196813000	1.566169000	-1.321701000
N	-1.280771000	-1.277033000	-1.506959000
C	-1.694073000	-1.389297000	2.444091000
C	-1.626439000	1.189940000	2.611040000
C	-1.004447000	-0.149003000	3.024477000
H	-2.768725000	-1.360275000	2.681754000
H	-1.281997000	-2.285138000	2.924443000
H	-1.067523000	-0.218482000	4.117376000
H	0.059057000	-0.159689000	2.760574000
H	-1.173396000	1.993829000	3.204084000
H	-2.702827000	1.185076000	2.842013000
C	-1.489166000	-2.520291000	-1.126185000
C	-1.661310000	-2.614906000	0.338818000
C	-1.339028000	2.759606000	-0.783844000
C	-1.514854000	2.674000000	0.681394000
C	-1.539211000	-3.687930000	-2.060331000
H	-2.541419000	-4.134484000	-2.080400000
H	-1.286640000	-3.364100000	-3.071541000
H	-0.835751000	-4.471213000	-1.755040000
C	-1.947976000	-3.932169000	1.002164000
H	-1.082896000	-4.268978000	1.588746000
H	-2.796445000	-3.849208000	1.689990000
H	-2.176117000	-4.707383000	0.269976000
C	-1.320318000	4.038236000	-1.560703000
H	-0.567220000	4.731330000	-1.167907000
H	-1.093858000	3.831326000	-2.608132000
H	-2.292535000	4.544482000	-1.510454000
C	-1.734286000	3.908547000	1.509147000
H	-2.585622000	3.781837000	2.186587000
H	-0.852647000	4.123498000	2.127500000
H	-1.922521000	4.781581000	0.883437000
O	-1.084465000	-0.980204000	-2.823911000
O	-1.009712000	1.431113000	-2.666231000
H	-1.014336000	0.231470000	-2.839925000
C	1.640468000	-1.181554000	-0.049874000
C	1.701484000	1.122441000	0.138197000
C	3.036423000	-1.265079000	0.021881000
H	1.047742000	-2.082660000	-0.155460000
C	3.095443000	1.119248000	0.216085000
H	1.154067000	2.056355000	0.183801000
C	3.812864000	-0.097314000	0.158025000

H	3.497133000	-2.244083000	-0.031280000
H	3.607773000	2.070005000	0.320579000
N	0.963504000	-0.009788000	0.004930000
C	5.345324000	-0.108016000	0.237295000
C	5.922831000	-1.537091000	0.174760000
H	5.665401000	-2.040642000	-0.765214000
H	7.016207000	-1.488289000	0.236288000
H	5.570062000	-2.155759000	1.009240000
C	5.789464000	0.544986000	1.573210000
H	6.884601000	0.548899000	1.635649000
H	5.445518000	1.582253000	1.655460000
H	5.399193000	-0.014590000	2.432236000
C	5.917458000	0.709733000	-0.951303000
H	5.567340000	1.748206000	-0.937398000
H	7.012969000	0.723310000	-0.896708000
H	5.627381000	0.263561000	-1.910468000
N	-3.639536000	0.145733000	-0.376219000
C	-4.800854000	0.181274000	-0.514914000
C	-6.247003000	0.223884000	-0.688091000
H	-6.529274000	-0.252162000	-1.632004000
H	-6.742800000	-0.303438000	0.132575000
H	-6.596758000	1.260562000	-0.700493000

Co^{II}(prdioxH)(CH_3CN)(Cl) (low-spin)

