***Supporting information for***

# Understanding Light-driven $H_2$ Evolution through the Electronic Tuning of Aminopyridine Cobalt Complexes

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# Experimental Section

## 1. General materials, reagents

All procedures were carried out under $N_2$ using standard vacuum line, Schlenk, and inert atmosphere glovebox techniques. Reagents and solvents were purchased from commercial sources as used as received unless otherwise stated. Triethylamine ($Et_3N$) ≥ 99 % purity and ascorbic acid (≥ 99 %) were purchased from Sigma-Aldrich and used without further purification. $[Ir(bpy)(ppy)_2]PF_6$ (**$PS_{Ir}^+$**)[1] was synthesized according to the literature procedure. Anhydrous acetonitrile was purchased from Sigma Aldrich. Water (18.2 MΩ·cm) was purified with a Milli-Q Millipore Gradient AIS system. All the solvents were strictly degassed and stored in anaerobic conditions. All water reduction catalytic reactions were performed under $N_2$.

## 2. Instrumentation

**Nuclear magnetic resonance** (NMR) spectra were recorded on Bruker Fourier300, AV400, AV500 and AVIII500 spectrometers using standard conditions (300 K). All $^1H$ chemical shifts are reported in ppm and have been internally calibrated to the residual protons of the deuterated solvent. The $^{13}C$ chemical shifts have been internally calibrated to the carbon atoms of the deuterated solvent. The coupling constants were measured in Hz.

**Elemental analyses** were performed using a CHNS-O EA-1108 elemental analyzer from Fisons.

**Mass Spectrometry**. Electrospray ionization mass spectrometry (ESI-MS) experiments were performed on a Bruker Daltonics Esquire 3000 Spectrometer using a 1 mM solution of the analysed compound, by introducing the sample directly into the ESI-source using a syringe. High-resolution mass spectra (HRMS) were recorded on a Bruker MicroTOF-Q IITM instrument with an ESI source. Samples were introduced into the mass spectrometer ion source by direct infusion through a syringe pump and were externally calibrated using sodium formate.

**Electrochemistry.** All the electrochemical experiments were performed with a VSP potentiostat from Bio-Logic, equipped of the EC-Lab software. CV measurements were carried out under Ar atmosphere by using 1 mM solutions of **$1^R$** complexes in $CH_3CN$, with tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as supporting electrolyte (0.1 M). A single-compartment cell was employed, with glassy carbon (GC) working electrodes (3 mm and 1 mm diameter). Additionally, a Pt wire was used as a counter electrode and an Ag/AgCl wire as pseudo-reference, immerged in a bridge tube containing the same electrolyte solution (0.1 M $TBAPF_6/CH_3CN$) and separated from the working solution by a porous tip. Ferrocene (Fc) was added to the solution as an internal standard and all the potentials are referenced *vs.* the $Fc^{+/0}$ redox couple. The working electrodes were polished by using 0.05 µm alumina powder (CHInstruments) on a polishing pad wet with distilled $H_2O$, followed by rinsing with distilled water/acetone and sonication to remove the residues of alumina over the electrode.

**X-Ray crystallography.** Single crystals of **$1^R$** complexes were mounted on a nylon loop for X-ray structure determination. The measurements were carried out on a BRUKER SMART APEX CCD diffractometer using graphite-monochromated MoKα radiation (λ=0.71073 Å). Programs used: data collection, Smart version 5.631 (Bruker AXS 1997-02); data reduction, Saint+ version 6.36A (Bruker AXS 2001); absorption correction, SADABS version 2.10 (Bruker AXS 2001). Structure solution and refinement was done using SHELXTL Version 6.14 (Bruker AXS 2000–2003). The structure was solved by direct methods and refined

by full-matrix least-squares methods on F2. The non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed in geometrically optimised position and forced to ride on the atom to which they are attached.

**UV-Vis** spectra were recorded on an Agilent 8453 diode array spectrophotometer (190-1100 nm range) in 1 cm quartz cells. A cryostat from Unisoku Scientific Instruments was used for the temperature control.

**FT-IR. FT-IR** spectra were measured in the solid state on a Bruker Alpha FTIR Spectrometer equipped with Platinum ATR single reflection diamond ATR module.

**Online MS measurements** have been performed using Omnistar GSD 301 C (Pfeiffer) quadrupole mass spectrometer apparatus.

**Gas chromatography identification and quantification of gases.** Gases at the headspace were analysed with an Agilent 7820A GC System equipped with columns Washed Molecular Sieve 5A, 2m x 1/8'' OD, Mesh 60/80 SS and Porapak Q, 4m x 1/8'' OD, SS. Mesh: 80/100 SS and a Thermal Conductivity Detector. The quantification of the $H_2$ obtained was measured through the interpolation of a previous calibration using different $H_2/N_2$ mixtures.

**In-house developed parallel photoreactor.** The parallel photoreactor that we have used for these studies is the same that was previously reported for the light-driven reduction of ketones and aldehydes studies in our group.

*Light source*: The reactions were performed using Royal-Blue ($\lambda$ = 447±20 nm) LUXEON Rebel ES LED, mounted on a 10mm Square Saber - 1030 mW @ 700mA (Datasheet: https://www.luxeonstar.com/assets/downloads/ds68.pdf) as a light source.

*Temperature Control:* Reaction temperature was controlled by a high precision thermoregulation Hubber K6 cryostat. Likewise, to guarantee a stable irradiation the temperature of the LEDs was also controlled and set up at 22 °C.

**Parallel Pressure Transducer Hardware.** The parallel pressure transducer sensors that we used for these studies are the same that those previously reported for the water oxidation studies in our group.[2] This system is composed by 8 differential pressure transducers (Honeywell-ASCX15DN, ± 15 psi) connected to a hardware data-acquisition system (base on Atmega microcontroller) controlled by a home-developed software program. The differential pressure transducer Honeywell-ASCX15DN is a 100 microseconds response, signal-conditioned (high level span, 4.5 V) output, calibrated and temperature compensated (0 ºC to 70 ºC) sensor. The differential sensor has two sensing ports that can be used for differential pressure measurements. The pressure devices were offset and span calibrated (± 0.5 matm) *via* software with a high precision pressure transducer (PX409-030GUSB, 0.08 % Accuracy). Each of the 8 differential pressure transducers (Honeywell-ASCX15DN, ±15 psi) produce a voltage outputs that can be directly transformed to a pressure difference between the two measuring ports. The voltage outputs were digitalized with a resolution of 0.25 matm from 0 to 175 matm and 1 matm from 176 to 1000 matm using an Atmega microcontroller with an independent voltage auto-calibration. Firmware Atmega microcontroller and control software were home-developed. The sensitivity of $H_2$ analytics allows for quantification of the gas formed when low $H_2$ volumes are generated. However, it could not be discarded that small amounts of $H_2$ were produced by inactive complexes.

## 3. Experimental procedures

**Photocatalytic experiments and gas-chromatographic detection of gases**

In a typical photocatalytic run, MeCN:$H_2O$:$Et_3N$ (4:6:0.2 mL) solvent mixtures containing 50 μM of **1$^R$** and 150 μM of [Ir(ppy)$_2$(bpy)](PF$_6$) (**PS$_{Ir}$**) were irradiated by a LED source (λ = 447 nm) and temperature was held constant at 25 ºC throughout the experiment. Each reaction vial was connected to one of the ports of a differential pressure transducer sensor (Honeywell-ASCX15DN) and the other port to a reference reaction. Reference reactions, have all components of the reaction except the catalyst. The reaction and reference vials are kept under the same experimental conditions to compensate the noise due to temperature-pressure fluctuations. In order to ensure a constant and stable irradiation, the LED sources were equipped with a water refrigeration system. This is composed for a refrigerated aluminum block by a Huber cryothermostat (refrigeration system, Minichiller -40°C-20°C). This block is shaken by an Orbital Shaker (IKA KS 260 Basic Package) which provides the agitation of the reaction vessels during the irradiation time. The aluminum block accommodates 16 vials (20 mL) capped with septum in which the reaction takes place. Each vial is submitted and located over a LED irradiation source (Royal-Blue Rebel LEDs (λ = 447±20 nm). The reaction began when the LEDs were turned on. At this point, the hydrogen evolved from the reactions was monitored by recording the increase in pressure of the headspace (1 second interval). The pressure increment is the result of the difference in pressure between the reaction and reference vials. After the hydrogen evolution reached a plateau the amount of the gas formed was measured equilibrating the pressure between reaction and reference vials. The gases at the headspace of the reaction vials and references in each of the reactions were quantified by the analysis of an aliquot of gas at the headspace (0.2 mL) by gas chromatography.

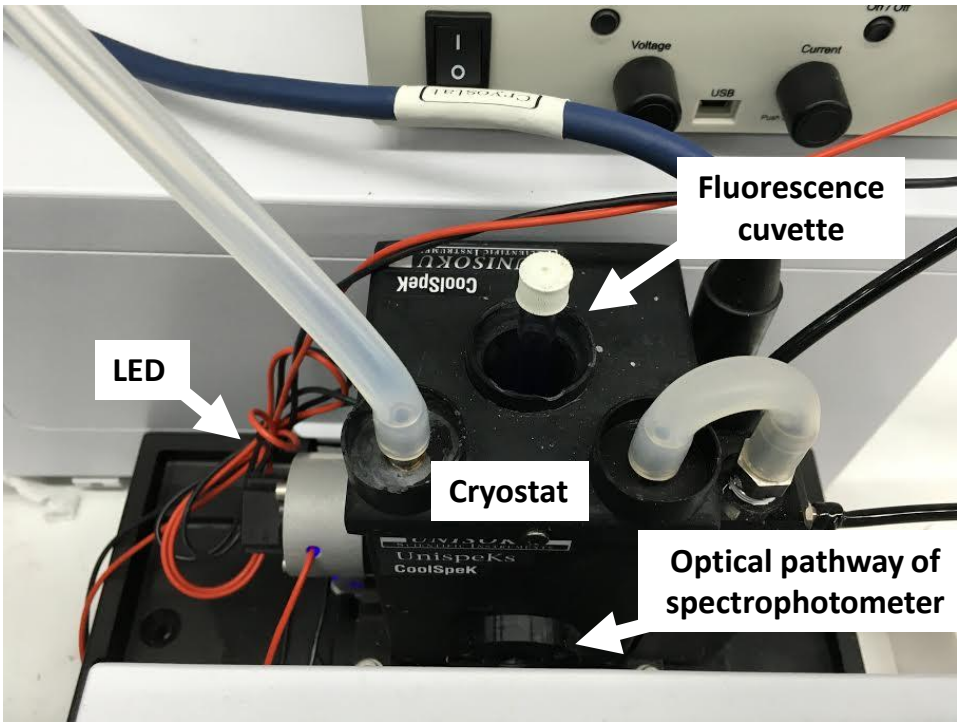
**Photophysics and UV-Vis quenching studies**

The solution of [Ir(ppy)$_2$(bpy)](PF$_6$) (**PS$_{Ir}$**) was prepared in water acetonitrile mixture (1.2:0.8 mL). The concentration of **PS$_{Ir}$** was fixed to 10 μM. The reference cuvette was with the same water-acetonitrile mixture. UV-Vis measurements were carried out on a Shimadzu UV-2401PC spectrophotometer equipped with a photomultiplier detector, double beam optics and $D_2$ and W light sources. The absorption kinetics were studied on an Agilent 8453 diode array spectrophotometer (190–1100 nm range) in 1 cm quartz cells. A cryostat from Unisoku Scientific Instruments was used for the temperature control under inert atmosphere.

**Luminescence measurements** were carried out on an Aminco-Bowman Series 2 Luminescence spectrofluorometer equipped with a high voltage PMT detector and continuum Xe light source. Sample preparation was the same as that of absorption experiments. Luminescence lifetimes were determined using an Edinburgh Instruments LifeSpec-II luminescence spectrometer equipped with a PMT detector, double subtractive monochromator and picosecond pulsed diode lasers source (470 nm). Exponential deconvolution fit was used to fit the emission decay by the FAST software from Edinburgh Instruments Ltd., with $\chi^2$ values and intensity residuals used to determine goodness of fit. For all fitting results reported here, $\chi^2$ values were close to unity. Where a single exponential fit result was unsatisfactory, a dual-exponential fit was used. Laser flash photolysis experiments were carried out by using the third harmonics (355 nm) of a pulsed Nd-YAG laser. The single pulses were ca. 10 ns duration and the energy of the laser beam was ca. 8 mJ/pulse. A xenon lamp was employed as detecting light source. The signal from the monochromator/photomultiplier detection system was captured by a Tektronix TDS640A digitizer. The output signal from the oscilloscope was transferred to a personal computer for study. Samples were prepared in 1x1 cm cells quartz and were deaerated with dry nitrogen prior to use.

### UV-Vis measurements with on-line irradiation

The UV-Vis measurements with on-line irradiation were performed on a self-made apparatus using 1 cm quartz fluorescence cuvette in a fluorescence cuvette holder. LED (Royal blue, 447 nm) was placed perpendicular to the optical pathway of Agilent 8453 diode array spectrophotometer (190-1100 nm range). A cryostat from Unisoku Scientific Instruments was used for the temperature control.




Setup for UV/Vis measurement with on-line irradiation.

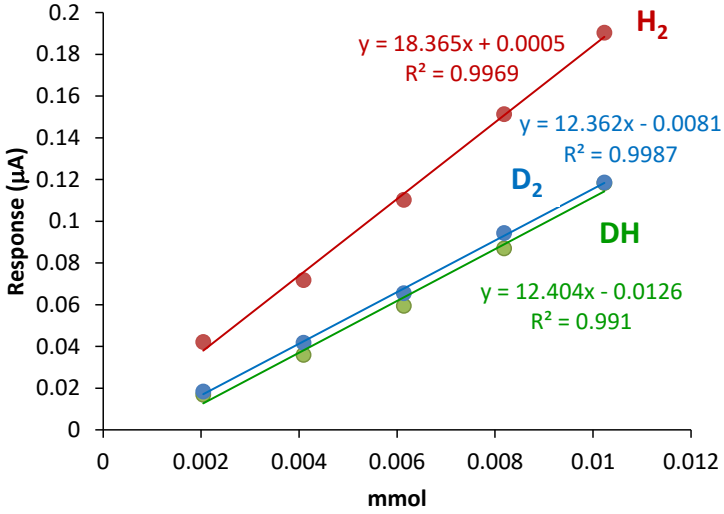
### Actinometry

We have calculated the quantum yield of the reactions by Ferrioxalate Actinometer Experiments following the recently reported procedure by Scaiano, J. C. and co. *Scientific Reports* **2015**, *5:16397.*

$$\Phi = 2 * (\text{moles of } H_2 \text{ per unit time}) / (\text{moles of photons per unit time})$$

**Calibration of the on-line MS monitoring formation of $H_2$, HD and $D_2$.**

We calibrated the response of $H_2$, HD and $D_2$ in the on-line mass spectrometer apparatus. The calibration was done by measuring known amounts of $H_2$, HD and $D_2$ in the headspace, and the response was plotted against the amount of gas.




Calibration of the response of $H_2$, DH and $D_2$ in the on-line mass spectrometer apparatus.

The HD and $D_2$ products for the injection were generated by reacting NaH with $D_2O$, and Li with $D_2O$, respectively.

**Kinetic Isotopic experiments**

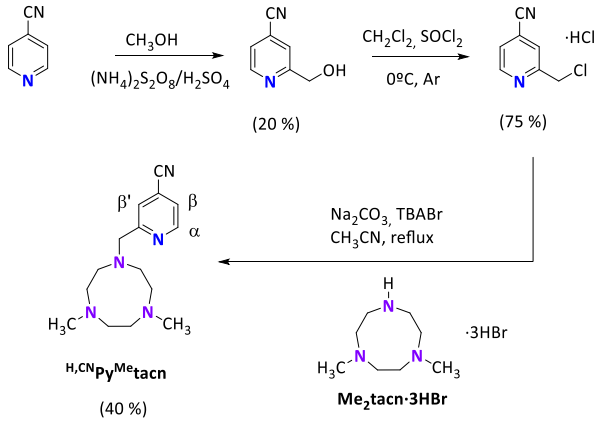
**On-line monitoring of $H_2$, HD and $D_2$.** $H_2$, HD and $D_2$ MS monitoring during the irradiation time was performed irradiating ($\lambda$ = 447 nm) a solution of $CH_3CN$:$H_2O$:$D_2O$ (0.8:0.6:0.6 mL) containing $\mathbf{1}^{H}$ (50 μM), $\mathbf{PS_{Ir}}^{+}$ (150 μM) and $Et_3N$ (40 μL) (reaction volume = 2 mL) under $N_2$ atmosphere. The headspace of the vial that contained the resulting solution was monitored by using an atmospheric pressure quadrupole mass spectrometer apparatus (Omnistar GSD 301 C Pfeiffer; m/z 2, 3 and 4 were monitored). The ion current response was calibrated with $H_2$, HD and $D_2$ authentic samples.

**Kinetics using $D_2O$.** Isotopic Kinetic experiments using $H_2O$, $D_2O$ (99.9% D) and a mixture of $H_2O$:$D_2O$ were performed in a $CH_3CN$:$H_2O$:$Et_3N$ (4:6:0.2 mL), $CH_3CN$:$D_2O$:$Et_3N$ (4:6:0.2 mL) or $CH_3CN$:$H_2O$:$D_2O$:$Et_3N$ (2:3:3:0.1 mL) solvent mixture containing 50 μM of $\mathbf{1}^{R}$ and 150 μM of ($\mathbf{PS_{Ir}}^{+}$). The solution was irradiated by a LED source ($\lambda$ = 447 nm) and the temperature was held constant at 25 °C throughout the experiment. The amount of gas evolved was monitored through the Parallel Pressure Transducer Hardware described above and quantified by the analysis of an aliquot of gas at the headspace (0.2 mL) by gas chromatography.

## 4. Synthesis and characterization

All the ligands discussed in the manuscript were synthesized by adopting slight modification of the procedure described in the literature.[3] The synthetic route used to obtain the novel **$^{H,CN}$Py$^{Me}$tacn** ligand as well as all the Co complexes is reported below.

### *4.1. Synthesis of $^{H,CN}$Py$^{Me}$tacn ligand*




**Scheme S1.** Synthesis of **$^{H,CN}$Py$^{Me}$tacn** ligand.

**4-nitrile-2-hydroxymethylpyridine**. A solution of 4-pyridinecarbonitrile (5.51 g) in MeOH (80 ml) was prepared in a rounded bottom flask, $H_2SO_4$ 98% (0.5 ml) was added to the solution at room temperature under argon. After stirring the solution for 30 min, a solution of ammonium persulfate in water (19.24 g in 35 ml) was added dropwise during 30 min under argon and under reflux. A white solid appeared during the addition. After the addition, the solution was refluxed for 1 hour and became bright yellow. Finally, the solution was cooled at room temperature and the MeOH was removed under reduced pressure. A saturated solution of $Na_2CO_3$ was added to the mixture to pH = 9 and the mixture was extracted with AcOEt (40 ml x 4) and dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure and a yellow solid was obtained. The compound was purified by silica column chromatography with hexane/AcOEt (9:1) to give 1.50 g of 4-nitrile-2-hydroxymethylpyridine as a white crystalline solid (20.1 % yield). $^1$H-NMR ($CDCl_3$, 400 MHz) $\delta$, ppm: 8.76 (dd, J = 5.0, J = 0.9 Hz, **H$_6$** of py), 7.61 (m, **H$_3$** of py), 7.43 (m, **H$_5$** of py), 4.87 (d, J = 5.3 Hz, 2H, C**H$_2$**OH), 3.34 (t, J = 5.3 Hz, O**H**).

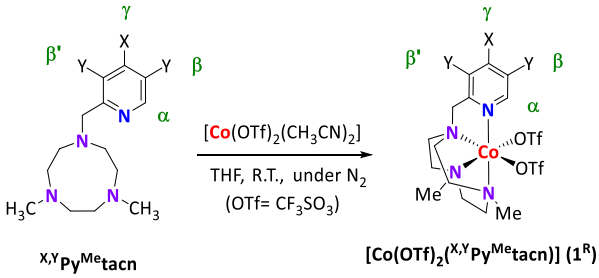
**2-chloromethyl-4-cyano-pyridine hydrochloride.** $SOCl_2$ (2.43 ml, 33.3 mmol) was added dropwise to an ice-cooled solution of 4-ethoxycarbonyl-2-hydroxymethylpyridine (1.36 g, 10.2 mmol) in $CH_2Cl_2$ anhydrous (35 mL) under $N_2$ with stirring. The mixture was stirred overnight at room temperature. After that, the $CHCl_3$ and the excess of $SOCl_2$ were removed by rotary evaporator to give a solid which was washed several times with $Et_2O$ to yield 1.43 g of 4-ethoxycarbonyl-2-chloromethylpyridine hydrochloride as a white solid (7.6 mmol, 74.5 %). $^1$H-NMR ($CD_3CN$, 500 MHz) $\delta$, ppm: 8.84 (d, J = 5.5 Hz, **H$_6$** of py), 8.25 (s, **H$_3$** of py), 8.09 (dd, J= 5.5 Hz, **H$_5$** of py), 5.50 (broad, N-**H** of py-H$^+$), 5.07 (s, 2H, C**H$_2$**Cl).

**1,4-dimethyl-7-(4-cianopyridin-2-ylmethyl)-triazacyclononane.** 2-chloromethyl-4-cianopyridine (0.48 g, 2.5 mmol), $Me_2$tacn·3HBr (1.00 g, 2.5 mmol) and anhydrous acetonitrile (40 ml) were mixed in a 100 mL flask. $Na_2CO_3$ (1.90 g) and tetrabutylammonium bromide, TBABr (80 mg) were added directly as solids and the resulting mixture was heated at reflux under $N_2$ for 20 hours. After cooling to room temperature, the resulting yellow mixture was filtered and the filter cake was washed with $CH_2Cl_2$. The combined filtrates

were evaporated under reduced pressure. To the resulting residue, 2 M NaOH (15 ml) was added and the mixture was extracted with $CH_2Cl_2$ (4 x 40 ml). The combined organic layers were dried over anhydrous $MgSO_4$ and the solvent was removed under reduced pressure. The resulting residue was treated with *n*-hexane (100 ml) and stirred for 12 hours. The mixture was filtered and the solvent from the yellow filtrates was removed under reduced pressure to yield 0.28 g of a pale yellow oil (1.0 mmol, 40 %). $^1$H-NMR ($CDCl_3$, 400 MHz) $\delta$, ppm: 8.71 (d, J = 5.1 Hz, **H$_2$** of py), 7.92 (s, J = 5.1 Hz, 1H, **H$_3$** of py), 7.39 (d, J = 5.1 Hz, 1H, **H$_5$** of py), 3.94 (s, 2H, C**H$_2$**-py), 2.88-2.85 (m, 4H, N-C**H$_2$**-$CH_2$), 2.71-2.68 (m, 4H, N-C**H$_2$**-$CH_2$), 2.76 (s, 4H, $CH_3$-N-C**H$_2$**-C**H$_2$**-N-$CH_3$), 2.40 (s, 6H, N-C**H$_3$**). $^{13}$C-NMR ($CDCl_3$, 400 MHz) δ, ppm: 162.90 (s, **C$_6$** of py), 149.80 (s, **C$_2$** of py), 124.90 (s, **C$_3$** of py), 123.06 (s, **C$_5$** of py), 120.66 (s, **C$_4$** of py), 116.91 (s, py-**C**N), 63.85 (s, **C**$H_2$-py), 57.37 (s, N-**C**$H_2$-$CH_2$), 57.32 (s, N-**C**$H_2$-$CH_2$), 55.94 (s, N-**C**$H_2$-$CH_2$), 46.74 (s, N-**C**$H_3$). ESI-MS (*m/z*): 274.2028 $[M+H]^+$.

**Synthesis of Complexes**

**1$^{R}$** complexes were synthesized by reacting **$^{X,Y}$Py$^{Me}$tacn** with 1 eq. $[Co(OTf)_2(CH_3CN)_2]$. It is worth noting that inert working conditions are necessary (Glovebox, $[O_2] < 1$ ppm, $[H_2O] < 1$ ppm) due to high instability of the studied complexes in the presence of $O_2$.




| Catalyst | Y | X |
|---|---|---|
| $1^{CN}$ | H | CN |
| $1^{CO2Et}$ | H | $CO_2Et$ |
| $1^{Cl}$ | H | Cl |
| $1^{H}$ | H | H |
| $1^{DMM}$ | Me | OMe |
| $1^{NMe2}$ | H | $NMe_2$ |

**Scheme S2.** General scheme of the synthesis of **1$^{R}$** complexes.

**[Co(OTf)$_2$($^{H,H}$Py$^{Me}$tacn)] (1$^{H}$).** In a glovebox, a suspension of $[Co(OTf)_2(MeCN)_2]$ (442.05 mg, 1.00 mmol) in anhydrous THF (2 mL) was added dropwise to a vigorously stirred solution of $^{H,H}$Py$^{Me}$tacn (250 mg, 1.00 mmol) in THF (2 mL). The cobalt triflate salt was quickly solubilized, and after few minutes, the solution became cloudy and a pale red precipitate appeared. After stirring for an additional 3h the solution was filtered off and the resulting solid was dried under vacuum. This solid was dissolved with $CH_2Cl_2$, filtered with Celite and the slow diffusion of diethyl ether over the resultant solution afforded a red crystalline compound (518 mg, 0.85 mmol, 85% yield). $^1$H-NMR ($CD_3CN$, 500 MHz, 298 K) $\delta$, ppm: 222.94 (**H$_\alpha$**), 186.37 (C**H$_2^{tacn}$**), 131.99 (C**H$_2^{tacn}$**), 103.24 (C**H$_2^{tacn}$**), 84.78 (**H$_\beta$**), 81.61 (N-C**H$_3$**), 60.87 (**H$_{\beta'}$**), 26.33 (**H$_\gamma$**), 21.67. ESI-MS (*m/z*): 456.0 $[M - OTf]^+$, 153.5 $[M\text{-}2\cdot OTf]^{2+}$. Anal. Calculated for $C_{16}H_{24}CoF_6N_4O_6S_2$: C, 31.74; N, 9.25; H, 4.00 %. Found: C, 31.75; N, 9.18; H, 4.08 %. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$)= 256 (5500 $M^{-1}\cdot cm^{-1}$).

**[Co(OTf)$_2$($^{H,NMe2}$Py$^{Me}$tacn] (1$^{NMe2}$). 1$^{NMe2}$** was prepared in analogous manner to **1$^{H}$**. A purple compound was obtained (150 mg, 83% yield). $^1$H-NMR ($CD_3CN$, 500 MHz, 298 K) $\delta$, ppm: 239.96 (**H$_\alpha$**), 193.33 (C**H$_2^{tacn}$**), 127.14 (C**H$_2^{tacn}$**), 122.08 (C**H$_2^{tacn}$**), 94.04 (N-C**H$_3$**), 89.05 (**H$_\beta$**), 59.06 (**H$_{\beta'}$**), 28.19 (N(C**H$_3$**)$_2$), 18.34 (N(C**H$_3$**)$_2$), -13.95. ESI-MS (*m/z*): 499.1 $[M - OTf]^+$, 175.0 $[M\text{-}2\cdot OTf]^{2+}$. Anal. Calculated for $C_{18}H_{29}CoF_6N_5O_6S_2$: C, 33.34; N, 10.80; H, 4.51 %. Found: C, 33.45; N, 10.95; H, 4.69 %. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$)= 270 (17950 $M^{-1}\cdot cm^{-1}$), 372 (1090 $M^{-1}\cdot cm^{-1}$).

**[Co(OTf)$_2$($^{Me,OMe}$Py$^{Me}$tacn] (1$^{DMM}$). 1$^{DMM}$** was prepared in analogous manner to **1$^{H}$**. A red compound was obtained (310 mg, 86% yield). $^1$H-NMR ($CD_3CN$, 500 MHz, 298 K) $\delta$, ppm: 230.57 (**H$_\alpha$**), 183.60 (C**H$_2^{tacn}$**), 124.08 (C**H$_2^{tacn}$**), 109.97 (C**H$_2^{tacn}$**), 85.39 (N-C**H$_3$**), 25.63 (**Me$^{Py}$**), 20.14, 13.68 (**Me$^{Py}$**), 7.26 (O**Me**). ESI-MS (*m/z*): 514.1 $[M - OTf]^+$, 182.5 $[M\text{-}2\cdot OTf]^{2+}$. Anal. Calculated for $C_{19}H_{30}CoF_6N_4O_7S_2$: C, 34.39; N, 8.44; H, 4.56 %. Found: C, 34.45; N, 8.40; H, 4.61 %. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$)= 260 (5400 $M^{-1}\cdot cm^{-1}$).

**[Co(OTf)$_2$($^{H,Cl}$Py$^{Me}$tacn] (1$^{Cl}$). 1$^{Cl}$** was prepared in analogous manner to **1$^{H}$**. A skin coloured compound was obtained (120 mg, 70% yield). $^1$H-NMR ($CD_3CN$, 500 MHz, 298 K) $\delta$, ppm: 221.87 (**H$_\alpha$**), 190.03 (C**H$_2^{tacn}$**), 136.54 (C**H$_2^{tacn}$**), 102.29, 81.40 (N-C**H$_3$**), 80.10 (**H$_\beta$**), 56.51 (**H$_{\beta'}$**). ESI-MS (*m/z*): 490.0 $[M - OTf]^+$, 170.5 $[M\text{-}2\cdot OTf]^{2+}$. Anal. Calculated for $C_{16}H_{23}ClCoF_6N_4O_6S_2$: C, 30.03; N, 8.76; H, 3.62 %. Found: C, 30.29; N, 8.54; H, 3.87 %. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$)= 217 (13800 $M^{-1}\cdot cm^{-1}$).

**[Co(OTf)$_2$($^{H,CO2Et}$Py$^{Me}$tacn] ($1^{CO2Et}$).** $\mathbf{1^{CO2Et}}$ was prepared in analogous manner to $\mathbf{1^{H}}$. An orange compound was obtained (213 mg, 82% yield). $^1$H-NMR ($CD_3CN$, 500 MHz, 298 K) $\delta$, ppm: 215.30 ($\mathbf{H_\alpha}$), 184.89 (C$\mathbf{H_2}^{tacn}$), 140.95 (C$\mathbf{H_2}^{tacn}$), 135.63 (C$\mathbf{H_2}^{tacn}$), 97.22, 80.16 ($\mathbf{H_\beta}$ + N-C$\mathbf{H_3}$), 57.86 ($\mathbf{H_{\beta'}}$), 20.82, 8.33 ($CO_2C\mathbf{H_2}CH_3$), 4.54 ($CO_2CH_2C\mathbf{H_3}$). ESI-MS (*m/z*): 528.1 [M - OTf]$^+$, 189.5 [M-2·OTf]$^{2+}$. Anal. Calculated for $C_{19}H_{28}CoF_6N_4O_8S_2$: C, 33.68; N, 8.27; H, 4.17 %. Found: C, 33.52; N, 8.15; H, 4.05 %. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$)= 281 (6845 $M^{-1}\cdot cm^{-1}$).

**[Co($^{H,CN}$Py$^{Me}$tacn)($CH_3CN$)$_2$](OTf)$_2$ ($1^{CN}$).** In a glovebox, a solution of [Co(OTf)$_2$(MeCN)$_2$] in anhydrous THF (0.45 g, 1.0 mmol in 2 mL) was added dropwise to a vigorously stirred solution of $Me_2$Pytacn in THF (0.28 g, 1.0 mmol in 2mL). After few minutes, the solution became brown. After stirring overnight, the solution was filtered off and the resulting orange solid was dried under vacuum. This solid was dissolved in $CH_2Cl_2$ and the minimum quantity of $CH_3CN$ to completely dissolve the solid, stirred for two hours, filtered with Celite and the slow diffusion of diethyl ether into this solution produced brown crystals (0.51 g, 0.7 mmol 70 % yield). $^1$H-NMR ($CD_3CN$, 500 MHz, 300 K) $\delta$, ppm: 210.25 ($\mathbf{H_\alpha}$), 183.77, 144.36, 139.17, 93.40, 78.32, 74.98 ($\mathbf{H_\beta}$), 54.18 ($\mathbf{H_{\beta'}}$), 19.67. ESI-MS (*m/z*): 367.0953 [M-2·$CH_3CN$-2·OTf+Cl]$^{2+}$. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$) = 282 (5457 $M^{-1}\cdot cm^{-1}$). Anal. Calculated for $C_{21}H_{29}CoF_6N_7O_6S_2\cdot(CH_2Cl_2)_{0.5}$: C, 34.20; N, 12.99; H, 4.00 %. Found: C, 34.48; N, 13.16; H, 3.99 %. UV/Vis ($CH_3CN$) $\lambda_{max}$ ($\varepsilon$)= 281 (6845 $M^{-1}\cdot cm^{-1}$).

### 4.2. Characterization of the complexes

#### 4.2.1. FT-IR characterisation

The studied $\mathbf{1}^{R}$ complexes exhibited similar pattern, with $\mathbf{1}^{CO2Et}$ showing characteristic band at 1731 $cm^{-1}$ attributed to the C=O stretching frequency.

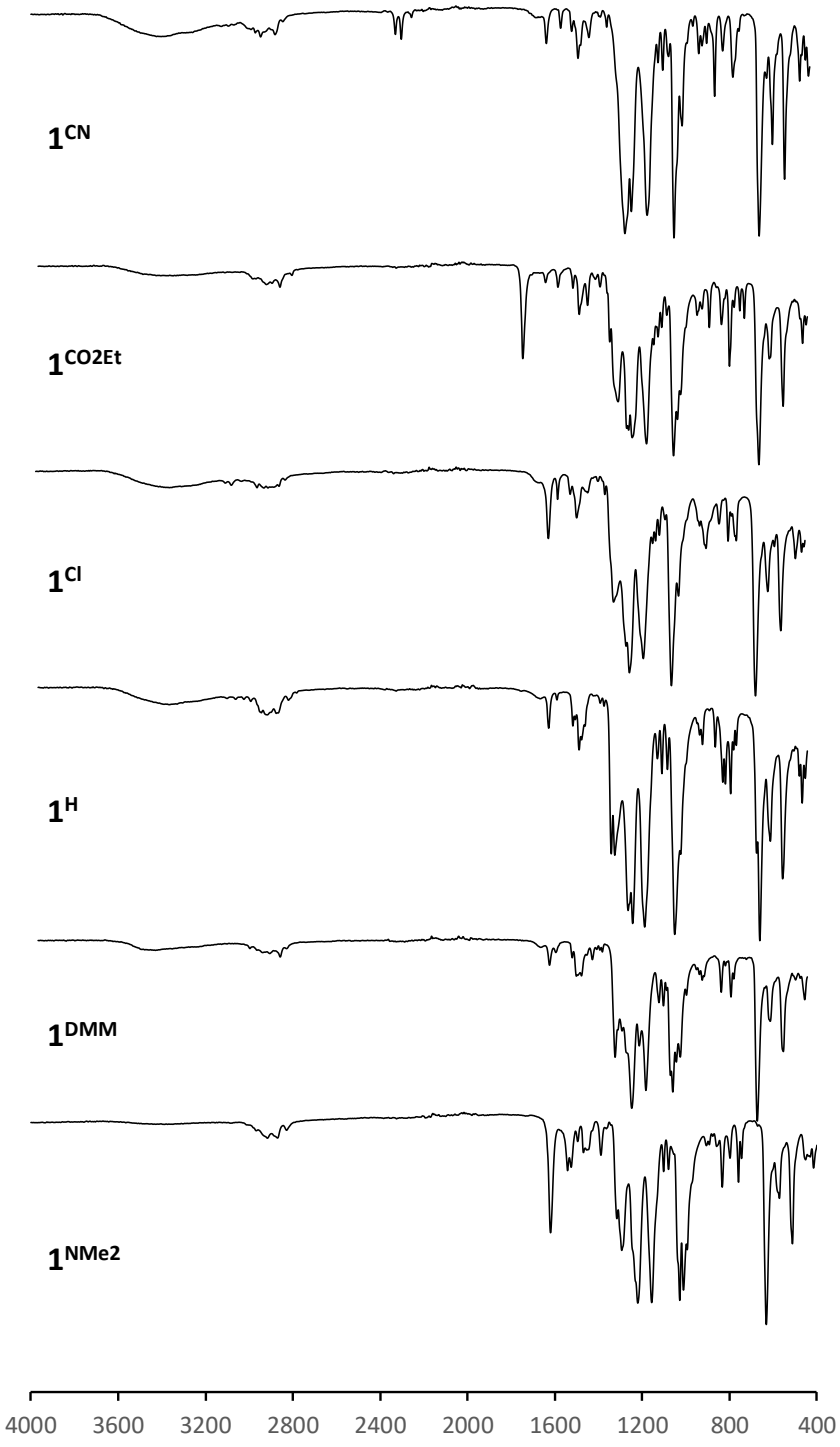



**Figure S1.** FT-IR spectra of $\mathbf{1}^{R}$ complexes.

### 4.2.2. $^{1}$H-NMR characterisation

The structures of complexes **1$^{R}$** were studied in detail in $CD_3CN$ by means of $^{1}$H-NMR spectroscopy. Since $Co^{II}$ complexes are paramagnetic, they are characterised by fast nuclear relaxation (short T1) with a line broadening of around 2-50 Hz, consistent with $Co^{II}$ high spin complexes.[4] The $^{1}$H-NMR spectra at room temperature of complexes **1$^{R}$** are collected in the Figure S2. All of the **1$^{R}$** complexes exhibit spectra windows ranged from -14 to 240 ppm, which is in agreement with $t_{2g}^{5}$ $e_g^{2}$ or $t_{2g}^{6}$ $e_g^{1}$ configuration of $Co^{II}$ paramagnetic species.

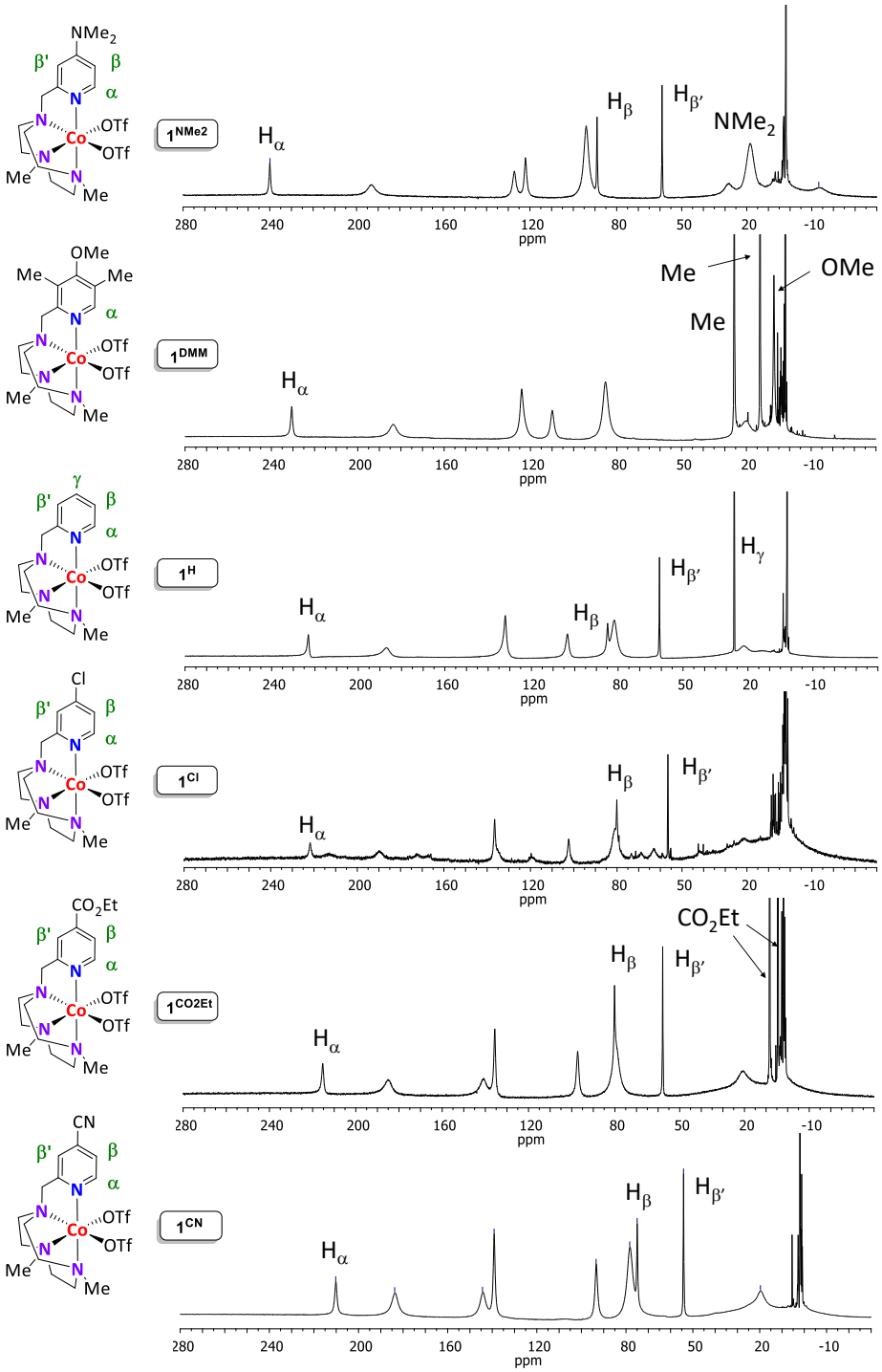



**Figure S2.** Paramagnetic $^{1}$H-NMR spectra of **1$^{R}$** complexes in $CD_3CN$ at 298 K.

The assignment of protons have been done on the basis of their relative integration, relative peak width (Δδ, measured at half-peak intensity) and the comparison of the $^1$H-NMR spectra within the **1$^R$** series. The integration of peaks for **1$^H$** (280 K) at 242.9 (Δδ = 0.60), 91.9 (Δδ = 0.10), 65.6 (Δδ = 0.12) and 28.9 (Δδ = 0.04) have about the same relative intensity (Figure S3), which can be set up to 1 and likely correspond to the aromatic hydrogens of the pyridine moiety. Signal at 242.9 ppm with the highest Δδ value (Δδ = 0.60, d(Co-H$_\alpha$) = 3.1900 Å) can be assigned to the H$_\alpha$, since this is the hydrogen closest to the paramagnetic Co$^{II}$ centre. This is in agreement with the characteristic field upshift behavior of H$_\alpha$ derived from Fermi contact interactions with the metal centre. The narrow signals at 91.9 (Δδ = 0.10, d(Co-H$_\beta$) = 5.1312 Å) and 65.6 (Δδ = 0.12, d(Co-H$_{\beta'}$) = 4.923 Å) can be attributed to the H$_\beta$ and H$_{\beta'}$ according to the integration and similar Δδ values. The distinction between H$_\beta$ and H$_{\beta'}$ protons was done on the basis of the cobalt-H$_\beta$ distances obtained by X-Ray crystallography and Δδ compared with the Δδ values. The assignment of H$_\beta$ was confirmed by their absent in the β substituted **1$^{DMM}$**, but present in the other *para*-substituted cobalt complexes (Figure S2). Finally, according to the lowest Δδ value, the peak at 28.9 (Δδ = 0.04) can be attributed to the γ proton since is located at the longest distance from the paramagnetic centre and is absent in all *para*-substituted complexes. The remaining broad paramagnetic $^1$H-NMR signals appeared downfield shifted (between 80 and 200 ppm) as compared with the H$_\beta$ protons and are consistent with the typical $^1$H-NMR patterns of related Co$^{II}$ polypyridyl complexes described in the literature.[5]

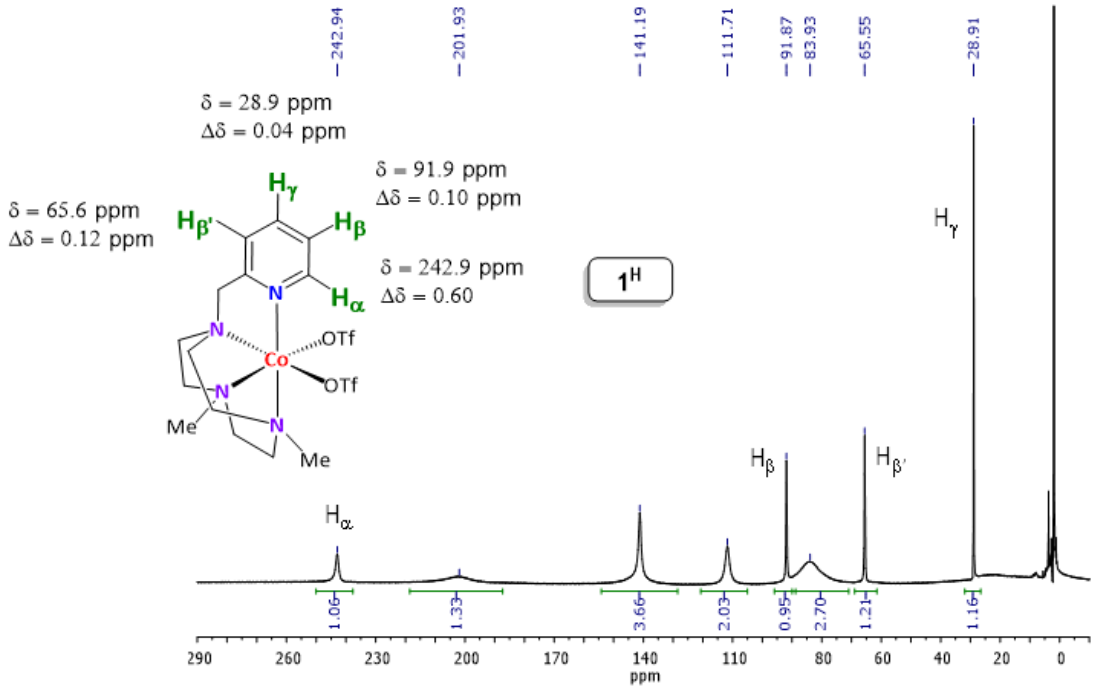



**Figure S3.** Paramagnetic $^1$H-NMR spectrum of **1$^H$** complex in $CD_3CN$ at 280 K. Peak width measured at half peak intensity (Δδ in ppm): 242.9 (0.6), 201.9 (4.3), 141.1 (0.61), 111.7 (0.81), 91.9 (0.10), 83.93 (4.24), 65.55 (0.12), 28.91 (0.04).

The $^{1}$H-NMR chemical shift of the $H_{\alpha}$ atoms was also found to linearly correlate with the electronic properties of the substituted pyridine in the series (Figure S4).

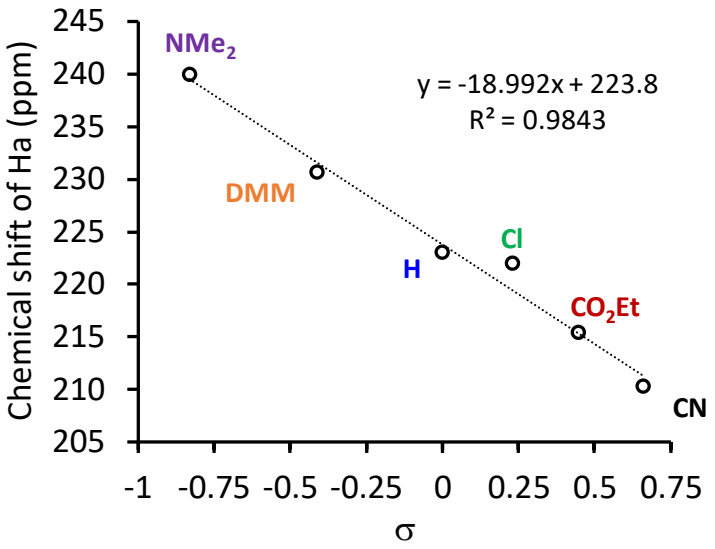



**Figure S4.** Linear plot of $H_{\alpha}$ chemical shift (T = 298 K) of the **1$^{R}$** complexes *vs.* the Hammett σ parameter.