Co	-1.363332000	0.018934000	-0.106259000
N	-1.593196000	-1.370237000	1.213893000
N	-1.467598000	1.569055000	1.038775000
N	-1.133138000	1.360093000	-1.441264000
N	-1.256303000	-1.484622000	-1.272128000
C	-1.793266000	-1.094954000	2.644131000
C	-1.676900000	1.484786000	2.491860000
C	-1.092461000	0.196371000	3.084253000
H	-2.875066000	-1.012598000	2.832683000
H	-1.420658000	-1.927168000	3.253231000
H	-1.181272000	0.265199000	4.175845000
H	-0.027188000	0.133205000	2.836655000
H	-1.222360000	2.345560000	2.996639000
H	-2.759296000	1.525394000	2.690241000
C	-1.380488000	-2.676965000	-0.730349000
C	-1.587609000	-2.589889000	0.728887000
C	-1.158369000	2.614693000	-1.045324000
C	-1.366934000	2.718213000	0.412554000
C	-1.306691000	-3.958957000	-1.500069000
H	-2.260802000	-4.499875000	-1.465269000
H	-1.067682000	-3.748413000	-2.544087000
H	-0.536060000	-4.622476000	-1.090139000
C	-1.766696000	-3.832132000	1.558176000
H	-0.886361000	-4.006025000	2.190923000
H	-2.635540000	-3.746061000	2.219335000
H	-1.902943000	-4.713508000	0.930276000
C	-0.983712000	3.787088000	-1.959767000
H	-0.178660000	4.444440000	-1.610951000
H	-0.740228000	3.438525000	-2.965063000
H	-1.900053000	4.388746000	-2.015054000
C	-1.443870000	4.059802000	1.088811000
H	-2.306763000	4.116011000	1.760910000
H	-0.544086000	4.242492000	1.691102000
H	-1.525715000	4.868069000	0.360987000
O	-1.060643000	-1.354693000	-2.617596000
O	-0.952152000	1.055533000	-2.760274000
H	-0.985493000	-0.156409000	-2.782888000
N	-3.585335000	0.090165000	-0.421805000
C	-4.739452000	0.114449000	-0.611138000
C	-6.175789000	0.143328000	-0.851407000
H	-6.378145000	0.222589000	-1.923897000
H	-6.641818000	-0.771875000	-0.473759000
H	-6.628053000	1.001586000	-0.345251000
Cl	1.303323000	-0.089203000	0.201963000

Co^{III}(prdioxH)($^{4\text{-}tBu}$py)(TFA) (low-spin)

Co	-1.025491000	-0.049991000	-0.482531000
N	-1.328090000	-1.591068000	0.623303000
N	-1.353260000	1.313119000	0.831374000
N	-0.877141000	1.464956000	-1.640481000
N	-0.857491000	-1.381409000	-1.844938000
C	-1.505553000	-1.531728000	2.086810000
C	-1.540734000	1.039009000	2.268447000
C	-0.885053000	-0.274454000	2.700950000

H	-2.580933000	-1.558815000	2.302009000
H	-1.043287000	-2.416285000	2.540059000
H	-1.004171000	-0.353423000	3.787665000
H	0.191466000	-0.244640000	2.503239000
H	-1.111482000	1.862874000	2.850163000
H	-2.618112000	1.002073000	2.471971000
C	-1.175660000	-2.607587000	-1.500239000
C	-1.456256000	-2.709743000	-0.050015000
C	-1.213638000	2.624508000	-1.124836000
C	-1.498247000	2.514247000	0.324045000
C	-1.223047000	-3.757558000	-2.450980000
H	-2.247312000	-4.138688000	-2.545395000
H	-0.879498000	-3.443182000	-3.437413000
H	-0.593122000	-4.583715000	-2.103108000
C	-1.815966000	-4.022158000	0.575186000
H	-0.945397000	-4.451202000	1.089715000
H	-2.610685000	-3.901713000	1.316992000
H	-2.146528000	-4.742185000	-0.173980000
C	-1.275921000	3.898327000	-1.900973000
H	-0.638421000	4.666679000	-1.449127000
H	-0.949272000	3.728625000	-2.927792000
H	-2.300610000	4.288761000	-1.921952000
C	-1.881944000	3.718085000	1.128539000
H	-2.686853000	3.483288000	1.831149000
H	-1.024220000	4.073800000	1.715411000
H	-2.208169000	4.537535000	0.487682000
O	-0.537683000	-1.063731000	-3.117702000
O	-0.551041000	1.337295000	-2.944457000
H	-0.486762000	0.144550000	-3.132622000
C	1.622495000	-1.219296000	-0.124317000
C	1.605938000	1.098058000	0.037570000
C	3.000183000	-1.257014000	0.091805000
H	1.081133000	-2.140131000	-0.275356000
C	2.979085000	1.124586000	0.258072000
H	1.049148000	2.021422000	0.014505000
C	3.730955000	-0.070461000	0.293192000
H	3.483192000	-2.225698000	0.098711000
H	3.447705000	2.091503000	0.400672000
N	0.914397000	-0.059991000	-0.153595000
C	5.241185000	-0.041233000	0.544846000
C	5.867148000	-1.450189000	0.501104000
H	5.726978000	-1.929932000	-0.475437000
H	6.945575000	-1.370536000	0.678608000
H	5.452357000	-2.105984000	1.276349000
C	5.499047000	0.574353000	1.947115000
H	6.578336000	0.611470000	2.136324000
H	5.109266000	1.595685000	2.024103000
H	5.033758000	-0.031594000	2.733955000
C	5.919676000	0.837742000	-0.539770000
H	5.547963000	1.868407000	-0.526468000
H	7.000482000	0.870001000	-0.358261000
H	5.752536000	0.424775000	-1.541844000
O	-2.873521000	-0.020579000	-1.013275000
C	-3.962701000	-0.101949000	-0.305777000
C	-5.207758000	-0.014074000	-1.240735000
O	-4.134428000	-0.226830000	0.922956000
F	-5.259466000	1.210217000	-1.915972000
F	-5.199294000	-1.012875000	-2.218833000
F	-6.403922000	-0.141134000	-0.546754000

Co^{II}(prdioxH)($^{4\text{-}tBu}$py)(TFA) (low-spin)

Co	-1.199286000	0.138631000	0.084438000
N	-1.411129000	-1.358956000	1.279371000
N	-1.263478000	1.568763000	1.374842000
N	-1.176569000	1.602787000	-1.133842000
N	-1.310861000	-1.239279000	-1.226866000
C	-1.451299000	-1.227578000	2.744064000
C	-1.317411000	1.347862000	2.828102000
C	-0.686153000	0.009542000	3.229551000
H	-2.503552000	-1.150425000	3.052860000
H	-1.028783000	-2.122550000	3.218227000
H	-0.661619000	-0.027509000	4.325948000
H	0.352053000	-0.034194000	2.880404000
H	-0.804472000	2.161702000	3.356172000
H	-2.373867000	1.358412000	3.129951000
C	-1.537502000	-2.462278000	-0.795933000
C	-1.612301000	-2.509488000	0.679098000
C	-1.287433000	2.811098000	-0.624321000

C	-1.355647000	2.769551000	0.851716000
C	-1.697438000	-3.652575000	-1.688810000
H	-2.712965000	-4.062991000	-1.620507000
H	-1.511894000	-3.364703000	-2.725179000
H	-0.999890000	-4.452848000	-1.415193000
C	-1.897181000	-3.796554000	1.401219000
H	-1.007766000	-4.146253000	1.942081000
H	-2.695978000	-3.662737000	2.138929000
H	-2.198705000	-4.584595000	0.710236000
C	-1.334808000	4.066066000	-1.438230000
H	-0.550492000	4.769051000	-1.133389000
H	-1.199931000	3.826900000	-2.494644000
H	-2.298930000	4.576369000	-1.319102000
C	-1.513195000	4.028147000	1.657915000
H	-2.327169000	3.927694000	2.384359000
H	-0.597075000	4.247511000	2.222244000
H	-1.727024000	4.887665000	1.021604000
O	-1.197367000	-0.986053000	-2.563353000
O	-1.082331000	1.427577000	-2.485151000
H	-1.113372000	0.226766000	-2.619581000
C	1.702701000	-1.157516000	0.039958000
C	1.818048000	1.150322000	0.131232000
C	3.098809000	-1.267402000	0.019360000
H	1.085837000	-2.048335000	0.010559000
C	3.214052000	1.121111000	0.114772000
H	1.290948000	2.096128000	0.175053000
C	3.903687000	-0.111432000	0.055971000
H	3.536791000	-2.257219000	-0.026646000
H	3.749783000	2.064141000	0.146676000
N	1.052769000	0.029270000	0.094044000
C	5.437807000	-0.150088000	0.032783000
C	5.983911000	-1.591392000	-0.032654000
H	5.653097000	-2.111524000	-0.940113000
H	7.079727000	-1.563121000	-0.046795000
H	5.678051000	-2.183425000	0.838850000
C	5.981894000	0.525780000	1.319593000
H	7.078731000	0.513863000	1.307265000
H	5.658460000	1.569737000	1.400539000
H	5.643587000	-0.008224000	2.216138000
C	5.944382000	0.627222000	-1.211394000
H	5.623295000	1.675039000	-1.196408000
H	7.040995000	0.612377000	-1.235167000
H	5.575225000	0.169351000	-2.137306000
O	-3.531597000	0.227911000	-0.138159000
C	-4.465254000	0.313692000	0.730622000
C	-5.889137000	0.236742000	0.071482000
O	-4.434611000	0.448239000	1.988796000
F	-6.109794000	1.292257000	-0.830470000
F	-6.068990000	-0.945264000	-0.666808000
F	-6.947191000	0.283284000	0.982164000

$Co^{III}(Cl)_2$(prdioxH) (low-spin)