Varied-temperature (230–320 K, Figures S5-S11) paramagnetic experiments on the **1$^{R}$** complexes showed a linear dependence of the $H_{\alpha}$ chemical shift on 1/T in agreement with the Curie's law, indicating no spin changes in the explored temperature range (Figures S10-S11).[6]
The $^{1}$H-NMR signals were assigned on the basis of their relative integration and peak width ($\Delta\delta$, measured at half-peak intensity) (Figures S2-S11).

Signals assigned to $CH_2$ fragments and N-Me groups became significantly broader when decreasing the temperature and could not be clearly distinguished at temperatures lower than 235 K. However, pyridine signals did not significantly change with the temperature.

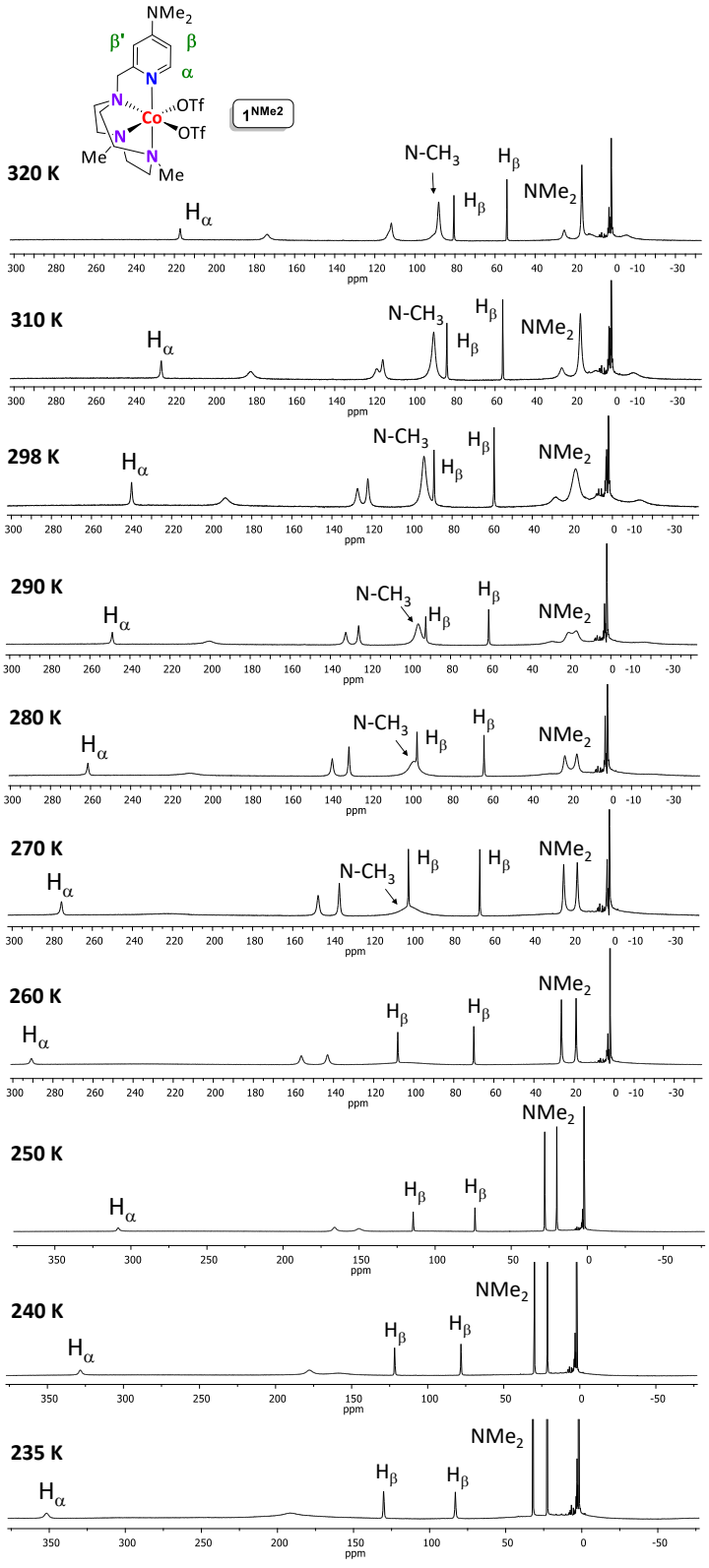



**Figure S5.** $^{1}$H-NMR spectra (500 MHz) of **1$^{NMe2}$** in $CD_3CN$ at different temperatures.

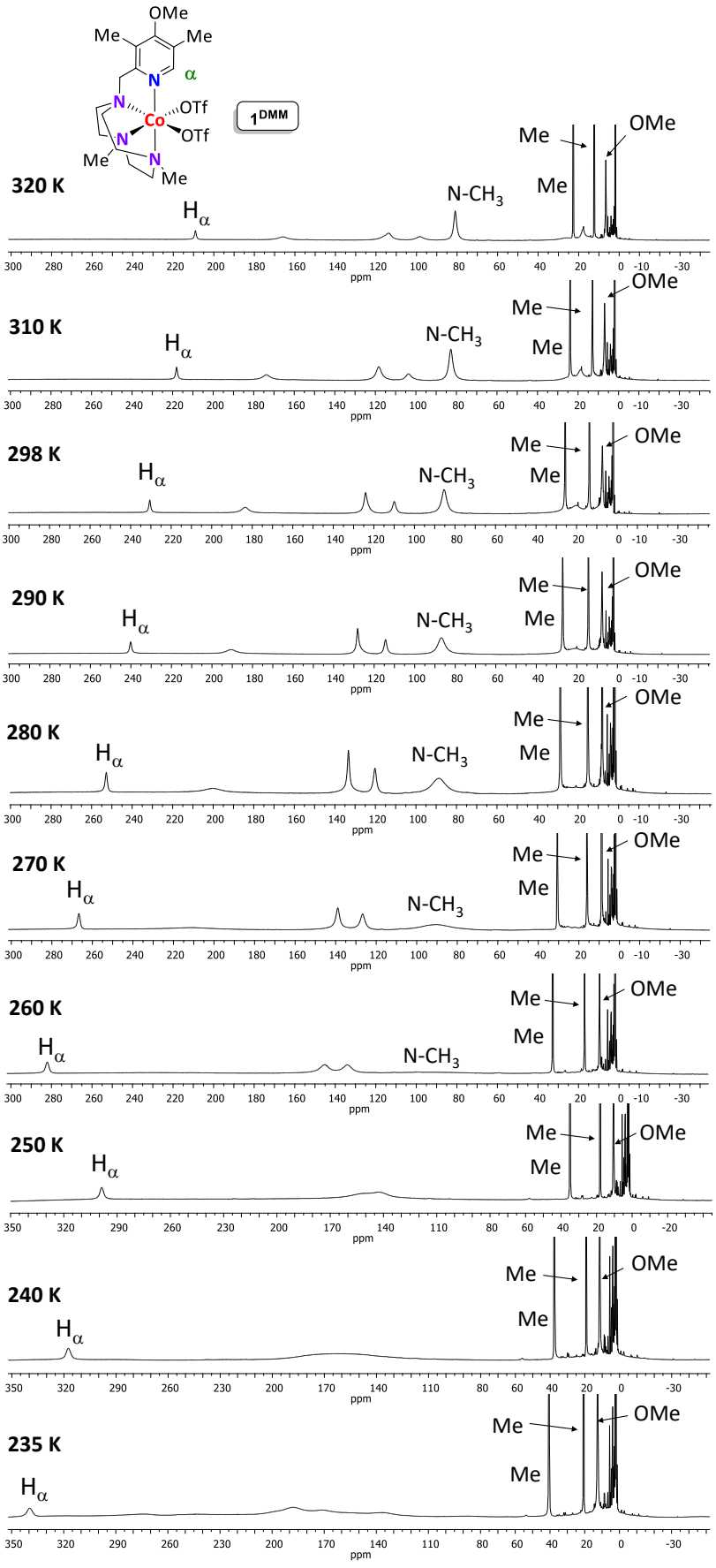



**Figure S6.** $^{1}$H-NMR spectra (500 MHz) of **1$^{DMM}$** in $CD_3CN$ at different temperatures.

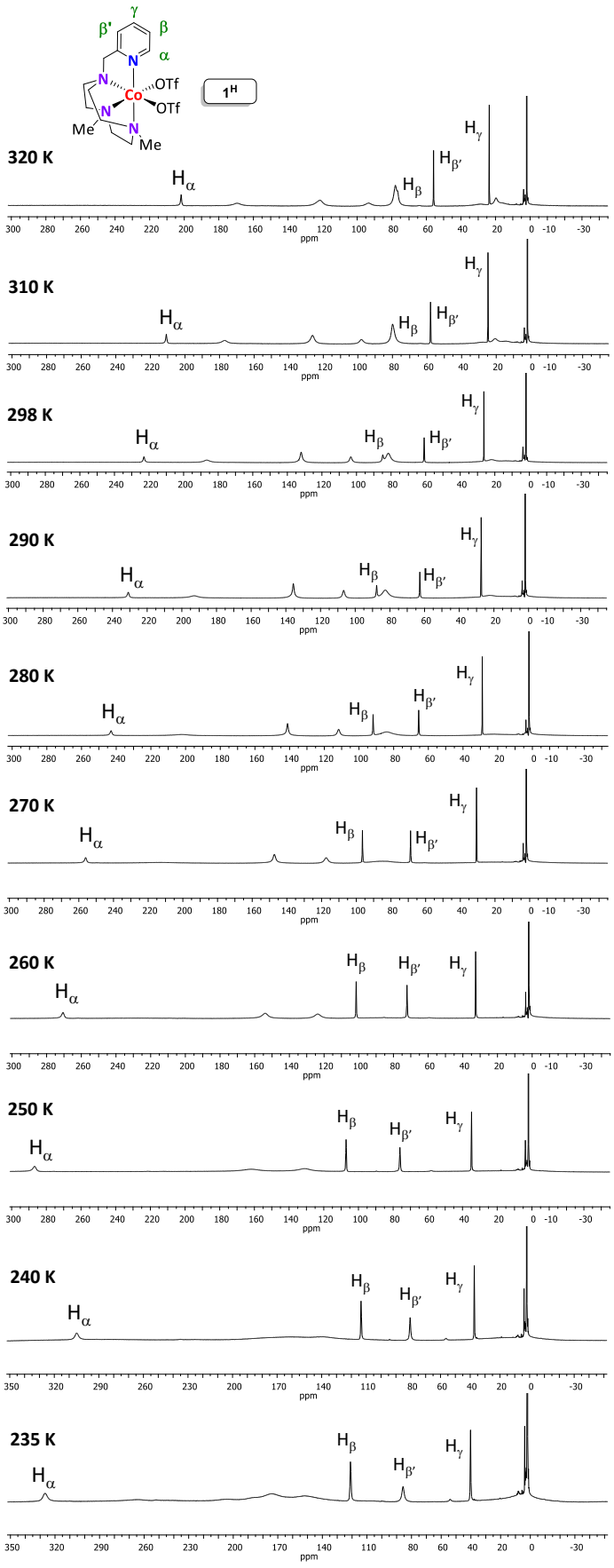



**Figure S7.** $^{1}$H-NMR spectra (500 MHz) of **1$^{H}$** in $CD_3CN$ at different temperatures.

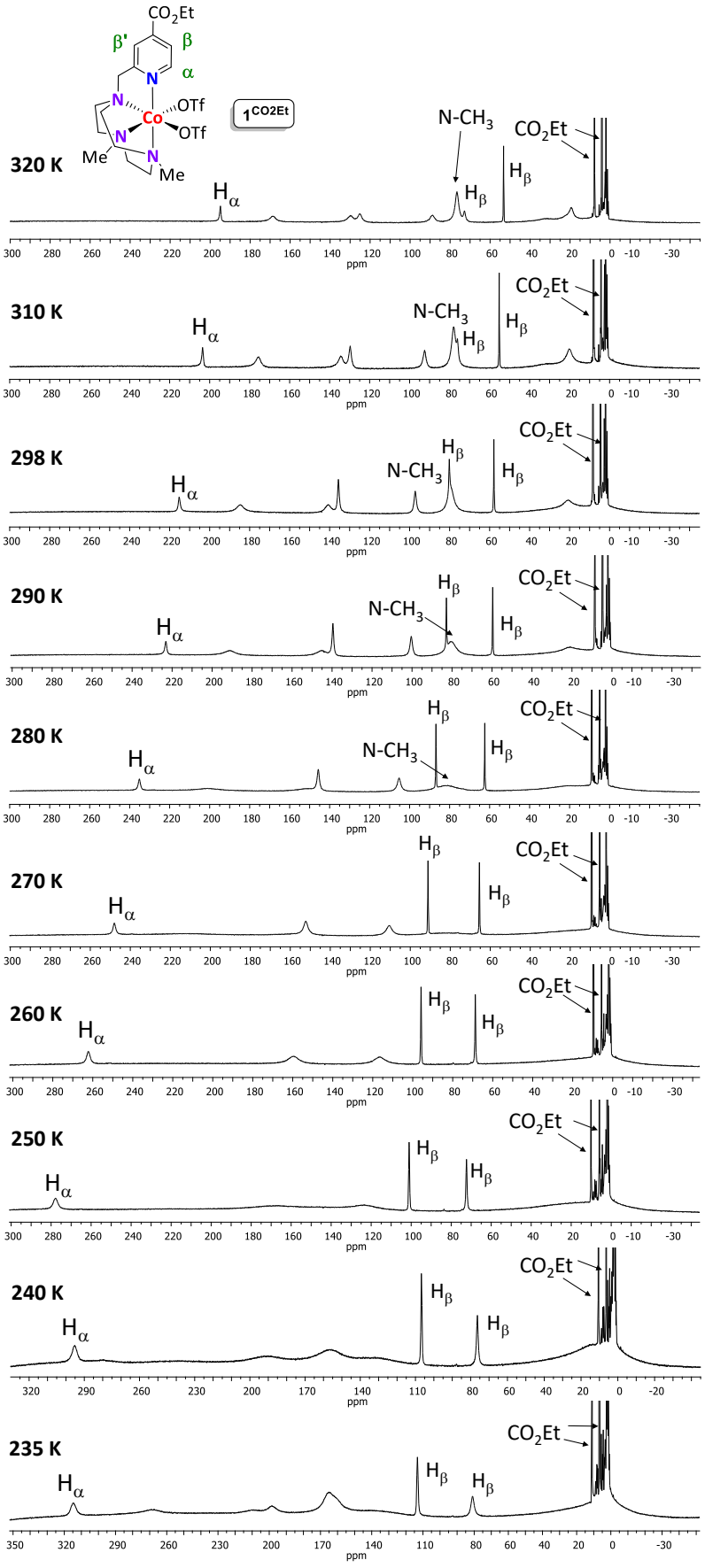



**Figure S8.** $^{1}$H-NMR spectra (500 MHz) of **1$^{CO2Et}$** in $CD_3CN$ at different temperatures.

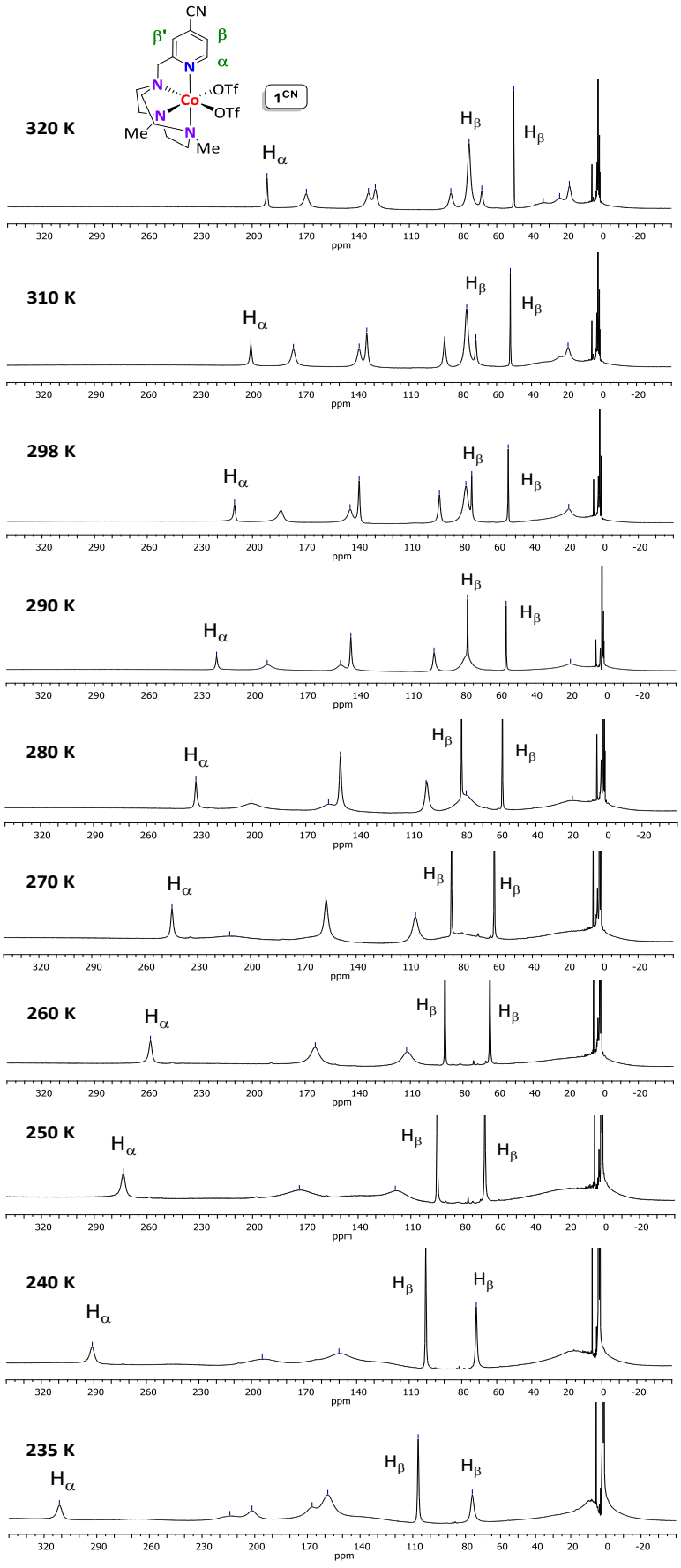



**Figure S9.** $^{1}$H-NMR spectra (500 MHz) of **1$^{CN}$** in $CD_3CN$ at different temperatures.

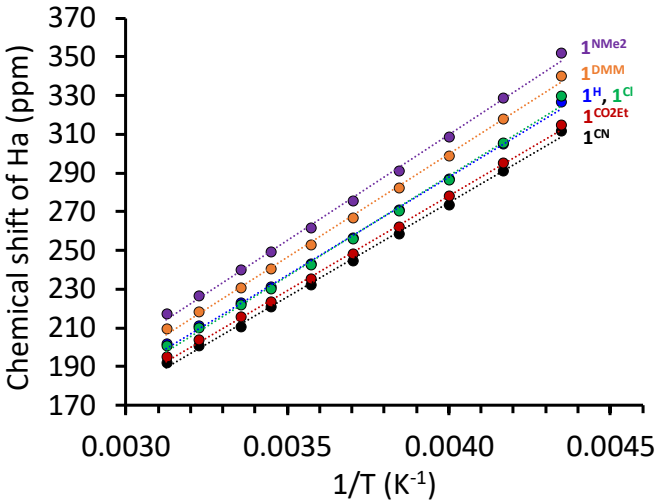



**Figure S10.** Representation of the chemical shift of $H_\alpha$ signals in front of temperature in the $^1$H-NMR spectrum of **1$^R$** complexes in $CD_3CN$.

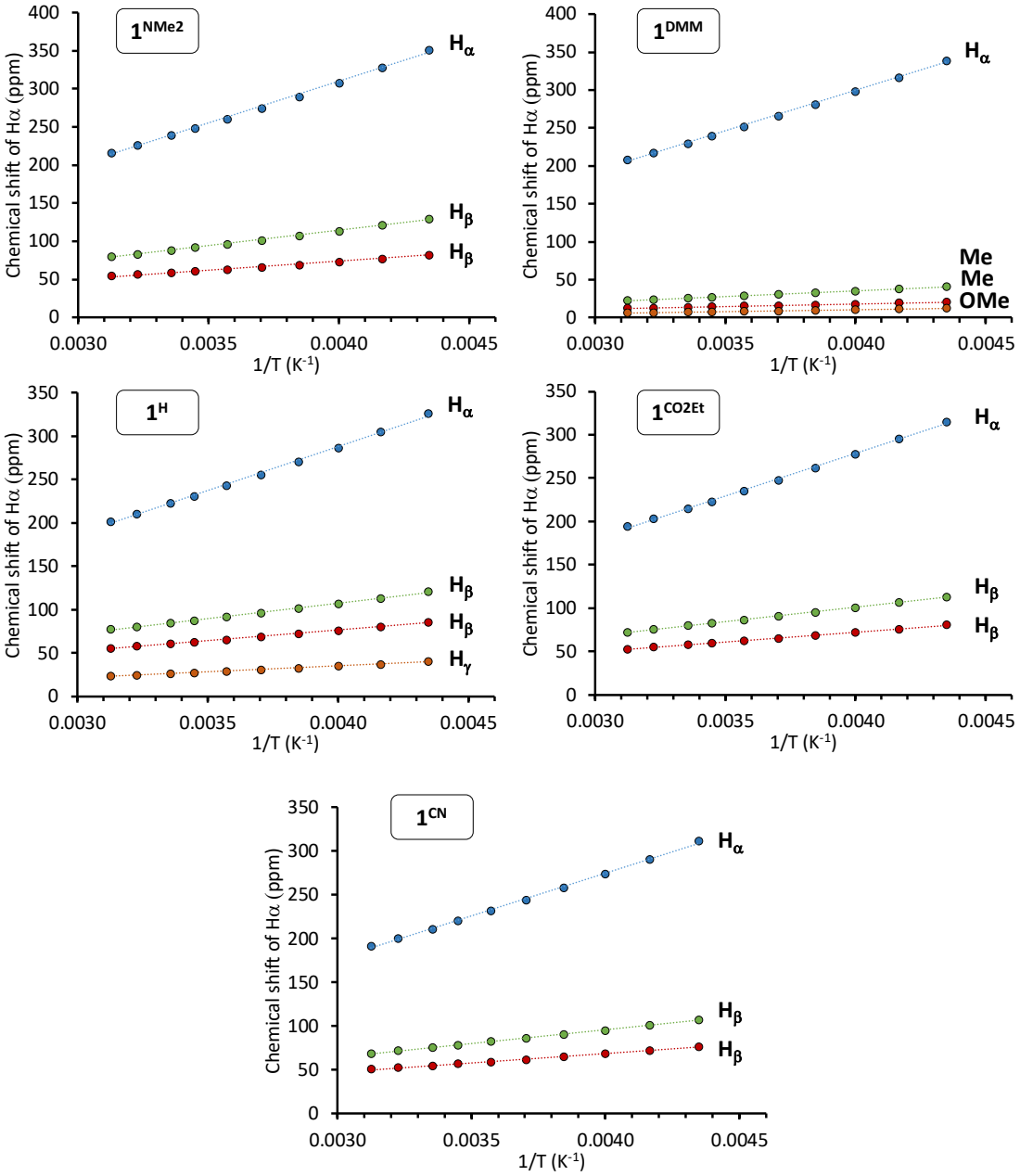



**Figure S11.** Representation of the chemical shift of aromatic protons of **1$^{R}$** complexes (in $CD_3CN$) in front of temperature in the $^{1}$H-NMR spectra.

### 4.2.3. Determination of the magnetic moment

The Evans' NMR method was also used to investigate the spin state of the **1$^{R}$** complexes,[7] providing constant $\mu_{eff}$ values (3.6-4.3 BM) for the series in the studied temperature range (235-330 K). These results are consistent with high-spin d$^7$ Co$^{II}$ complexes (S = 3/2) reported in the literature (expected $\mu_{eff}$ value: 3.9 BM).[8] However, for the corresponding low-spin (S = ½) Co$^{II}$ complexes, the $\mu_{eff}$ value is 1.7 MB.

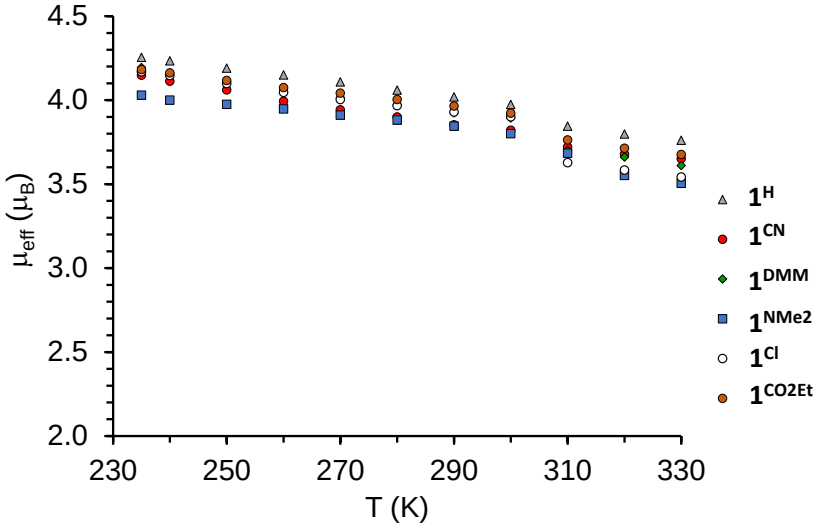



**Figure S12.** Representation of the effective magnetic moment ($\mu_{eff}$) of **1$^{R}$** complexes as a function of the temperature. $\mu_{eff}$ values were obtained in $CD_3CN$ using the Evans' method.[9]

### 4.2.4. $^{19}$F-NMR spectroscopy

Moreover, NMR studies gave useful information about the labile coordination sphere of the Co$^{II}$ center in the **1$^{R}$** complexes, formally represented by triflate groups. Actually, $^{19}$F-NMR of complex **1$^{H}$** showed a singlet at around -80 ppm, which is characteristic of a free triflate anion in $CD_3CN$ solution in diamagnetic species (Figure S13). The experimentally observed broadening and shift to higher fields of such $^{19}$F-NMR signal upon increasing the temperature could be due to a dynamic ligand exchange process of the triflate anion(s) with the solvent molecule(s) for the coordination with the metal centre (Figure S13). It is worth noting that a clear deeper colour change was generally observed when $CH_3CN$ was added to a solution of the starting triflate-containing **1$^{R}$** complexes in $CH_2Cl_2$. This behaviour, common for all the **1$^{R}$** series, suggests a highly favoured $CH_3CN$ coordination at room temperature. Finally, the replacement of triflate anions by $CH_3CN$ is also demonstrated by the X-Ray diffraction analysis of darker single crystals obtained from an acetonitrile solution containing **1$^{CN}$** (see manuscript).

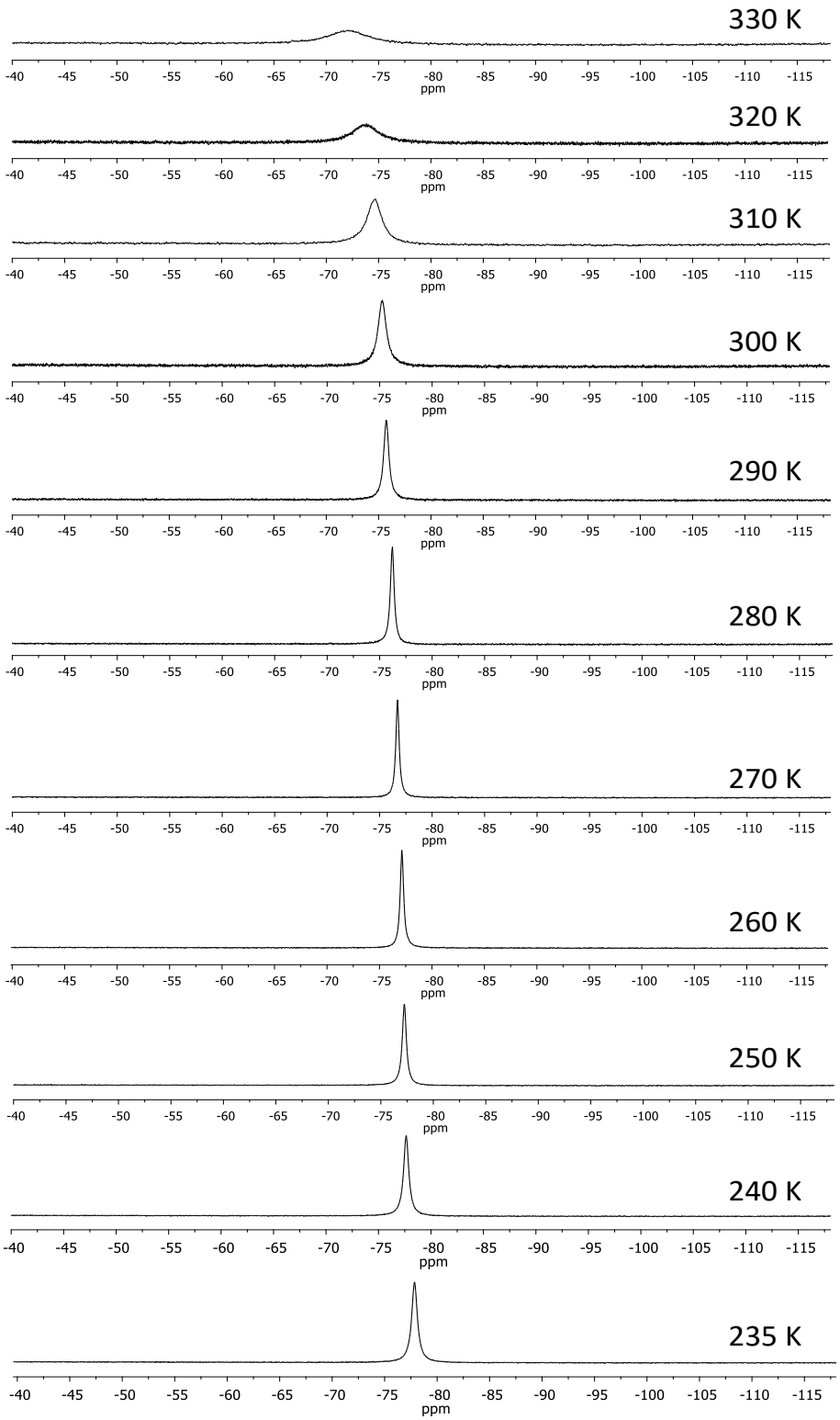



**Figure S13.** $^{19}$F-NMR spectra (500 MHz) of **1$^{H}$** in $CD_3CN$ at different temperatures.

### 4.2.5. X-ray crystallography

Crystals of the cobalt complexes $\mathbf{1}^{CO2Et}$, $\mathbf{1}^{Cl}$, $\mathbf{1}^{H}$, $\mathbf{1}^{DMM}$ and $\mathbf{1}^{NMe2}$ were grown by layering a solution of dichloromethane with diethyl ether. The compound $\mathbf{1}^{CN}$ was crystallized from an acetonitrile solution due to its insolubility in dichloromethane. Crystals of complexes $\mathbf{1}^{CN}$, $\mathbf{1}^{CO2Et}$, $\mathbf{1}^{Cl}$, $\mathbf{1}^{H}$ and $\mathbf{1}^{DMM}$ were measured at 100 K, whereas $\mathbf{1}^{NMe2}$ was measured at 298 K due to the low stability of the crystal at low temperature. $\mathbf{1}^{R}$ complexes crystallized in a monoclinic (for $\mathbf{1}^{CN}$, $\mathbf{1}^{CO2Et}$, $\mathbf{1}^{Cl}$, $\mathbf{1}^{DMM}$ and $\mathbf{1}^{NMe2}$) or orthorhombic (for $\mathbf{1}^{H}$) crystal system (see Tables S1-S4). Geometric distortions are probably the result of ligand constraints with only one carbon atom between tacn moieties with the pyridine ring. The $N^{CH2Py}{}_{tacn}$–Co–$N_{Py}$ angles are in the range of 78.0–80.3°, inducing a decrease in the $N^{Me}{}_{tacn}$–Co–$N_{Py}$ angle (155.7–163.6°) with respect to the ideal 180° (Tables S1-S4). More specifically, the pyridine arm coordinates *trans* to one of the N-methyl groups of the tacn ligand. This provides two accessible coordination sites in a relative *cis* configuration. In the bis-triflato complexes $\mathbf{1}^{CO2Et}$, $\mathbf{1}^{Cl}$, $\mathbf{1}^{H}$, $\mathbf{1}^{DMM}$ and $\mathbf{1}^{NMe2}$ the two free coordination sites are occupied by two triflate anions whereas in the case of $\mathbf{1}^{CN}$ the coordination sphere is completed by two acetonitrile molecules, leaving two free triflate anions. As previously mentioned however, coordinating solvent molecules replace triflate units in $CH_3CN$ solutions of $\mathbf{1}^{R}$ complexes at room temperature. The spatial distance between the Co atom and the pyridyl H atoms was correlated with the $^1$H-NMR $\Delta\delta$ values helping us to characterize the $H_\alpha$, $H_\beta$ and $H_{\beta'}$ atoms. In particular, a value of 3.190 Å was obtained for Co-$H_\alpha$, whereas distances of 5.131 Å and 4.923 Å were experimentally observed for Co-$H_\beta$ and Co-$H_{\beta'}$, respectively.

**Table S1.** Selected Bond Lengths (Å) and Angles (°) for $\mathbf{1}^{CN}$ $\mathbf{1}^{CO2Et}$ and $\mathbf{1}^{Cl}$.

| $\mathbf{1}^{CN}$ | | $\mathbf{1}^{CO2Et}$ | | $\mathbf{1}^{Cl}$ | |
|---|---|---|---|---|---|
| Co-N1 | 2.1068(10) | Co-N1 | 2.1175(17) | Co-N1 | 2.116(2) |
| Co-N2 | 2.1347(10) | Co-N2 | 2.1451(17) | Co-N2 | 2.154(2) |
| Co-N3 | 2.1679(9) | Co-N3 | 2.157(2) | Co-N3 | 2.155(2) |
| Co-N4 | 2.1293(9) | Co-N4 | 2.1436(18) | Co-N4 | 2.145(2) |
| Co-N5 | 2.0849(11) | Co-O1 | 2.0450(15) | Co-O1 | 2.0861(19) |
| Co-N6 | 2.1425(10) | Co-O2 | 2.2089(17) | Co-O2 | 2.175(2) |
| N1-Co-N2 | 80.26(4) | N1-Co-N2 | 78.00(7) | N1-Co-N2 | 79.92(9) |
| N1-Co-N3 | 96.81(4) | N1-Co-N3 | 110.39(7) | N1-Co-N3 | 101.19(8) |
| N1-Co-N4 | 163.55(4) | N1-Co-N4 | 155.68(7) | N1-Co-N4 | 161.69(9) |
| N1-Co-N5 | 98.12(4) | N1-Co-O1 | 99.25(7) | N1-Co-O1 | 104.77(8) |
| N1-Co-N6 | 84.21(4) | N1-Co-O2 | 82.81(6) | N1-Co-O2 | 85.26(8) |
| N2-Co-N3 | 82.61(4) | N2-Co-N3 | 81.59(7) | N2-Co-N3 | 82.01(8) |
| N2-Co-N4 | 83.53(4) | N2-Co-N4 | 84.06(7) | N2-Co-N4 | 83.30(9) |
| N2-Co-N5 | 176.35(4) | N2-Co-O1 | 169.72(7) | N2-Co-O1 | 170.61(8) |
| N2-Co-N6 | 92.90(4) | N2-Co-O2 | 100.94(7) | N2-Co-O2 | 100.02(9) |
| N3-Co-N4 | 83.82(4) | N3-Co-N4 | 82.69(7) | N3-Co-N4 | 83.57(8) |
| N3-Co-N5 | 94.37(4) | N3-Co-O1 | 90.23(7) | N3-Co-O1 | 89.04(8) |
| N3-Co-N6 | 175.14(4) | N3-Co-O2 | 166.77(7) | N3-Co-O2 | 173.52(8) |
| N4-Co-N5 | 98.23(4) | N4-Co-O1 | 101.15(7) | N4-Co-O1 | 92.90(8) |
| N4-Co-N6 | 93.86(4) | N4-Co-O2 | 84.65(7) | N4-Co-O2 | 90.53(8) |
| N5-Co-N6 | 90.18(4) | O1-Co-O2 | 88.44(6 | O1-Co-O2 | 88.57(8) |

**Table S2.** Selected Bond Lengths (Å) and Angles (°) for $\mathbf{1}^{H}$, $\mathbf{1}^{DMM}$ and $\mathbf{1}^{NMe2}$.

| $\mathbf{1}^{H}$ | | $\mathbf{1}^{DMM}$ | | $\mathbf{1}^{NMe2}$ | |
|---|---|---|---|---|---|
| Co-N1 | 2.0969(12) | Co-N1 | 2.0883(13) | Co-N1 | 2.088(4) |
| Co-N2 | 2.1309(12) | Co-N2 | 2.1263(13) | Co-N2 | 2.160(4) |
| Co-N3 | 2.1667(12) | Co-N3 | 2.1628(14) | Co-N3 | 2.172(5) |
| Co-N4 | 2.1458(12) | Co-N4 | 2.1427(13) | Co-N4 | 2.150(4) |
| Co-O1 | 2.1684(10) | Co-O1 | 2.0596(13) | Co-O1 | 2.083(4) |
| Co-O2 | 2.0689(10) | Co-O2 | 2.2230(12) | Co-O2 | 2.225(4) |
| N1-Co-N2 | 80.26(5) | N1-Co-N2 | 78.21(5) | N1-Co-N2 | 79.03(15) |
| N1-Co-N3 | 95.45(5) | N1-Co-N3 | 108.01(5) | N1-Co-N3 | 106.7(2) |
| N1-Co-N4 | 163.27(5) | N1-Co-N4 | 157.25(5) | N1-Co-N4 | 158.05(18) |
| N1-Co-O1 | 87.37(4) | N1-Co-O1 | 100.22(6) | N1-Co-O1 | 101.75(15) |
| N1-Co-O2 | 103.44(5) | N1-Co-O2 | 84.44(5) | N1-Co-O2 | 86.73(15) |
| N2-Co-N3 | 82.84(5) | N2-Co-N3 | 82.26(5) | N2-Co-N3 | 81.31(19) |
| N2-Co-N4 | 83.02(5) | N2-Co-N4 | 83.64(5) | N2-Co-N4 | 82.75(17) |
| N2-Co-O1 | 96.60(4) | N2-Co-O1 | 175.82(6) | N2-Co-O1 | 171.35(17) |
| N2-Co-O2 | 174.14(4) | N2-Co-O2 | 97.98(5) | N2-Co-O2 | 101.10(17) |
| N3-Co-N4 | 82.95(5) | N3-Co-N4 | 82.71(5) | N3-Co-N4 | 82.4(2) |
| N3-Co-O1 | 176.98(4) | N3-Co-O1 | 94.62(6) | N3-Co-O1 | 90.26(19) |
| N3-Co-O2 | 92.24(4) | N3-Co-O2 | 167.23(5) | N3-Co-O2 | 166.6(2) |
| N4-Co-O1 | 94.03(4) | N4-Co-O1 | 98.77(6) | N4-Co-O1 | 98.12(18) |
| N4-Co-O2 | 93.27(4) | N4-Co-O2 | 84.62(5) | N4-Co-O2 | 84.86(18) |
| O1-Co-O2 | 88.16(4) | O1-Co-O2 | 85.68(6) | O1-Co-O2 | 87.55(17) |

**Table S3.** Crystal Data for $\mathbf{1^{CN}}$ $\mathbf{1^{CO2Et}}$ and $\mathbf{1^{Cl}}$.

| **Compound** | $\mathbf{1^{CN}}$ | $\mathbf{1^{CO2Et}}$ | $\mathbf{1^{Cl}}$ |
|---|---|---|---|
| Empirical formula | $C_{21}H_{29}CoF_6N_7O_6S_2$ | $C_{19}H_{28}CoF_6N_4O_8S_2$ | $C_{16}H_{23}ClCoF_6N_4O_6S_2$ |
| Formula weight | 712.56 | 677.50 | 639.88 |
| Temperature | 100(2) K | 100(2) K | 100(2) K |
| Wavelength | 0.71073 Å | null Å | 0.71073 Å |
| Crystal system | Monoclinic | Monoclinic | Monoclinic |
| Space group | P2(1)/n | Cc | P 21/n |
| Unit cell dimensions | a = 14.2091(5) Å<br>$\alpha$ = 90°<br>b = 13.4658(4) Å<br>$\beta$ = 93.2950(8)°<br>c = 15.1840(5) Å<br>$\gamma$ = 90° | a = 12.8115(16) Å<br>$\alpha$ = 90°<br>b = 24.0973(19)Å<br>$\beta$ = 96.927(5)°<br>c = 8.7902(10)Å<br>$\gamma$ = 90° | a = 8.8511(7) Å<br>$\alpha$ = 90°<br>b = 24.5258(19) Å<br>$\beta$ = 97.0660(10)°<br>c = 11.1501(9) Å<br>$\gamma$ = 90° |
| Volume | 2000.46(16) $Å^3$ | 2693.9(5) $Å^3$ | 2402.1(3) $Å^3$ |
| Z | 4 | 4 | 4 |
| Density (calculated) | 1.632 $Mg/m^3$ | 1.670 $Mg/m^3$ | 1.769 $Mg/m^3$ |
| Adsorption coefficient | 0.824 $mm^{-1}$ | 0.885 $mm^{-1}$ | 1.088 $mm^{-1}$ |
| F(000) | 1460 | 1388 | 1300 |
| Crystal size | 0.20 x 0.20 x 0.20 $mm^3$ | 0.30 x 0.30 x 0.15 $mm^3$ | 0.25 x 0.15 x 0.08 $mm^3$ |
| $\Theta$ range for data collection | 1.909 to 30.518° | 1.811 to 32.527° | 1.661 to 28.302° |
| Index ranges | -19 ≤ h ≤ 20<br>-11 ≤ k ≤ 19<br>-18 ≤ l ≤ 21 | -19 ≤ h ≤ 19<br>-25 ≤ k ≤ 36<br>-12 ≤ l ≤ 6 | -8 ≤ h ≤ 11<br>-32 ≤ k ≤ 31<br>-13 ≤ l ≤ 14 |
| Reflections collected | 27923 | 16431 | 14849 |
| Independent reflections | 8496 | 6178 | 5575 |
| | [R(int) = 0.0223] | [R(int) = 0.0251] | [R(int) = 0.0250] |
| Completeness to $\Theta$ | 95.9% ($\Theta$= 30.518°) | 92.0% ($\Theta$ = 32.527°) | 99.9 % ($\Theta$ = 25.242°) |
| Absorption correction | Multi-scan | Multi-scan | Empirical |
| Max. and min. transmission | 0.853 and 0.728 | 0.879 and 0.777 | 1 and 0.783 |
| Refinement method | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 8496/0/392 | 6178/2/364 | 5575/0/327 |
| Goodness-of-fit on $F^2$ | 1.030 | 1.034 | 1.031 |
| Final R indices [I>2$\alpha$(I)] | R1 = 0.0269<br>wR2 = 0.0690 | R1 = 0.0259<br>wR2 = 0.0595 | R1 = 0.0426<br>wR2 = 0.1065 |
| R indices (all data) | R1 = 0.0309<br>wR2 = 0.0715 | R1 = 0.0280<br>wR2 = 0.0605 | R1 = 0.0538<br>wR2 = 0.1133 |
| Largest diff. peak and hole | 0.417 and -0.393 e·$Å^{-3}$ | 0.377 and -0.373 e·$Å^{-3}$ | 0.941 and -0.635 e·$Å^{-3}$ |

**Table S4.** Crystal Data for $\mathbf{1^{H}}$, $\mathbf{1^{DMM}}$ and $\mathbf{1^{NMe2}}$.

| Compound | $\mathbf{1^{H}}$ | $\mathbf{1^{DMM}}$ | $\mathbf{1^{NMe2}}$ |
|---|---|---|---|
| Empirical formula | $C_{16}H_{24}CoF_6N_4O_6S_2$ | $C_{19}H_{30}CoF_6N_4O_7S_2$ | $C_{18}H_{29}CoF_6N_5O_6S_2$ |
| Formula weight | 605.44 | 663.52 | 648.51 |
| Temperature | 100(2) K | 100(2) K | 298(2) K |
| Wavelength | 0.71073 Å | 0.71073 Å | 0.71073 Å |
| Crystal system | Orthorhombic | Monoclinic | Monoclinic |
| Space group | Pbca | P2(1)/c | P 21/n |
| Unit cell dimensions | a = 9.312(2) Å | a = 11.9921(9) Å | a = 8.802(2) Å |
| | $\alpha$ = 90 | $\alpha$= 90° | $\alpha$ = 90° |
| | b = 16.956(4) Å | b = 15.4423(14) Å | b = 24.936(6) Å |
| | $\beta$ =90° | $\beta$ = 108.403(2)° | $\beta$ = 94.038(5)° |
| | c=29.498(7) Å | c = 15.8756(13) Å | c = 12.694(3) Å |
| | $\gamma$ = 90° | $\gamma$ = 90° | $\gamma$ = 90° |
| Volume | 4657.5(19) Å$^3$ | 2789.6(4) Å$^3$ | 2779.3(12) Å$^3$ |
| Z | 8 | 4 | 4 |
| Density (calculated) | 1.727 Mg/m$^3$ | 1.580 Mg/m$^3$ | 1.550 Mg/m$^3$ |
| Adsorption coefficient | 1.006 mm$^{-1}$ | 0.850 mm$^{-1}$ | 0.849 mm$^{-1}$ |
| F(000) | 2472 | 1364 | 1332 |
| Crystal size | 0.20 x 0.20 x 0.05 mm$^3$ | 0.40 x 0.35 x 0.10 mm$^3$ | 0.35 x 0.20 x 0.12 mm$^3$ |
| $\Theta$ range for data collection | 2.402 to 27.573° | 1.790 to 30.537° | 2.292 to 27.498° |
| Index ranges | -11 ≤ h ≤ 12 | -15 ≤ h ≤ 17 | -11 ≤ h ≤ 11 |
| | -22 ≤ k ≤ 20 | -21 ≤ k ≤ 22 | -32 ≤ k ≤ 32 |
| | -38 ≤ l ≤ 38 | -16 ≤ l ≤ 22 | -16 ≤ l ≤ 16 |
| Reflections collected | 20276 | 29373 | 41842 |
| Independent reflections | 5153 | 8352 | 6388 |
| | [R(int) = 0.0216] | [R(int) = 0.0381] | [R(int) = 0.0479] |
| Completeness to $\Theta$ | 95.6% ($\Theta$ = 27.573°) | 97.89% ($\Theta$ = 30.537°) | 95.6% ($\Theta$ = 25.242°) |
| Absorption correction | Empirical | Multi-scan | Empirical |
| Max. and min. transmission | 0.951 and 0.732 | 0.920 and 0.733 | 1.0 and 0.843 |
| Refinement method | Full-matrix least-squares on F$^2$ | Full-matrix least-squares on F$^2$ | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters | 5153/6/318 | 8352/0/357 | 6388/6/330 |
| Goodness-of-fit on F$^2$ | 1.091 | 1.035 | 1.036 |
| Final R indices [I>2$\alpha$(I)] | R1 = 0.0227 | R1 = 0.0353 | R1 = 0.0767 |
| | wR2 = 0.0556 | wR2 = 0.0873 | wR2 = 0.2182 |
| R indices (all data) | R1 = 0.0251 | R1 = 0.0458 | R1 = 0.1031 |
| | wR2 = 0.0568 | wR2 = 0.0933 | wR2 = 0.2483 |
| Largest diff. peak and hole | 0.397 and -0.369 e·Å$^{-3}$ | 1.509 and -0.603 e·Å$^{-3}$ | 1.05 d -0.656 e·Å$^{-3}$ |

### 4.2.6. Electrochemistry

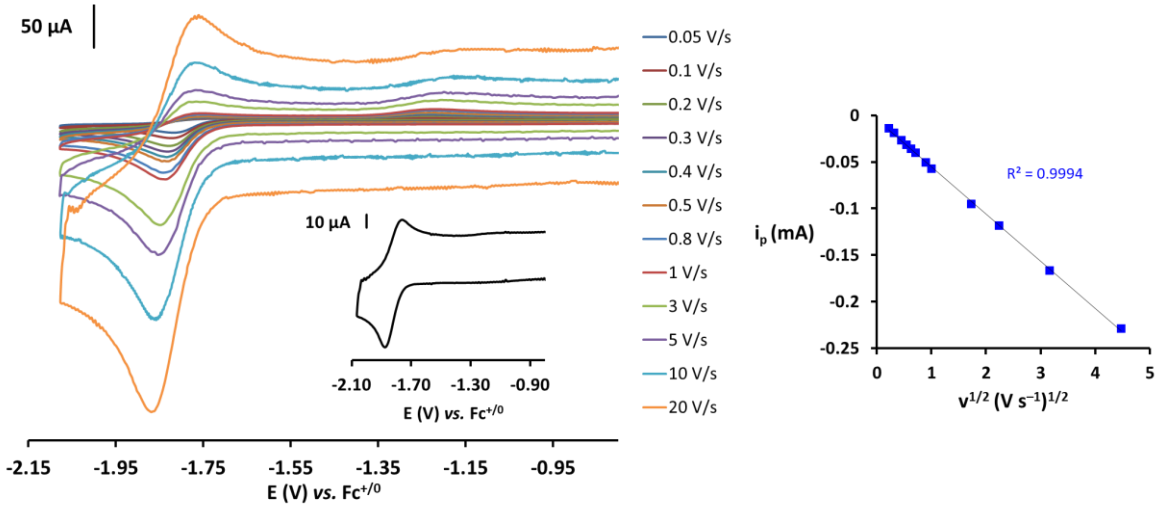



**Figure S14.** CVs of $\mathbf{1}^{\mathbf{NMe2}}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at different scan rates (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1, 3, 5, 10, 20 V $s^{-1}$) (left) and plot of the peak cathodic current *vs.* the square root of the scan rate (right). A GC working electrode of 3 mm diameter was employed. The inset shows a CV of $\mathbf{1}^{\mathbf{NMe2}}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at $v$=50 V $s^{-1}$ on a smaller size GC working electrode (1 mm diameter), providing $E_{1/2}(Co^{II/I})$ = –1.82 V.