Co	-1.386140000	0.018314000	-0.146246000
N	-1.621630000	-1.367137000	1.162077000
N	-1.510796000	1.555731000	0.998536000
N	-1.159142000	1.361906000	-1.479088000
N	-1.263853000	-1.478871000	-1.319004000
C	-1.874496000	-1.096084000	2.584883000
C	-1.767046000	1.468070000	2.444112000
C	-1.197565000	0.189988000	3.063454000
H	-2.962390000	-1.019506000	2.727834000
H	-1.521500000	-1.934993000	3.194228000
H	-1.346186000	0.256141000	4.147818000
H	-0.119701000	0.134268000	2.879923000
H	-1.333696000	2.335531000	2.953328000
H	-2.855319000	1.503088000	2.599464000
C	-1.379357000	-2.668714000	-0.778136000
C	-1.607127000	-2.583377000	0.675641000
C	-1.186843000	2.610162000	-1.075541000
C	-1.412716000	2.705109000	0.377937000
C	-1.294758000	-3.946131000	-1.550335000
H	-2.253839000	-4.478429000	-1.535571000
H	-1.032650000	-3.736600000	-2.588454000
H	-0.537985000	-4.613612000	-1.122831000
C	-1.816741000	-3.820715000	1.500553000
H	-0.974579000	-3.975849000	2.187013000
H	-2.725705000	-3.739571000	2.105851000
H	-1.903125000	-4.707469000	0.872544000

C	-1.011178000	3.783713000	-1.985017000
H	-0.225443000	4.452267000	-1.615633000
H	-0.741377000	3.442616000	-2.985624000
H	-1.937239000	4.367814000	-2.056623000
C	-1.524380000	4.039661000	1.057829000
H	-2.417097000	4.086221000	1.690069000
H	-0.653036000	4.220236000	1.700458000
H	-1.577341000	4.851434000	0.332168000
O	-1.057168000	-1.339180000	-2.650803000
O	-0.968956000	1.059048000	-2.785995000
H	-0.994876000	-0.146722000	-2.824546000
Cl	-3.666012000	0.082209000	-0.461368000
Cl	0.898888000	-0.047960000	0.139627000

Transition states:

$Co^{II}(Cl)(^{4\text{-}tBu}py)$(prdioxH) (low-spin)(loosing Cl^-)

Co	0.00402200	0.00220100	-0.17402500
Cl	0.09058100	-0.00669500	3.50973600
N	0.05397100	0.00451400	-2.32015700
N	-0.96947300	1.65173800	0.02136900
N	-1.47404600	-1.21945500	0.00521000
N	1.00458600	-1.61207200	-0.02580800
N	1.49470000	1.17756900	-0.01571900
C	-2.43942300	1.73865300	0.03049400
C	-2.88588500	-0.80148600	0.01436500
C	-3.09145200	0.54836400	-0.67995500
H	-2.78123700	1.77988100	1.07573100
H	-2.76563200	2.66744900	-0.45328800
H	-4.17084200	0.73811500	-0.72029900
H	-2.73461800	0.49223000	-1.71461000
H	-3.50587100	-1.55821900	-0.48191300
H	-3.22663700	-0.73756600	1.05886800
C	1.23771600	2.45538700	0.17667700
C	-0.21610000	2.71206400	0.21610900
C	0.32748300	-2.72745200	0.15573300
C	-1.12666500	-2.47363600	0.19623200
C	2.28761100	3.50880500	0.33056700
H	2.24668600	3.95998600	1.32978100
H	3.27680200	3.06984900	0.19078800
H	2.15233400	4.31394900	-0.40109600
C	-0.75608700	4.09214800	0.45488800
H	-1.22954000	4.48611200	-0.45430800
H	-1.51800000	4.08398300	1.24185800
H	0.03227400	4.78570100	0.74847500
C	0.95474200	-4.07718400	0.29941100
H	0.55843900	-4.78004300	-0.44289200
H	2.03522600	-4.00017100	0.16788600
H	0.75538900	-4.49860600	1.29245200
C	-2.10440000	-3.58754800	0.43348700
H	-2.81665900	-3.32053900	1.22180700
H	-2.68508300	-3.79586900	-0.47505400
H	-1.59898200	-4.50835900	0.72562600
O	2.78258700	0.73904700	-0.10386100
O	2.36524100	-1.63786700	-0.11064100
H	2.67546200	-0.46791400	-0.13181600
C	0.28606800	1.14044300	-3.02149700
C	-0.14694700	-1.13473300	-3.03285700
C	0.32515200	1.17981600	-4.41984000
H	0.44616900	2.04499800	-2.44725800
C	-0.12190700	-1.17110400	-4.42728700
H	-0.33258200	-2.03819000	-2.46502700
C	0.11892700	0.00611900	-5.17132500
H	0.51760300	2.13033500	-4.90216300
H	-0.29103900	-2.12226900	-4.92057900
C	0.15178200	-0.03032400	-6.70480600
C	1.28223300	-0.99153300	-7.16062900
C	-1.21195700	-0.55287800	-7.23030600
C	0.41378900	1.36175900	-7.31576500
H	1.31053500	-1.03345100	-8.25635000
H	2.25988100	-0.64363000	-6.80532600
H	1.12563900	-2.01059400	-6.78898300
H	-2.03120900	0.10829900	-6.92225500
H	-1.19408600	-0.58851200	-8.32641500
H	-1.43099400	-1.56288600	-6.86543800
H	-0.36976900	2.08027700	-7.04494600
H	1.38302400	1.76920500	-7.00266300
H	0.42623900	1.28103200	-8.40895800