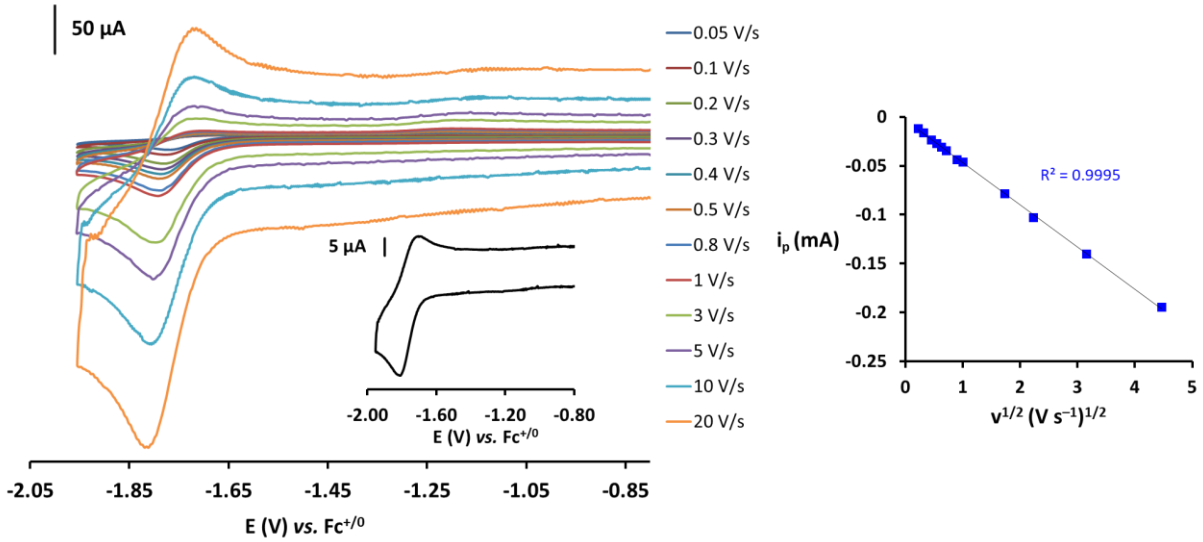



**Figure S15.** CVs of $\mathbf{1}^{\mathbf{DMM}}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at different scan rates (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1, 3, 5, 10, 20 V $s^{-1}$) (left) and plot of the peak cathodic current *vs.* the square root of the scan rate (right). A GC working electrode of 3 mm diameter was employed. The inset shows a CV of $\mathbf{1}^{\mathbf{DMM}}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at $v$=20 V $s^{-1}$ on a smaller size GC working electrode (1 mm diameter), providing $E_{1/2}(Co^{II/I})$ = –1.76 V.

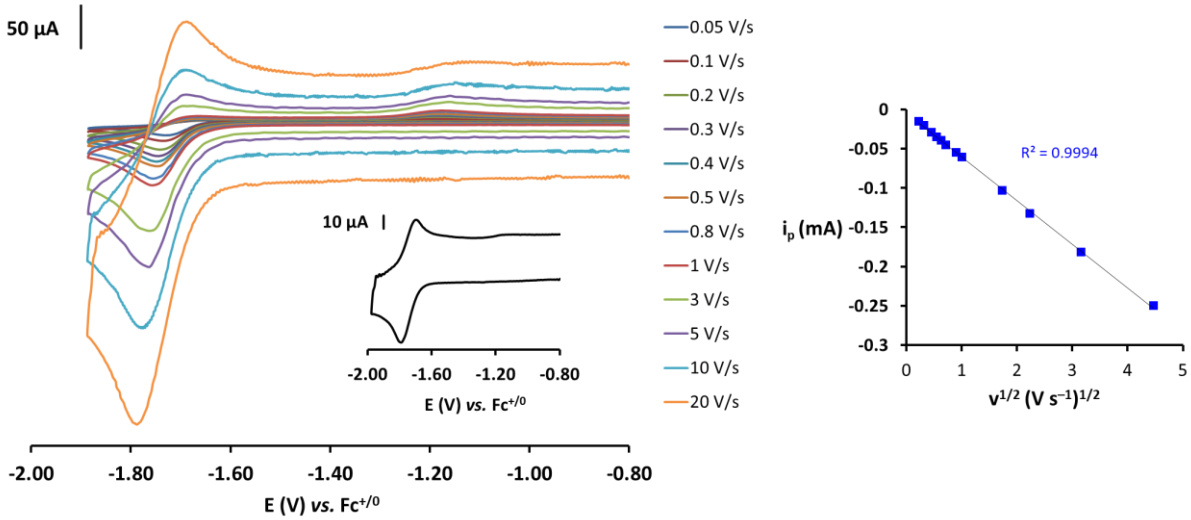



**Figure S16.** CVs of $\mathbf{1}^{H}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at different scan rates (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1, 3, 5, 10, 20 V $s^{-1}$) (left) and plot of the peak cathodic current *vs.* the square root of the scan rate (right). A GC working electrode of 3 mm diameter was employed. The inset shows a CV of $\mathbf{1}^{H}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at *v*=50 V $s^{-1}$ on a smaller size GC working electrode (1 mm diameter), providing $E_{1/2}(Co^{II/I})$ =–1.74 V.

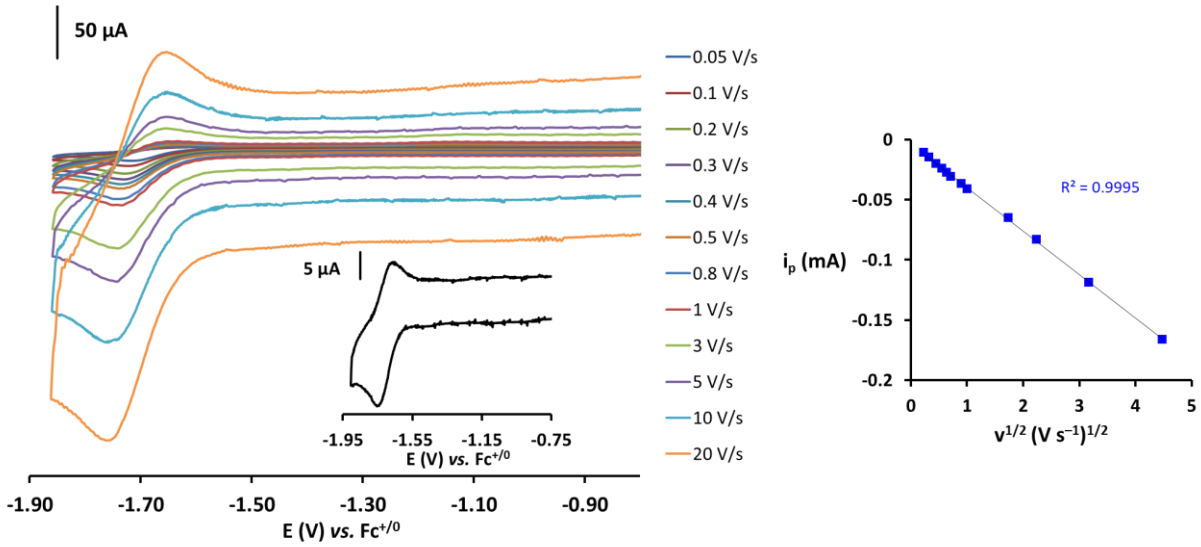



**Figure S17.** CVs of $\mathbf{1}^{Cl}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at different scan rates (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1, 3, 5, 10, 20 V $s^{-1}$) (left) and plot of the peak cathodic current *vs.* the square root of the scan rate (right). A GC working electrode of 3 mm diameter was employed. The inset shows a CV of $\mathbf{1}^{Cl}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at *v*=10 V $s^{-1}$ on a smaller size GC working electrode (1 mm diameter), providing $E_{1/2}(Co^{II/I})$ = –1.71 V.

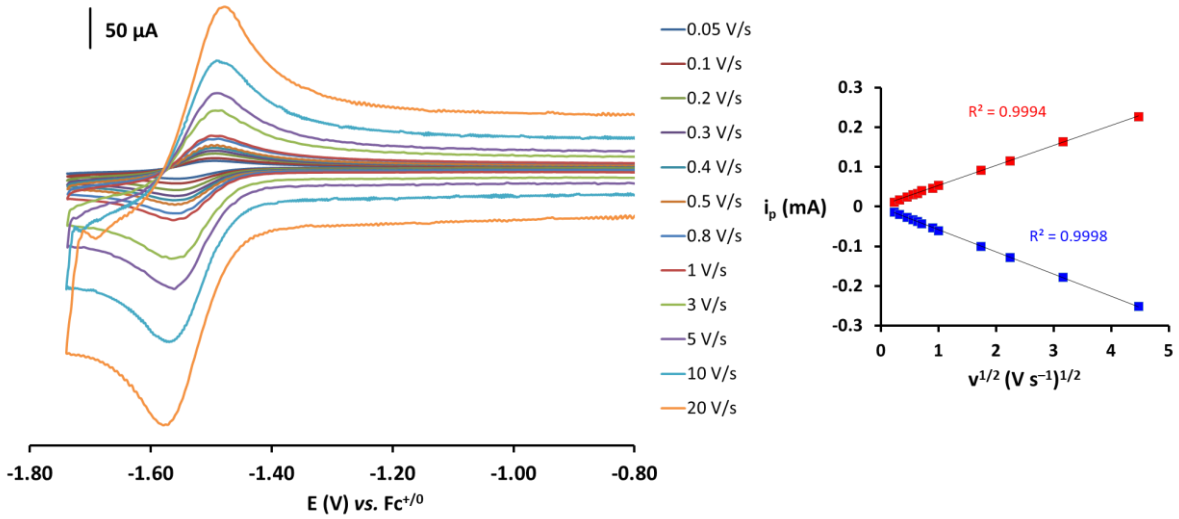



**Figure S18.** CVs of $\mathbf{1}^{CO2Et}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at different scan rates (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 1, 3, 5, 10, 20 V $s^{-1}$) (left) and plot of the peak current (anodic and cathodic) *vs.* the square root of the scan rate (right). A GC working electrode of 3 mm diameter was employed.

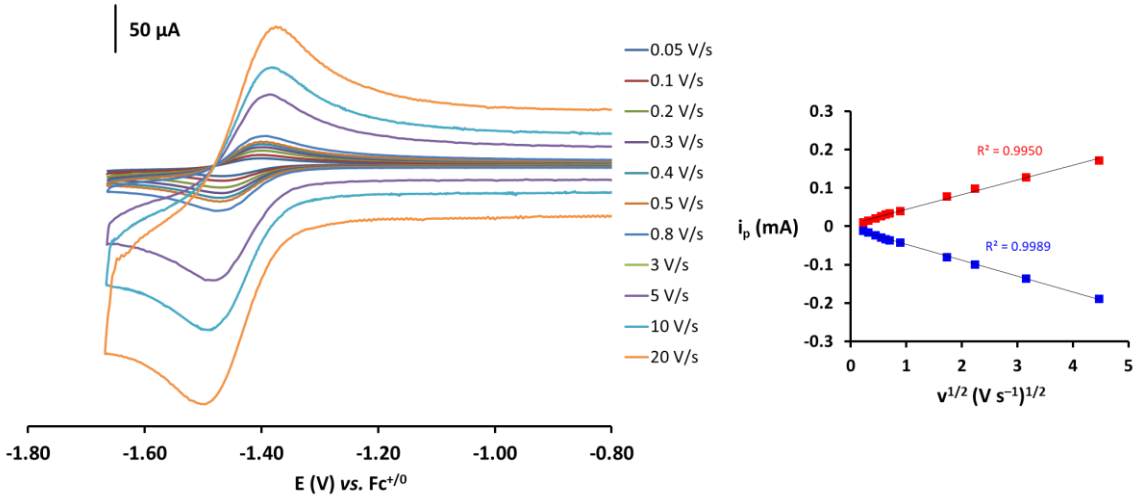



**Figure S19.** CVs of $\mathbf{1}^{CN}$ (1 mM) in 0.1 M $TBAPF_6/CH_3CN$ at different scan rates (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.8, 3, 5, 10, 20 V $s^{-1}$) (left) and plot of the peak current (anodic and cathodic) *vs.* the square root of the scan rate (right). A GC working electrode of 3 mm diameter was employed.

## 5. Photocatalytic reactions

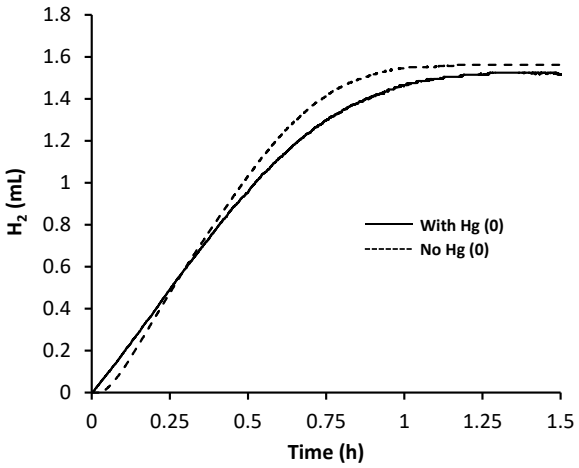



**Figure S20.** Photocatalytic hydrogen production in the presence (dashed line) and absence (solid line) of $Hg^0$. Conditions: $\mathbf{1}^{H}$ (50 μM), $\mathbf{PS}_{Ir}$ (250 μM) using $CH_3CN$:$H_2O$:$Et_3N$ (4:6:0.2 mL) as solvent and irradiated (λ = 447 nm) at 25 °C under nitrogen. The reaction using $Hg^0$ was performed using 1.5 mL of $Hg^0$ (15 % of the total volume of the reaction).

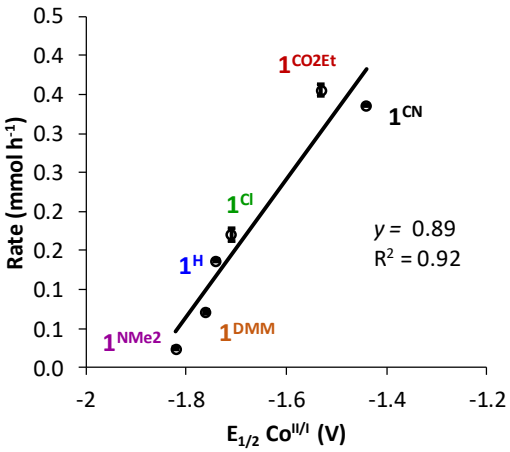



**Figure S21.** Plot of the initial rates in $H_2$ evolution measured at 10% conversion vs. the experimental $E_{1/2}$ $Co^{II/I}$ (V) values. Conditions: $\mathbf{1}^{R}$ (50 μM) and $\mathbf{PS}_{Ir}^{+}$ (150 μM) in $CH_3CN$:$H_2O$:$Et_3N$ (4:6:0.2 mL) irradiated ( λ = 447 nm) at 25 °C under nitrogen.

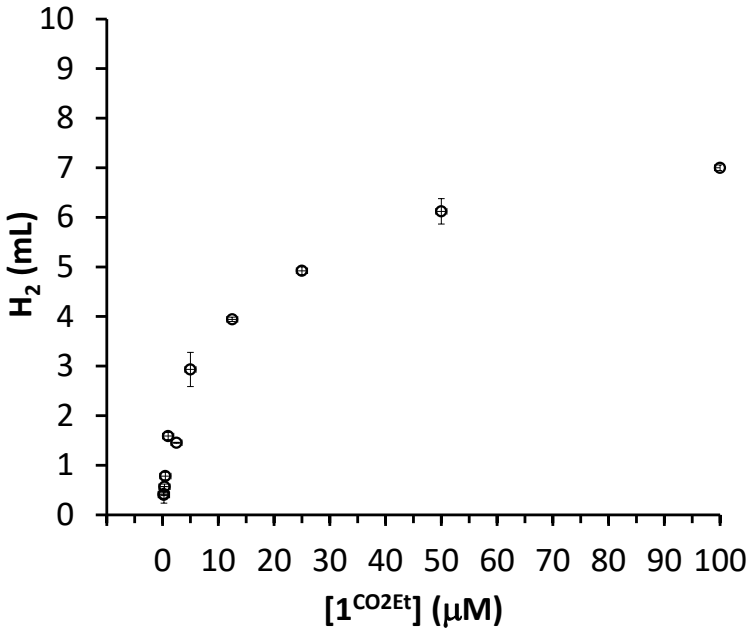



**Figure S22.** Hydrogen production (mL $H_2$) *vs.* the concentration of $\mathbf{1}^{CO2Et}$. Experimental conditions: $\mathbf{1}^{CO2Et}$ (0.25-100 μM), $\mathbf{PS}_{Ir}$ (150 μM) using $CH_3CN$:$H_2O$:$Et_3N$ (4:6:0.2 mL) as solvent and irradiated (λ = 447 nm) at 25 °C under nitrogen.

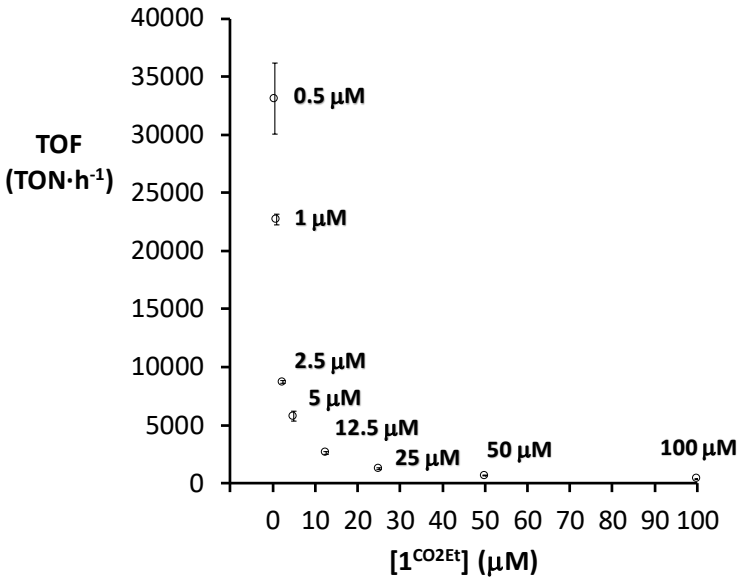



**Figure S23.** Dependence of the light-driven $H_2$ evolution activity on catalyst ($\mathbf{1}^{CO2Et}$) concentration. Conditions: $\mathbf{1}^{CO2Et}$ (0.25-100 μM), $\mathbf{PS}_{Ir}$ (150 μM) using $CH_3CN$:$H_2O$:$Et_3N$ (4:6:0.2 mL) as solvent and irradiated (λ = 447 nm) at 25 °C under nitrogen.

## 6. Photochemistry and UV-Vis quenching studies

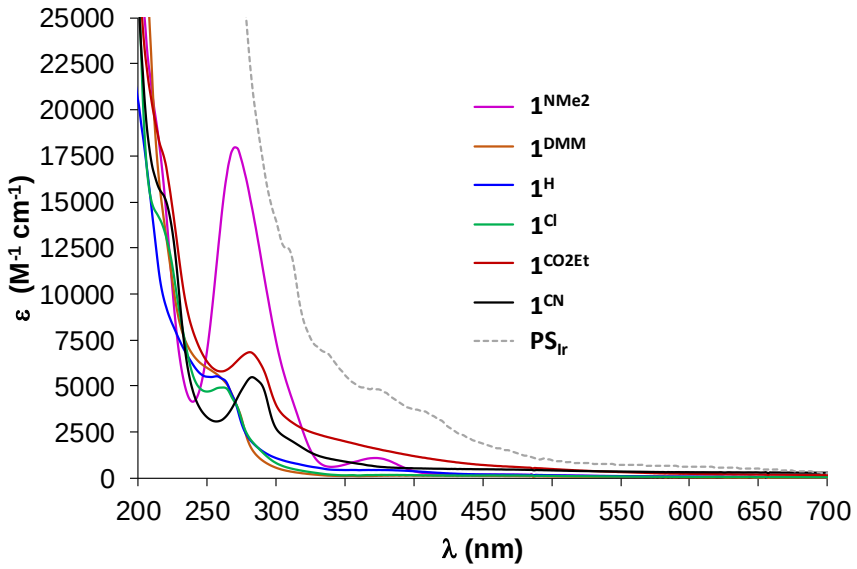



**Figure S24.** UV/Vis spectra of 0.1M solution of $\mathbf{1}^{NMe2}$ (purple), $\mathbf{1}^{DMM}$ (orange), $\mathbf{1}^{H}$ (blue), $\mathbf{1}^{Cl}$ (green), $\mathbf{1}^{CO2Et}$ (red) and $\mathbf{1}^{CN}$ (black), in MeCN at 298 K. The dashed grey spectrum corresponds to the absorption of 0.02 mM solution of $\mathbf{PS}_{Ir}$ in MeCN.

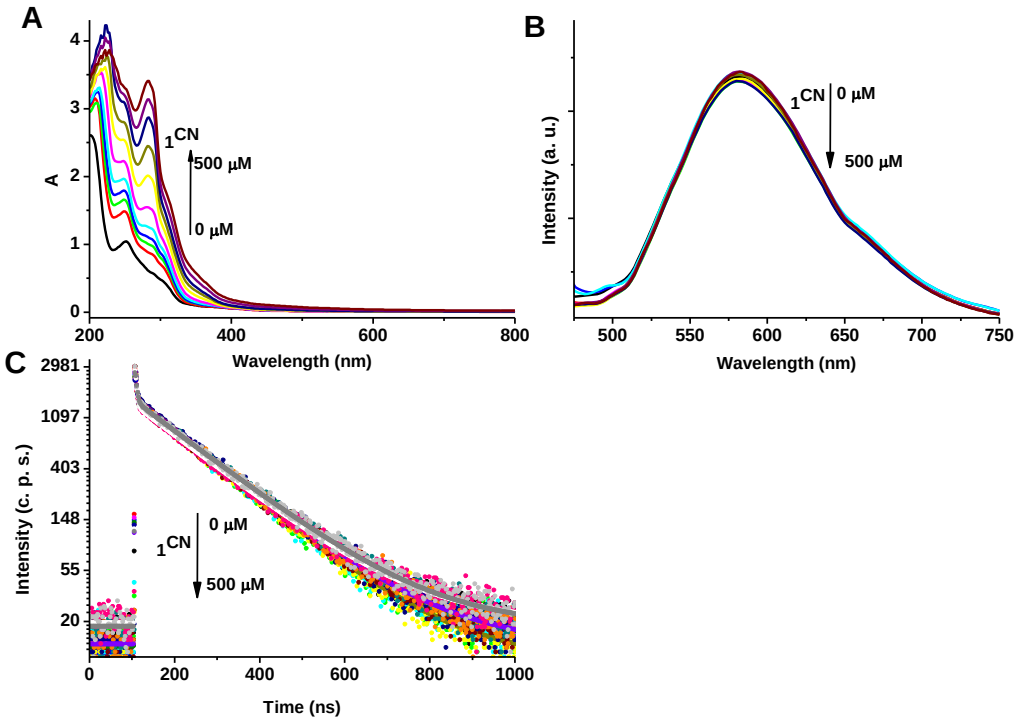



**Figure S25.** Steady state absorption spectra (**a**), emission spectra (**b**) and time resolved luminescence decays (**c**) of $\mathbf{PS_{Ir}^{+}}$ in presence varying concentrations of $\mathbf{1^{CN}}$. $\lambda_{ex}$= 470 nm.[$\mathbf{PS_{Ir}^{+}}$]= 10 μM in $H_2O$:$CH_3CN$ 6:4 solvent mixture, (V=2 ml); cell path length b =1 cm; temperature= 25 °C.

**Table. S5.** Fitting parameters of luminescence decays of $\mathbf{PS_{Ir}^+}$ in presence of varying concentrations of $\mathbf{1^{CN}}$.

| $\mathbf{1^{CN}}$ (μM) | $\tau_1$/ ns | $\tau_2$/ ns | A1 (%) | A2 (%) | $\chi^2$ |
|---|---|---|---|---|---|
| 0 | 3 | 146 | 3 | 97 | 1.2 |
| 50 | 2.7 | 146 | 4 | 96 | 1.3 |
| 100 | 2.6 | 147 | 4 | 96 | 1.3 |
| 200 | 2.7 | 150 | 4 | 96 | 1.3 |
| 300 | 3 | 150 | 4 | 96 | 1.3 |
| 400 | 3 | 150 | 4 | 96 | 1.4 |
| 500 | 3 | 150 | 4 | 96 | 1.4 |

The luminescence decay of $\mathbf{PS_{Ir}^+}$ in $H_2O$:$CH_3CN$ 6:4 solvent mixture is fitted with bi-exponentials and the luminescence lifetimes appear to be with fast and slow components, 146 ns and 3 ns, respectively. A1 and A2 correspond to the relative contributions of the two lifetimes, $\tau_1$ and $\tau_2$ in the case of bi-exponential decay. $\mathbf{PS_{Ir}^+}$= 10 μM in $H_2O$:$CH_3CN$ 6:4 solvent mixture.

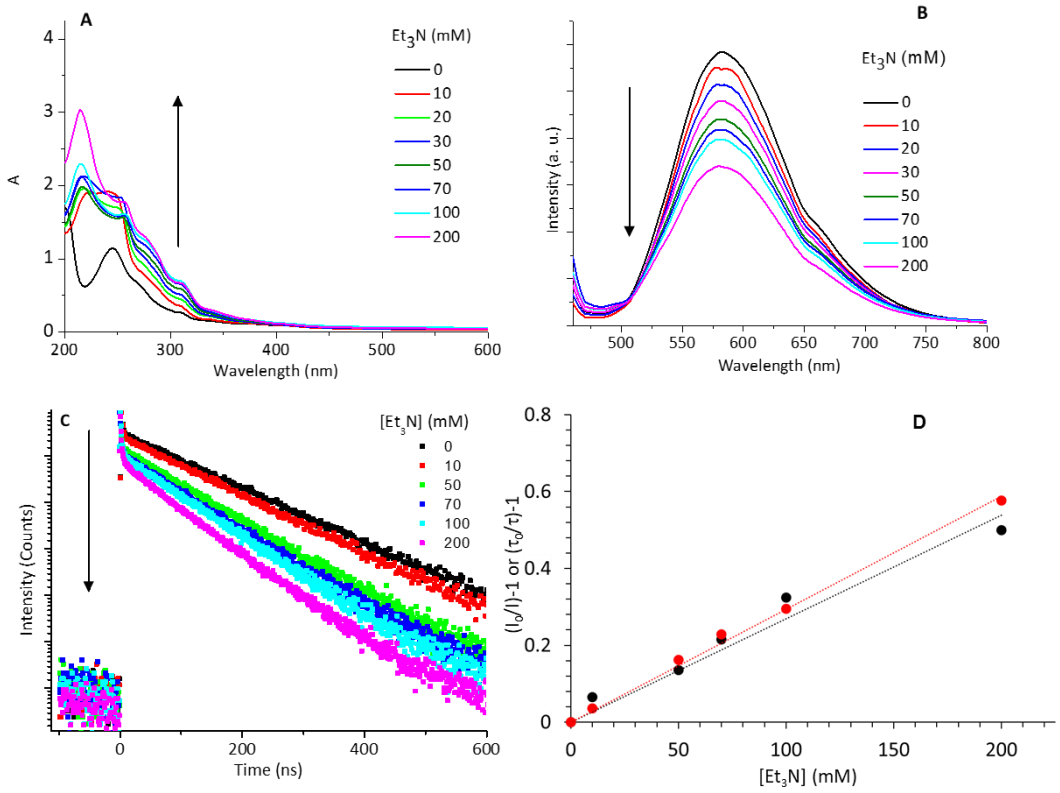



**Figure S26.** (A) Absorption spectra of $\mathbf{PS_{Ir}^+}$ at different concentrations of $Et_3N$; [$Et_3N$]/mM: 0-300 mM. (B) Steady-state emission spectra of $\mathbf{PS_{Ir}^+}$ ($\lambda_{ex}$=450 nm at isosbestic point) at different concentrations of $Et_3N$. (C) Time-resolved luminescence decay of $\mathbf{PS_{Ir}^+}$ and its exponential fits at different concentrations of $Et_3N$; excitation with 470 nm laser. (D) Stern-Volmer quenching analysis on $\mathbf{^*PS_{Ir}^+}$ lifetimes (red circle) or intensity changes (black circle) at 584 nm as a function of [$Et_3N$]. [$\mathbf{PS_{Ir}^+}$] = 10 μM in $H_2O$:$CH_3CN$ 6:4 solvent mixture (V = 2 mL), cell path length 1 cm, Temperature = 25 °C.

**Table S6.** The biexponential fitting parameters of excited state lifetime decay of $\mathbf{PS_{Ir}^+}$ obtained by time correlated single photon counting upon addition of different concentrations of $Et_3N$.

| $Et_3N$ (mM) added to the $\mathbf{PS_{Ir}^+}$ solution | $\tau_1$/ ns | $\tau_2$/ ns | A1 (%) | A2 (%) | $\chi^2$ |
|---|---|---|---|---|---|
| 0 [a] | 3 | 146 | 3 | 97 | 1.2 |
| 10 | 1.2 | 140 | 2.5 | 97.5 | 1.3 |
| 20 | 2 | 126 | 3 | 97 | 1.3 |
| 30 | 2 | 118 | 4 | 96 | 1.3 |
| 50 | 2 | 112 | 4 | 96 | 1.27 |
| 70 | 1.5 | 92 | 4 | 96 | 1.3 |
| 100 | 2 | 82 | 6 | 94 | 1.32 |
| 200 | 2 | 70 | 7 | 93 | 1.3 |

The decay is fitted with biexponential function with fast and slow lifetime components *ca.*, 3 ns and 145 ns with the corresponding amplitude of 3 % and 97 % respectively, as according to the solvent medium. $A_1$ and $A_2$ correspond to the relative contributions of the two lifetimes, $\tau_1$ and $\tau_2$. [a]fitting parameters of $\mathbf{PS_{Ir}^+}$ alone in 2 mL water:acetonitrile (60:40 %) solvent mixture.

The Stern-Volmer analysis is based on eqs. S1-S2:

$$\frac{I_0}{I_Q}\left(or\ \frac{\tau_0}{\tau_Q}\right) = 1 + K_{SV}[Et_3N] \qquad (S1)$$

$$K_{SV} = k_q\tau_0 \qquad (S2)$$

where $I_0$, $I_Q$, $\tau_0$ and $\tau_Q$ are the luminescence intensities and excited state lifetime at emission peak (584 nm) in the absence or in the presence of $Et_3N$, respectively, and $K_{SV}$ is the Stern-Volmer quenching constant. The bimolecular quenching rate constant ($k_q$ [1]) was obtained from the slope of the linear fitting of the plot using eq. (S2) and $\tau_0$ is the $^*\mathbf{PS_{Ir}^+}$ lifetime.

**6.1.- Absorption kinetics studies. Estimation of the photogenerated $PS_{Ir}$.**

To estimate the concentration of photogenerated $\mathbf{PS_{Ir}}$ (see main text) we titrated solution with different $\mathbf{1^{CN}}$ (**Figures S27 and S28**) while monitoring the $\mathbf{PS_{Ir}}$ absorption (527 nm) decay. We selected $\mathbf{1^{CN}}$ for the titration since the redox potential difference between $Co^{I/II}$ and $\mathbf{PS_{Ir}}/\mathbf{PS_{Ir}}^{+}$ (–1.44 V and -1.04, respectively) is 400 mV, which is enough to safely consider that the $Co^{II}$ species are fully consumed by the photogenerated $\mathbf{PS_{Ir}}$. In other words, the equilibrium between the $\mathbf{PS_{Ir}}$ and the Co(II) catalyst is completely shifted to the products. Full consumption of the photogenerated $\mathbf{PS_{Ir}}$ was achieved after 15 μM of $\mathbf{1^{CN}}$ (**Figures S27 and S28**), therefore we estimate that *c.a.* 15 μM of $\mathbf{PS_{Ir}}$ is formed under our experimental conditions ($\mathbf{PS_{Ir}}^{+}$ (100 μM) and $Et_3N$ (1000 eq.) in degased acetonitrile at -20 ºC under $N_2$ and irradiated at 447 nm with a 3 W LED).

$$\mathbf{PS_{Ir}} \quad + \quad Co^{II} \quad \rightleftharpoons \quad \mathbf{PS_{Ir}}^{+} \quad + \quad Co^{I}$$

In order to validate the obtained value of $\mathbf{PS_{Ir}}$ concentration, we studied the reaction of different $\mathbf{1^{R}}$ (14.5 μM, 97% of the [$\mathbf{PS_{Ir}}$]) catalysts with $\mathbf{PS_{Ir}}^{+}$ (**Figures SI.29 and SI.30**) In this regard, the $\mathbf{PS_{Ir}}$ absorption (527 nm) decay was proportional to the $\mathbf{1^{R}}$ redox potential following the Nernst equation.

$$\begin{array}{ccccccc} \mathbf{PS_{Ir}} & + & Co^{II} & \rightleftharpoons & \mathbf{PS_{Ir}}^{+} & + & Co^{I} \\ 15\text{-}\alpha & & 14.5\text{-}\alpha & & 85+\alpha & & \alpha \end{array}$$

$[\mathbf{PS_{Ir}}^{+}]_{initial} = [\mathbf{PS_{Ir}}] + [\mathbf{PS_{Ir}}^{+}] = 100$ μM, after 20 s of [$\mathbf{PS_{Ir}}$] irradiation is maximized, therefore [$\mathbf{PS_{Ir}}^{+}$] = 85 μM and [$\mathbf{PS_{Ir}}$] = 15 μM. Then, the Nernst equation for the redox equilibrium is:

$$\Delta E = E_{1/2}(PS_{Ir}{}^{+}/PS_{Ir}) - E_{1/2}(Co^{II/I}) = -0.059 \log \frac{[Ir(III)][Co(I)]}{[Co(II)][Ir(II)]} \qquad (S3)$$

$$\Delta E = E_{1/2}\left(\frac{PS_{Ir}{}^{+}}{PS_{Ir}}\right) - E_{1/2}(Co^{II/I}) = -0.059 \log \frac{[85+\alpha][\alpha]}{[15-\alpha][14.5-\alpha]} \qquad (S4)$$

Where the remaining $\mathbf{PS_{Ir}}$ is 15-α (absorption at 527 nm) and α is the concentration of $Co^{I}$ that is formed in solution (see main text). The values obtained for α are consistent with the expected theoretical response for the Nernst equation, see figure 7 in the main text.

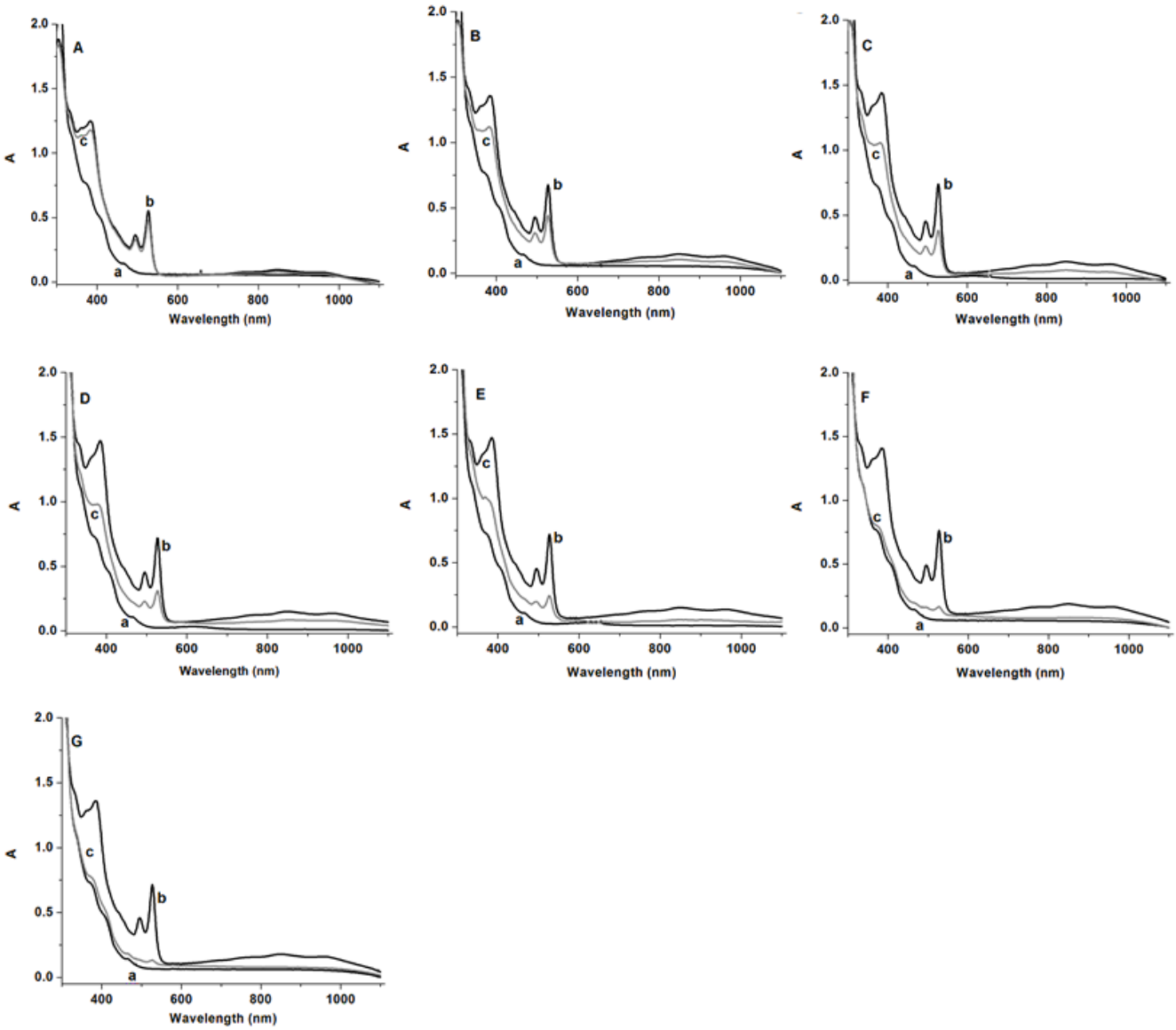



**Figure S27.** Titration studies of $\mathbf{PS_{Ir}^{+}}$ (100 μM) in acetonitrile at -20 °C in the presence of $Et_3N$ (1000 eq.) by the addition of different amounts of $\mathbf{1^{CN}}$: (A) 2.5 μM $\mathbf{1^{CN}}$, (B) 5 μM $\mathbf{1^{CN}}$, (C) 7.5 μM $\mathbf{1^{CN}}$, (D) 10 μM $\mathbf{1^{CN}}$, (E) 12.5 μM $\mathbf{1^{CN}}$, (F) 15 μM $\mathbf{1^{CN}}$, (G) 20 μM $\mathbf{1^{CN}}$. a) Steady state absorption spectra of $\mathbf{PS_{Ir}^{+}}$ in the dark. b) UV-Vis spectrum after generation of the reduced $\mathbf{PS_{Ir}}$ species by irradiating at 447 nm. c) UV-Vis spectrum of the photogenerated $\mathbf{PS_{Ir}}$ species just after the addition of $\mathbf{1^{CN}}$.

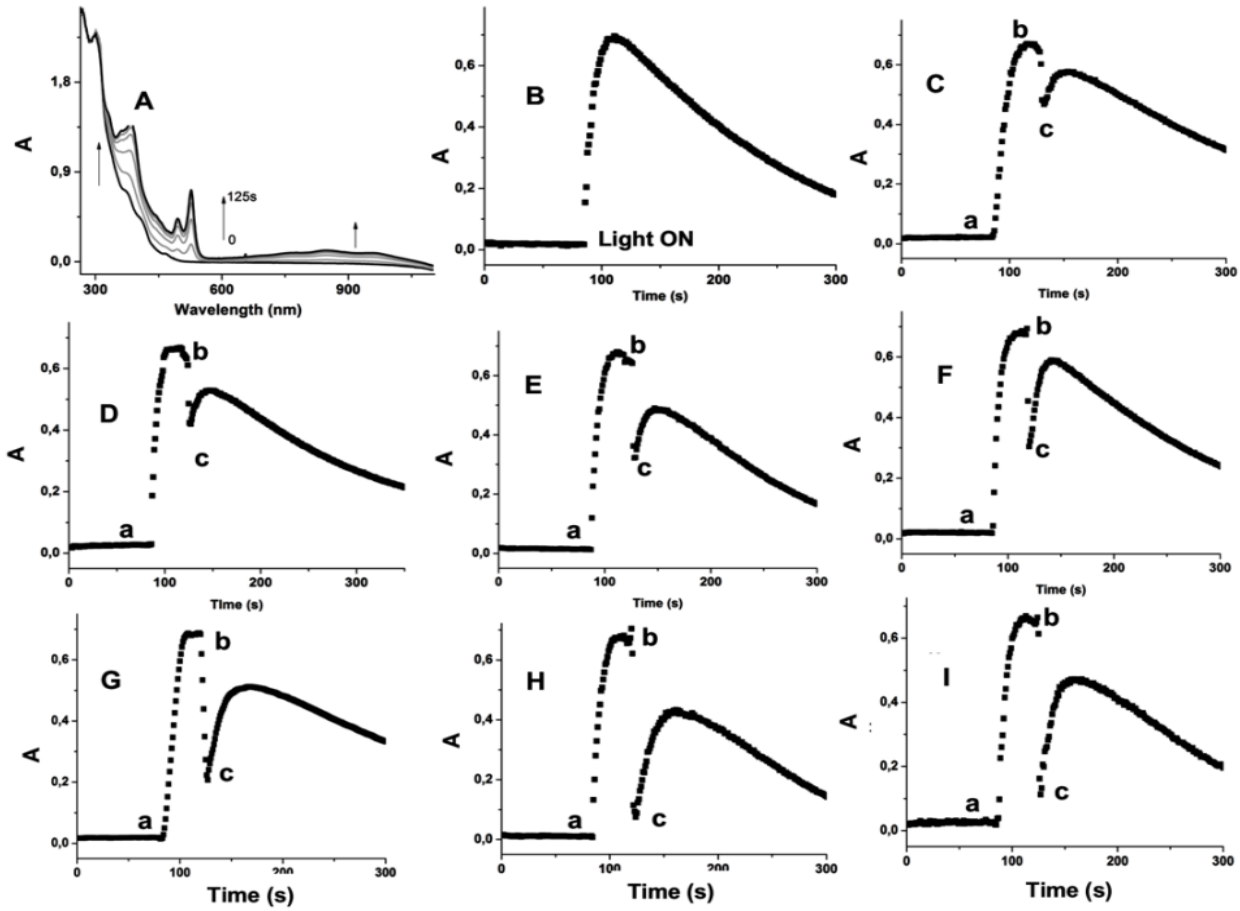



**Figure S28.** The absorption kinetic the reaction of $PS_{Ir}^{+}$ (100 µM) with varying concentration of $\mathbf{1}^{CN}$ and $Et_3N$ (1000 eq.) in neat acetonitrile at -20 °C; A) steady state absorption spectra of $PS_{Ir}$ upon irradiation with 447 nm from 0 to 125 seconds; B) absorbance of $PS_{Ir}$ at 527 nm in the dark and irradiating at 447 nm in the absence of catalyst; C) absorbance of $PS_{Ir}$ at 527 nm in the dark (a) and irradiating at 447 nm in the absence (b) and in the presence of 2.5 µM $\mathbf{1}^{CN}$ (D) 5 µM $\mathbf{1}^{CN}$, (E) 7.5 µM $\mathbf{1}^{CN}$, (F) 10 µM $\mathbf{1}^{CN}$, (G) 12.5 µM $\mathbf{1}^{CN}$, (H) 15 µM $\mathbf{1}^{CN}$, (I) 20 µM $\mathbf{1}^{CN}$.