$Co^{II}(Cl)(^{4\text{-}tBu}py)(prdioxH)$ (low-spin)(loosing $^{4\text{-}tBu}py$)

Co	0.00275600	-0.04357500	-0.21836100
N	0.09695200	-0.35212700	3.27449200
C	1.22973700	-0.19793500	4.00122600
C	-1.07694100	-0.31192400	3.95768400
C	1.23776500	-0.00517500	5.39257300
H	2.16473800	-0.23044000	3.44843300
C	-1.15502000	-0.12407500	5.34257800
H	-1.98081400	-0.43612700	3.36801300
C	0.02353800	0.03708200	6.10730700
H	2.19075400	0.10966500	5.89532400
H	-2.13424300	-0.10504500	5.81058400
C	-0.05423000	0.24239200	7.62772300
C	-0.88564700	1.51820000	7.92643500
C	-0.75110100	-0.98690600	8.26939300
C	1.34051900	0.40511500	8.26635900
H	-0.95323600	1.67053500	9.01086500
H	-0.41530800	2.40506000	7.48408900
H	-1.90604200	1.44094900	7.53374400
H	-0.18029800	-1.90431600	8.07943000
H	-0.82391600	-0.84694800	9.35513400
H	-1.76567800	-1.12860300	7.87960200
H	1.96555800	-0.48319400	8.11195000
H	1.87174800	1.27766100	7.86633800
H	1.23077200	0.54993200	9.34766600
Cl	-0.02200200	0.40419700	-2.70215900
N	1.49088700	-1.26156300	-0.33411800
N	-1.44267500	-1.31388000	-0.31873000
N	-1.43616600	1.15800700	0.10925200
N	1.40117800	1.20837200	0.09578300
C	1.33825100	-2.69248200	-0.63516100
C	-1.24323200	-2.73933500	-0.61931200
C	0.06128000	-3.27479900	-0.01780700
H	1.30787200	-2.81404300	-1.72808600
H	2.20247500	-3.25809900	-0.26884500
H	0.07995100	-4.35953100	-0.18052200
H	0.06479600	-3.11015300	1.06651300
H	-2.08214200	-3.33423000	-0.24052700
H	-1.22314200	-2.86311200	-1.71222200
C	2.63615500	0.75355600	0.06207000
C	2.67071500	-0.69687800	-0.20867700
C	-2.65481300	0.66039300	0.08460700
C	-2.64057200	-0.79045600	-0.18476900
C	3.84803400	1.60842100	0.25964700
H	4.44191900	1.67083600	-0.66114100
H	3.54614600	2.61839200	0.54224300
H	4.49692800	1.20160900	1.04381100
C	3.97725900	-1.42799100	-0.34501400
H	4.10142000	-2.16201900	0.46144300
H	4.02382300	-1.97273300	-1.29461300
H	4.82382100	-0.74212400	-0.30537900
C	-3.89415500	1.47277300	0.29082400
H	-4.52035300	1.04656800	1.08308600
H	-3.62519500	2.49394700	0.56649200
H	-4.49887000	1.51034200	-0.62419100
C	-3.92153500	-1.56740300	-0.30918800
H	-3.95358400	-2.12081300	-1.25428300
H	-4.01600300	-2.29907900	0.50351600
H	-4.79133600	-0.91121300	-0.27023300
O	1.16577500	2.53353300	0.32184300
O	-1.24538100	2.49049300	0.33307500
H	-0.04042900	2.61377100	0.33757700