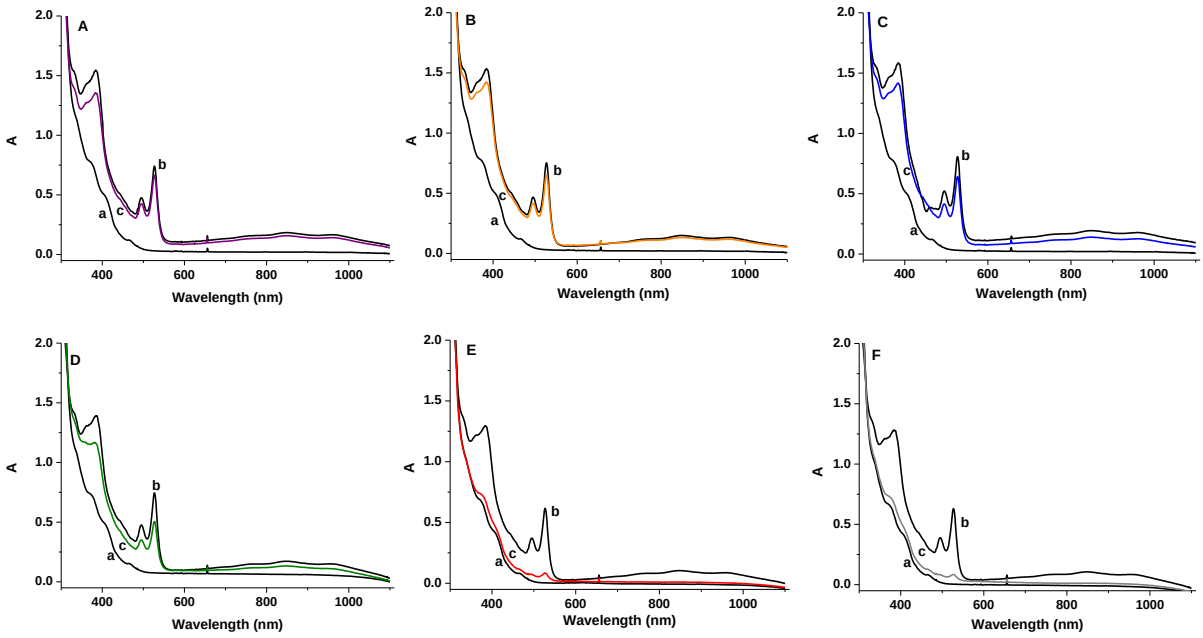



**Figure S29.** Absorption spectra of $\mathbf{PS_{Ir}}$ (100 μM) in the presence of $NEt_3$ (100 mM, 1000 eq.) and 14 μM $\mathbf{1^R}$ catalysts in neat acetonitrile; (A) absorbance of $\mathbf{PS_{Ir}}$ at 527 nm in the dark (**a**) and irradiating at 447 nm in the absence (**b**) and in the presence of catalyst (**c**), $\mathbf{1^{NMe2}}$ (B) $\mathbf{1^{DMM}}$, (C) $\mathbf{1^{H}}$, (D) $\mathbf{1^{Cl}}$, (E) $\mathbf{1^{CO2Et}}$, (F) $\mathbf{1^{CN}}$.

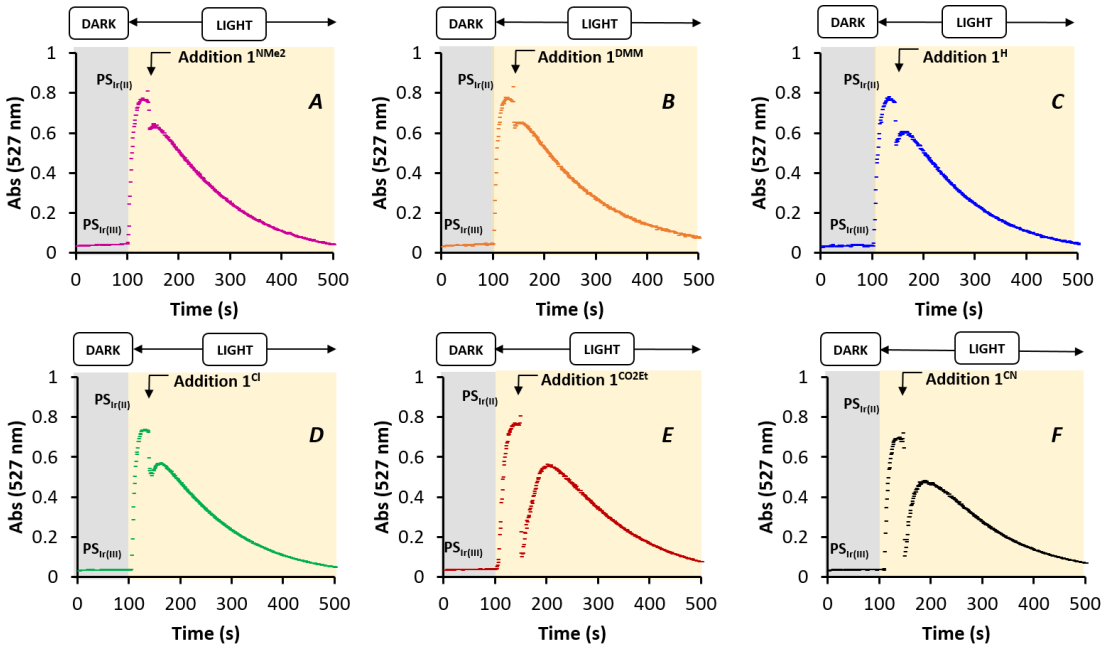



**Figure S30.** Titration studies of $\mathbf{PS_{Ir}^+}$ (100 μM) by the addition of $\mathbf{1^R}$ (15 μM) in the presence of $NEt_3$ (100 mM, 1000 eq.) in acetonitrile at −20 °C and irradiated at 447 nm. UV-Vis traces at 527 nm of the titration with different $\mathbf{1^R}$ (15 μM) ($\mathbf{1^{NMe2}}$ (A), $\mathbf{1^{DMM}}$ (B), $\mathbf{1^{H}}$ (C), $\mathbf{1^{Cl}}$ (D), $\mathbf{1^{CO2Et}}$ (E), $\mathbf{1^{CN}}$ (F)).

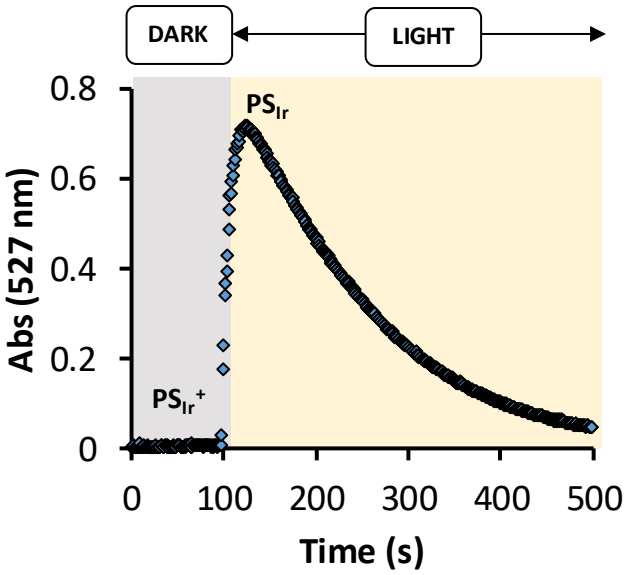



**Figure S31.** Monitoring of the absorbance at 527 nm corresponding of the self-decay of the photogenerated **$PS_{Ir}$** species by irradiating at $\lambda$ = 447 nm. Conditions: [**$PS_{Ir}^{+}$**] = 0.1 mM, [$Et_3N$] = 100 mM, $CH_3CN/H_2O$ (0.8:1.2 mL) at -20 °C.

### 6.2.- Transition absorption spectroscopy (TAS)

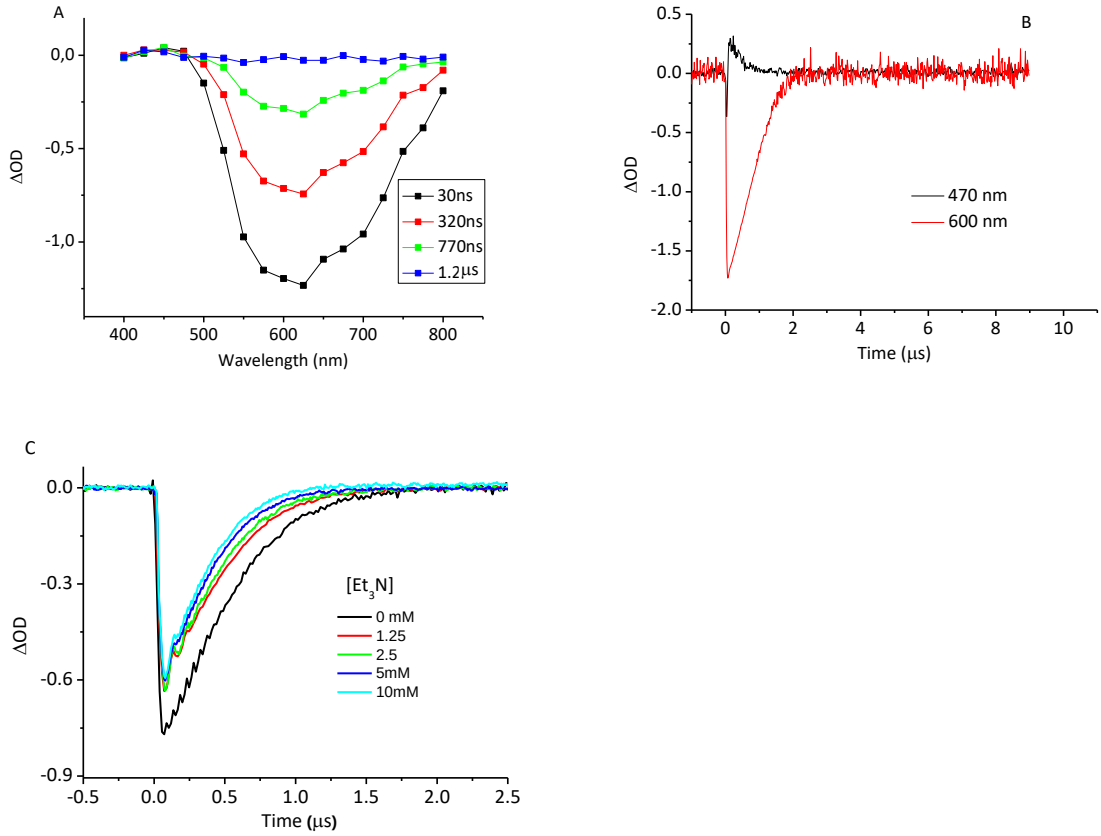



**Figure S32.** (A) Nanosecond transient absorption spectra of $\mathbf{PS_{Ir}}^+$ ($50 \times 10^{-6}$ M) at different times after laser excitation in acetonitrile ($\lambda_{ex}$ = 355 nm), (B) and the respective kinetics at 470 and 600 nm. (C) Kinetic decay profile of $\mathbf{PS_{Ir}}^+$ ($50 \times 10^{-6}$ M) in the presence of different concentrations of $Et_3N$ monitored at 600 nm. Conditions: All measurements were carried out in nitrogen-saturated $CH_3CN$ at room temperature.

**Table S7.** Kinetic fitting parameters of $\mathbf{PS_{Ir}}^+$ obtained by exponential curve fit of each kinetic at 600 nm in presence of varying concentration of $Et_3N$ ([$\mathbf{PS_{Ir}}^+$] = 50 μM in acetonitrile).

| [$Et_3N$] (mM) | **τ (μs)** | **$R^2$** |
|---|---|---|
| 0 | 0.330 | 0.99 |
| 1.25 | 0.307 | 0.90 |
| 2.5 | 0.278 | 0.95 |
| 5 | 0.244 | 0.98 |
| 10 | 0.180 | 0.96 |
| $K_{SV}$= 84 $M^{-1}$ | **$k_q(Et_3N)$ = 2.5X $10^8$ $M^{-1}s^{-1}$** | |

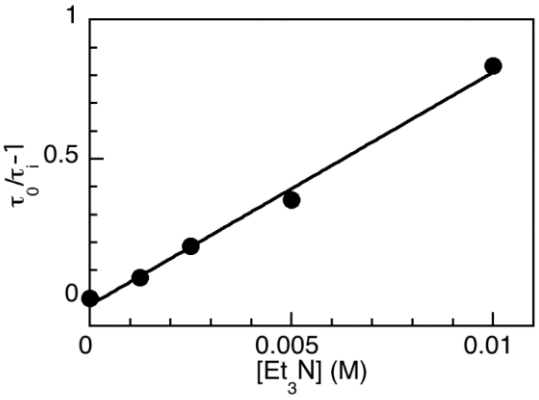



**Figure S33.** Stern-Volmer quenching analysis of $PS_{Ir}^{+}$ (50 x $10^{-6}$ M) in presence of varying concentration of $Et_3N$ obtained by fitting the kinetics at 600 nm.

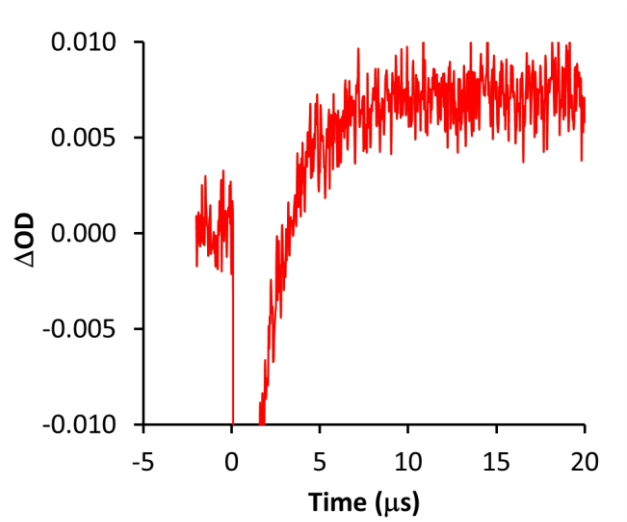
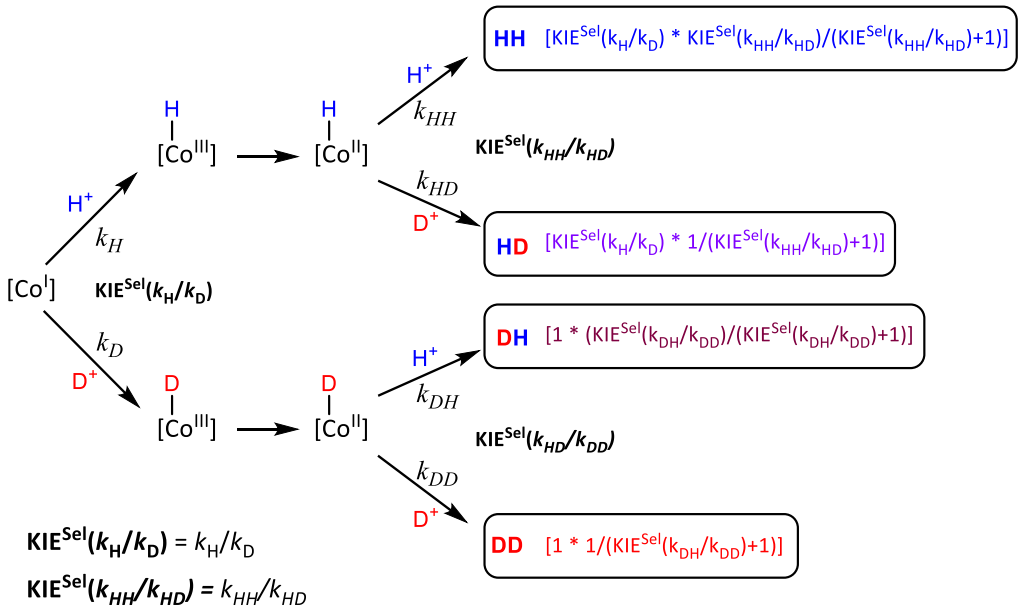



**Figure S34.** Decay profile at 500 nm of a mixture containing **$PS_{Ir}$** (50 μM), $Et_3N$ (20 mM) and **$1^{CO2Et}$** (80 μM) in acetonitrile under $N_2$ at room temperature ($\lambda_{exc}$ = 355 nm, FWHM = 10 ns, E = 8 mJ per pulse).

## 7. Kinetic Isotope Effect (KIE)




**KIE$^{Sel}$($k_H/k_D$)** = $k_H/k_D$

**KIE$^{Sel}$($k_{HH}/k_{HD}$)** = $k_{HH}/k_{HD}$

**KIE$^{Sel}$($k_{HD}/k_{DD}$)** = $k_{HD}/k_{DD}$

**KIE$^{Sel}$($H_2/D_2$)** = [KIE$^{Sel}$($k_H/k_D$) * KIE$^{Sel}$($k_{HH}/k_{HD}$)/(KIE$^{Sel}$($k_{HH}/k_{HD}$)+1)] / [1 * 1/(KIE$^{Sel}$($k_{DH}/k_{DD}$)+1)]

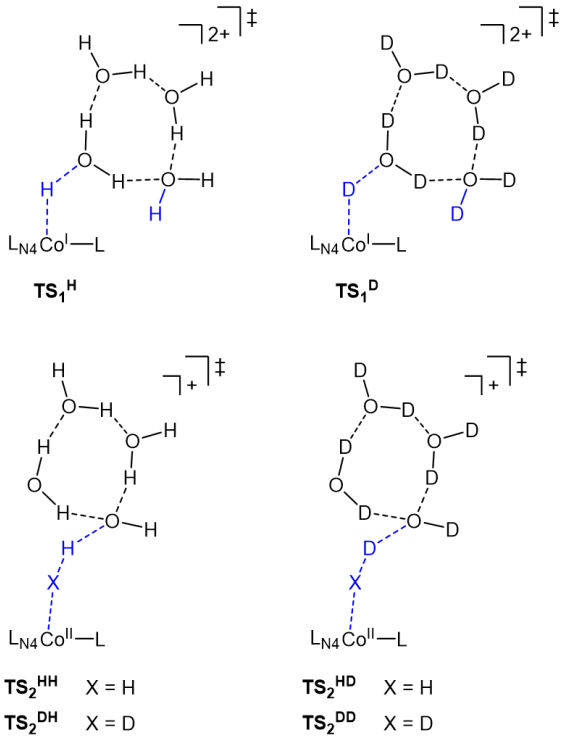
**KIE$^{Sel}$(HD/$D_2$)** = ([KIE$^{Sel}$($k_H/k_D$) * 1/(KIE$^{Sel}$($k_{HH}/k_{HD}$)+1)] + [1 * (KIE$^{Sel}$($k_{DH}/k_{DD}$)/(KIE$^{Sel}$($k_{DH}/k_{DD}$)+1)]) / [1 * 1/(KIE$^{Sel}$($k_{DH}/k_{DD}$)+1)]

**Scheme S3.** Elementary steps where H/D selectivity can take place in the water reduction reaction and the equations used to calculate the **KIE$^{Sel}$** values.

$$KIE\left(\frac{k_H}{k_D}\right) = \frac{e^{\left(\frac{-\Delta G^{\ddagger}\left(TS1^{H}\right)}{RT}\right)}}{e^{\left(\frac{-\Delta G^{\ddagger}\left(TS1^{D}\right)}{RT}\right)}} = e^{\left(\frac{-\Delta\Delta G^{\ddagger}\left(TS_1{}^{H} - TS_1{}^{D}\right)}{RT}\right)}$$

$$KIE\left(\frac{k_{HH}}{k_{HD}}\right) = e^{\left(\frac{-\Delta\Delta G^{\ddagger}\left(TS_2{}^{HH} - TS_2{}^{HD}\right)}{RT}\right)}$$

$$KIE\left(\frac{k_{DH}}{k_{DD}}\right) = e^{\left(\frac{-\Delta\Delta G^{\ddagger}\left(TS_2{}^{DH} - TS_2{}^{DD}\right)}{RT}\right)}$$




| Species | G (Hartree) |
|---|---|
| $TS_1{}^{H}$ | -2588.735803 |
| $TS_1{}^{D}$ | -2588.765127 |
| $[L_{N4}Co^{I}]^{+}$ + [H3O_3H2O]$^{+}$ | -2588.747044 |
| $[L_{N4}Co^{I}]^{+}$ + [D3O_3D2O]$^{+}$ | -2588.777626 |
| $TS_2{}^{HH}$ | -2588.892708 |
| $TS_2{}^{DH}$ | -2588.895138 |
| $TS_2{}^{HD}$ | -2588.91836 |
| $TS_2{}^{DD}$ | -2588.920819 |
| $[L_{N4}Co^{II}\text{-}H\_H_2O\_3H_2O]^{+}$ | -2588.898394 |
| $[L_{N4}Co^{II}\text{-}H\_D_2O\_3D_2O]^{+}$ | -2588.925891 |
| $[L_{N4}Co^{II}\text{-}D\_H_2O\_3H_2O]^{+}$ | -2588.900732 |
| $[L_{N4}Co^{II}\text{-}D\_D_2O\_3D_2O]^{+}$ | -2588.928237 |

***Scheme S4.*** *Top) Equations employed for the calculation of the theoretical KIE and the corresponding energies for the TS. The* $\Delta\Delta G^{\ddagger}$ terms have been calcualted as the energy difference between barriers with default $G_{corr}$ and $G_{corr}$ obtained by replacing the required H by D. In the case of $\Delta\Delta G^{\ddagger}\left(TS_1{}^{H} - TS_1{}^{D}\right)$ and $\Delta\Delta G^{\ddagger}\left(TS_2{}^{HH} - TS_2{}^{HD}\right)$ the $H_2O$ molecules were replaced by $D_2O$ and involves the metal protonation and $H_2$ formation TS. In the case of $\Delta\Delta G^{\ddagger}\left(TS_2{}^{DH} - TS_2{}^{DD}\right)$ the Co-H $H_2O$ molecules are replaced by Co-D and and $D_2O$, respectively. Bottom) Line drawing for the employed TS (Left) and absolute Gibbs energies for the corresponding species.

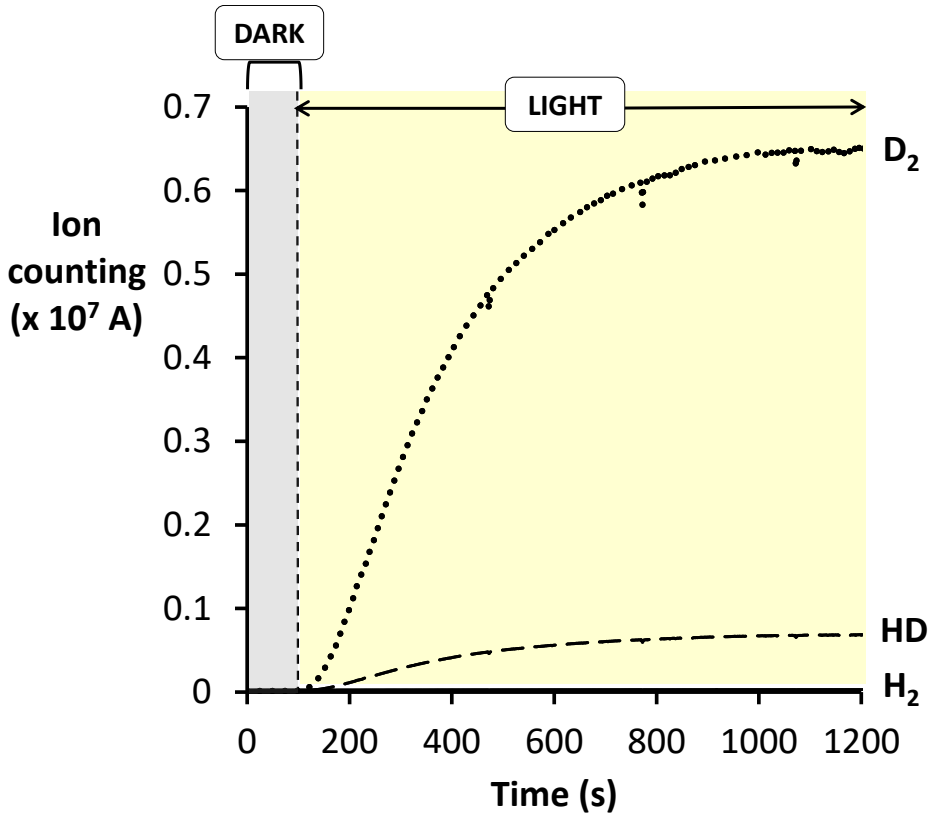



**Figure S35.** On-line monitoring of $H_2$ (Solid trace), HD (dashed trace) and $D_2$ (dotted line) formation *vs.* time using $D_2O$ (99 % in deuterium). The current response was corrected relative to a previous calibration of HD and $D_2$. Conditions: $\mathbf{1}^{CO2Et}$ (50 μM), $\mathbf{PS}_{Ir}$ (150 μM), MeCN:$D_2O$ (0.8:1.2 mL), $Et_3N$ (40 μL), reaction volume = 2 mL, irradiated at λ = 447 nm, under $N_2$ atmosphere.

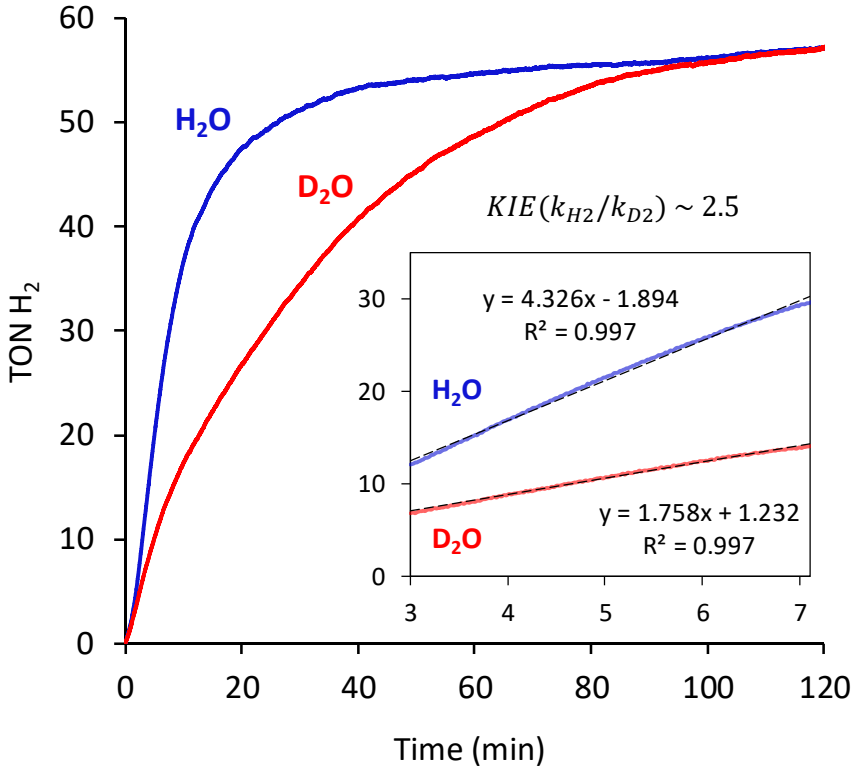



**Figure S36.** On-line hydrogen evolution monitored using $H_2O$ (blue trace), $D_2O$ 99.9% in deuterium (red trace) *vs.* time. Magnification of the linear region employed in the calculation of the initial rates (*k* = slope of the linear correlation) and the subsequent estimation of the KIE($k_{H2}/k_{D2}$). Conditions: **1**$^{H}$ (50 μM), **PS**$_{Ir}$ (150 μM), MeCN:$H_2O$:$Et_3N$ (4:6:0.2 mL) or MeCN:$D_2O$:$Et_3N$ (4:6:0.2 mL), reaction volume = 10.2 mL, irradiated at λ = 447 nm, under $N_2$ atmosphere.

***Calculation of the Quantum yield.***

Calculations for quantum yields have performed following a slightly modified procedure recently reported by Scaiano, J. C., and co. (Pitre, S. P.; McTiernan, C. D.; Vine, W.; DiPucchio, R.; Grenier, M.; Scaiano, J. C. *Scientific Reports* **2015**, *5:16397*).

Two solutions (sample and control) containing a freshly prepared potassium ferrioxalate solution (0.15 M, 3 mL, 0.1 M $H_2SO_4$) were prepared. The Sample solution (3 mL) was irradiated for 10 s in a slot of the parallel photoreactor employing the same vial type used for the hydrogen evolution studies at different powered current intensities (See table). The control solution was left in the dark in a cuvette. After irradiation, 180 µL of the irradiated and control solution was added to independent cuvettes containing 0.02% buffered phenanthroline solution ($H_2O$, 10 mL). After 5 min stirring in the dark, the absorption spectra at 510 nm were measured.

The amount of $Fe^{2+}$ produced during irradiation was obtained by the difference in the absorption spectra between the irradiated sample and dark control cuvettes (ε(510 nm) = 11100 $M^{-1}$ $cm^{-1}$). Quantum yield for $Fe^{2+}$ production is 1.0 and that the potassium ferrioxalate solution absorbs> 99 % of incoming radiation.

Table containing the absorption at 510 nm of the sample irradiated in a slot of the parallel photoreactor with a LED powered by the current intensity conditions employed in hydrogen evolution experiments.

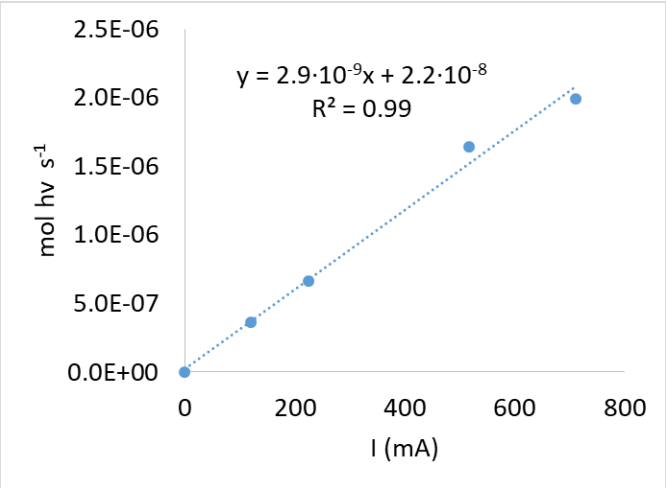
| Repetition | Irradiated sample ($A_{light}$) | Dark sample ($A_{dark}$) | $A_{light}$- $A_{Dark}$ |
|---|---|---|---|
| 1 (714 mA) | 1.40 | 0.1 | 1.30 |
| 2 (713 mA) | 1.49 | 0.1 | 1.39 |
| 3 (711 mA) | 1.43 | 0.1 | 1.33 |
| Average (713) | 1.44±0.05 | 0.1 | 1.34±0.05 |

$$[Fe(II)] = (A_{light}-A_{dark})/(\varepsilon_{510\ nm} * l)$$

$$n(Fe(II)) = [Fe(II)] * V$$

$$\frac{Nh\nu}{t} = \frac{n(Fe(II))}{\Phi t F}\ ;\ \Phi = 1$$

| I(mA, LED) | Irrad. sample ($A_{light}$) | $A_{light}$- $A_{Dark}$ | [$Fe^{2+}$] (x $10^{-6}$ M) | N. photons (x $10^{17}$ hν/s) |
|---|---|---|---|---|
| 0 | 0.10 | 0 | 0 | 0 |
| 120 | 0.34 | 0.24 | 3.6 | 2.2 |
| 226 | 0.55 | 0.45 | 6.7 | 4.0 |
| 517 | 1.19 | 1.09 | 16.4 | 9.9 |
| 713 | 1.44 | 1.34 | 19.9 | 12 |




Hydrogen evolution experiments have been performed at LED current intensity of 700 mA. Therefore under reaction conditions, there are $2.05 \cdot 10^{-3}$ mmol·hν/s; obtained from the regression line. Quantum yields were calculated using the following expression: $\Phi(H_2)$ = n($H_2$)*2 / n(photons)*100.

| Complex | $H_2$ (mmol/s) | Φ (%) |
|---|---|---|
| $\mathbf{1}^{NMe2}$ | 6.9E-06 | 0.7±0.1 |
| $\mathbf{1}^{DMM}$ | 2.0E-05 | 1.9±0.2 |
| $\mathbf{1}^{H}$ | 3.8E-05 | 3.7±0.4 |
| $\mathbf{1}^{Cl}$ | 4.7E-05 | 4.6±0.5 |
| $\mathbf{1}^{CO2Et}$ | 9.9E-05 | 9.7±1.0 |
| $\mathbf{1}^{CN}$ | 9.3E-05 | 9.1±0.9 |

## Quantum-mechanical (DFT) calculations

### *Computational details*

The DFT calculations have been performed with the *Gaussian09* software package using the B3LYP density functional.[10] Geometry optimizations and subsequent frequency calculations have been performed at the B3LYP/6-31+G* level of theory. The effect of the solvent (acetonitrile or water) and London interactions are considered through the SMD model[11] and Grimme-$D_3$ dispersion correction,[12] respectively. The free energy (G) was calculated following equation *S7,* in which $E_{elec}$ is obtained through a single point calculation (over the B3LYP/6-31+G* optimized geometry) using a more flexible basis set and the Gibbs corrections ($\Delta G_{corr}$) were obtained from the previous frequency calculation.

$$G = E_{elec} + \Delta G_{corr} + \Delta G^{o/*} \qquad (S7)$$

$\Delta G^{o/*}$ is the free energy change associated with the conversion from a standard-state gas-phase pressure of 1 atm to a standard-state gas-phase concentration of the desired concentration.

$$\Delta G^{o/*} = RT \ln(24.4 \cdot c) \qquad (S8)$$

R is the universal gas constant (1.987 cal·mol$^{-1}$·K$^{-1}$), T is the temperature in Kelvin and *c* the concentration in mol·L$^{-1}$. Its value at 1 M concentration and 298.15 K is 1.89 kcal·mol$^{-1}$. [13]

In the calculation of the $pK_a$ values, redox and PCET potentials in acetonitrile, the single point calculations have been performed at the B3LYP-$D_3$(SMD)/cc-pVTZ level of theory. In contrast, to construct the the reaction profile in water the basis set has been upgraded to a modified aug-cc-pVTZ (i.e. (aug-cc-pVTZ(-d$^{H}$, -f$^{C,N,O}$, -g$^{Co}$)). The latter basis set has been simplified in order to reduce the computational cost of the calculation but maintaining the diffuse character of the basis set needed for a proper description of anionic intermediates. Thus, the (aug-cc-pVTZ(-d$^{H}$, -f$^{C,N,O}$, -g$^{Co}$) excludes the g basis functions of Co, the f basis functions of C, O and N and the d basis functions of H (aug-cc-pVTZ(-d$^{H}$, -f$^{C,N,O}$, -g$^{Co}$)).

In the cases where spin contamination was more than 10 %, the energy values were corrected using the following expressions:

$$G = E_{elec} + \Delta G_{corr} + \Delta G^{o/*} + E_{spin-corr} \qquad (S9)$$

$$E_{spin-corr} = \frac{E_S - a \cdot E_{(S+1)}}{1 - a} \qquad (S10)$$

$$a = \frac{\langle S_S^2 \rangle - S \cdot (S+1)}{\langle S_{(S+1)}^2 \rangle - S \cdot (S+1)} \qquad (S11)$$

where $E_S$ and $\langle S_S^2 \rangle$ are the UB3LYP/cc-pVTZ electronic energy and square total spin angular momentum of the S spin state obtained by means of an unrestricted calculation. $E_{(S+1)}$ and $\langle S_{(S+1)}^2 \rangle$ are the electronic energy and square total spin angular momentum obtained for the *S+1* spin state computed with the same level of theory and at the geometry of the S spin state. $E_{spin-corr}$ is the spin-corrected electronic energy.[14-15]

The redox potentials (E°) have been evaluated through the Nernst equation in standard state conditions and using the Standard Hydrogen Electrode ($SHE$) as the reference (Eq. *S12*). To compare with the experimental values, the potentials are reported versus the $Fc^{+/0}$ reference.

$$\mathrm{E^o(V)} = -\left(\frac{\Delta \mathrm{G^\circ}}{\mathrm{nF}} - \frac{\Delta \mathrm{G^\circ_{SHE}}}{\mathrm{F}}\right) \qquad (S12)$$

where *n* is the number of electrons involved in the reduction step, *F* is the Faraday constant, $\Delta G^\circ_{SHE}$ = -4.28 eV.

The standard free energy dissociation ($\Delta G^o$) of an acid (HA) to form its conjugate base ($A^-$) in solution may be defined as:

$$\Delta \mathrm{G_s^o} = \mathrm{G(A_s^-)} + \mathrm{G(H_s^+)} - \mathrm{G(AH_s)} \qquad (S13)$$

where $\mathrm{G(AH_s)}$, $\mathrm{G(A_s^-)}$ and $\mathrm{G(H_s^+)}$ are standard free energies of the acid, its conjugate base and the proton in solution, respectively. The solvation energy of a proton ($\Delta \mathrm{G_{solv}^{H+}}$) cannot be computed through an implicit model of the solvent, since the dielectric environment does not describe the strong hydrogen bonding interactions that establish the proton within polar solvents. Therefore, $\mathrm{G(H_s^+)}$ is calculated as follows:

$$\mathrm{G(H_s^+)} = \mathrm{G\left(H_{gas}^+\right)} + \Delta \mathrm{G_{solv}^{H+}} \qquad (S14)$$

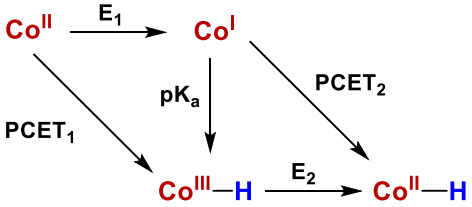
where $\Delta \mathrm{G_{solv}^{H+}}$ is taken from the experimental solvation free energy in a given solvent ($\Delta \mathrm{G_{solv}^{H+}}(in\ acetonitrile) = -260.2\ \mathrm{kcal \cdot mol^{-1}}$), and the gas-phase free energy $\mathrm{G\left(H_{gas}^+\right)}$ is computed from the translational partition function (-6.3 kcal·mol$^{-1}$).

Taking into account the previous equations, the $pK_a$ of an acid HA in solution is computed as:

$$\mathrm{pK_a} = \frac{\Delta \mathrm{G_s^o}}{\mathrm{RT\ ln(10)}} \qquad (S15)$$

For the calculations of the reduction potentials and $pK_a$, the most stable isomers have been taken to calculate the $\Delta G^o$ associated to each process. The change on the solvent concentration has been corrected through the addition of $\Delta G^{o/*}$.

**Table S8.** Theoretical thermodynamic parameters and redox potentials.[§]




| Catalyst | $E_1$ (V) *vs.* $Fc^{+/0}$ | $Co^{III}$-H $pK_a$ | $PCET_1$ (V) *vs.* $Fc^{+/0}$ | $E_2$ (V) *vs.* $Fc^{+/0}$ | $PCET_2$ (V) *vs.* $Fc^{+/0}$ |
|---|---|---|---|---|---|
| $\mathbf{1}^{NMe2}$ | -1.92 (0.0) | 15.4 (0.0) | -1.69 (0.0) | -1.53 (0.0) | -1.27 (0.0) |
| $\mathbf{1}^{DMM}$ | -1.92 (0.0) | 14.7 (-1.0) | -1.73 (0.9) | -1.49 (-0.9) | -1.27 (0.1) |
| $\mathbf{1}^{H}$ | -1.85 (-1.9) | 12.9 (-3.4) | -1.75 (1.4) | -1.46 (-1.6) | -1.35 (1.7) |
| $\mathbf{1}^{Cl}$ | -1.82 (-2.3) | 11.9 (-4.7) | -1.80 (2.6) | -1.42 (-2.6) | -1.36 (2.1) |
| $\mathbf{1}^{COOEt}$ | -1.74 (-3.5) | 11.5 (-5.2) | -1.80 (2.4) | -1.44 (-2.2) | -1.40 (3.1) |
| $\mathbf{1}^{CN}$ | -1.59 (-6.8) | 8.4 (-9.5) | -1.84 (3.4) | -1.36 (-3.9) | -1.51 (5.6) |

[§]The PCET potential values have been adjusted to pH = 11. The corresponding relative free energy change (in kcal/mol) with respect to $\mathbf{1}^{NMe2}$ is shown in parenthesis. Reduction redox potentials versus $Fc^{+/0}$.

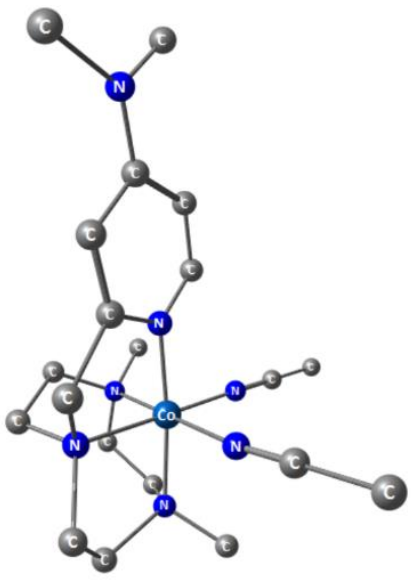
***Cartesian coordinates of optimized geometries in acetonitrile***

For the calculation of the thermodynamic parameters (reduction potentials, PCET and $pK_a$), the geometries were optimized at the UB3LYP-$D_3$/6-31+G* level of theory for different spin states and different coordination isomers were evaluated. In parenthesis, the ground spin states, the number of coordinating acetonitrile molecules (n AC where n = 1, 2) and the associated free energy values ($G = E_{elec} + \Delta G_{corr}$, in Hartrees) are indicated. Irrelevant hydrogen atoms are omitted for clarity in the inserted figures.

The ground spin state of the different species involved in the catalytic cycle has been determined optimizing all the different intermediates in the S = 0 and S = 1 spin states for formal $Co^{I}$ and $Co^{III}$-H species and S = 1/2 and S = 3/2 spin states for formal $Co^{II}$ and $Co^{II}$-H. The open shell singlet states have been considered by using the unrestricted formalism for the B3LYP hybrid functional.

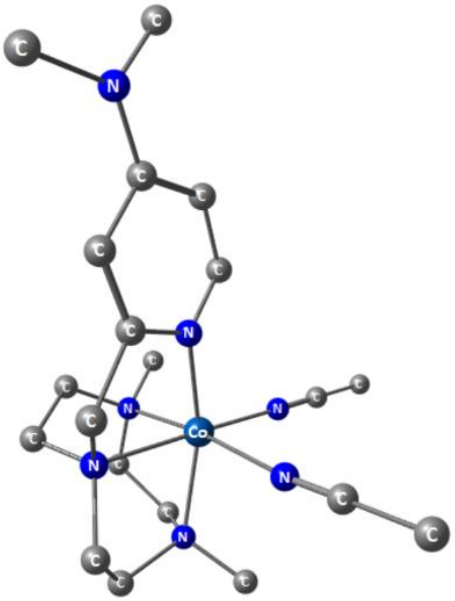
**$1^{NMe2}$-$Co^{III}$ (singlet, 2 AC, G = -2549.04890249)**

| | | | |
|---|---|---|---|
| 27 | 0.983191000 | 0.026577000 | 0.004550000 |
| 7 | 0.604980000 | -1.774046000 | 0.646524000 |
| 7 | -0.954823000 | 0.159297000 | -0.159564000 |
| 7 | 1.223604000 | -0.764254000 | -1.809964000 |
| 7 | 2.924128000 | -0.344410000 | 0.322689000 |
| 6 | -0.730021000 | -1.719355000 | 1.321151000 |
| 1 | -0.590710000 | -1.314320000 | 2.325673000 |
| 1 | -1.144690000 | -2.725269000 | 1.417949000 |
| 6 | -1.621041000 | -0.803632000 | 0.532572000 |
| 6 | -2.993994000 | -0.889392000 | 0.554926000 |
| 1 | -3.452062000 | -1.694848000 | 1.114082000 |
| 6 | -3.778179000 | 0.072628000 | -0.144286000 |
| 6 | -3.055996000 | 1.095505000 | -0.824861000 |
| 1 | -3.563009000 | 1.884005000 | -1.364609000 |
| 6 | -1.680356000 | 1.098735000 | -0.804281000 |
| 1 | -1.127955000 | 1.873411000 | -1.320353000 |
| 6 | 1.713805000 | -2.106923000 | 1.596841000 |
| 1 | 1.689841000 | -3.174983000 | 1.835383000 |
| 1 | 1.544465000 | -1.540584000 | 2.512176000 |
| 6 | 3.035356000 | -1.715146000 | 0.959855000 |
| 1 | 3.821509000 | -1.693753000 | 1.717510000 |
| 1 | 3.343954000 | -2.429045000 | 0.198034000 |
| 6 | 3.536897000 | -0.327162000 | -1.041126000 |
| 1 | 4.554317000 | -0.730077000 | -0.993567000 |
| 1 | 3.590304000 | 0.715127000 | -1.358611000 |
| 6 | 2.679535000 | -1.138845000 | -1.985480000 |
| 1 | 2.971939000 | -0.951448000 | -3.020701000 |
| 1 | 2.789276000 | -2.207574000 | -1.808473000 |
| 6 | 0.358340000 | -1.984700000 | -1.815348000 |
| 1 | 0.617195000 | -2.610855000 | -2.675551000 |
| 1 | -0.673215000 | -1.653173000 | -1.928460000 |
| 6 | 0.562841000 | -2.739594000 | -0.518584000 |
| 1 | -0.246791000 | -3.454143000 | -0.362336000 |
| 1 | 1.493458000 | -3.302756000 | -0.525447000 |
| 6 | 3.628761000 | 0.650130000 | 1.179210000 |
| 1 | 4.700362000 | 0.425076000 | 1.161414000 |
| 1 | 3.263472000 | 0.576275000 | 2.202043000 |
| 1 | 3.460879000 | 1.655342000 | 0.794554000 |
| 6 | 0.818024000 | 0.110400000 | -2.946185000 |
| 1 | 0.877113000 | -0.478550000 | -3.867405000 |
| 1 | 1.495301000 | 0.959601000 | -3.017593000 |
| 1 | -0.204923000 | 0.453827000 | -2.807589000 |
| 7 | 1.319542000 | 1.806069000 | -0.614284000 |
| 7 | 0.757727000 | 0.790432000 | 1.756561000 |
| 6 | 1.502649000 | 2.904667000 | -0.909893000 |
| 6 | 0.558430000 | 1.346599000 | 2.745708000 |
| 6 | 1.738665000 | 4.279174000 | -1.296709000 |
| 1 | 2.308998000 | 4.300176000 | -2.231061000 |
| 1 | 0.778955000 | 4.785932000 | -1.441590000 |
| 1 | 2.305419000 | 4.785863000 | -0.508865000 |
| 6 | 0.319884000 | 2.028380000 | 3.999791000 |
| 1 | 1.277527000 | 2.238619000 | 4.487336000 |
| 1 | -0.208932000 | 2.967857000 | 3.808514000 |
| 1 | -0.289908000 | 1.390722000 | 4.648223000 |
| 7 | -5.125921000 | 0.018365000 | -0.158157000 |
| 6 | -5.830097000 | -1.014668000 | 0.600315000 |
| 1 | -6.902756000 | -0.879305000 | 0.466771000 |
| 1 | -5.558113000 | -2.016326000 | 0.247164000 |
| 1 | -5.600005000 | -0.944663000 | 1.670403000 |
| 6 | -5.896735000 | 1.020669000 | -0.892734000 |
| 1 | -5.599841000 | 1.045713000 | -1.947304000 |
| 1 | -6.953152000 | 0.760358000 | -0.838683000 |
| 1 | -5.759634000 | 2.021212000 | -0.463800000 |



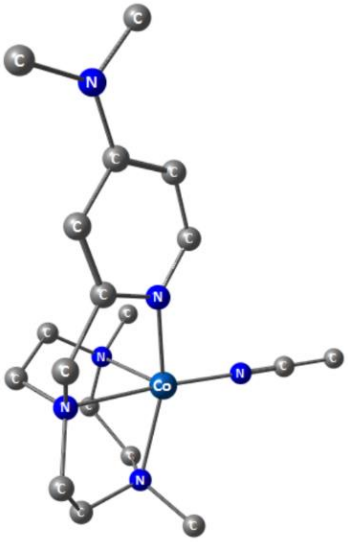
**$1^{NMe2}$-$Co^{II}$ (quartet, 2 AC, G = -2549.225026)**

| | | | |
|---|---|---|---|
| 27 | 0.999298000 | 0.128174000 | -0.060886000 |
| 7 | 0.388663000 | -1.702735000 | 0.944465000 |
| 7 | -1.092458000 | 0.360597000 | -0.050092000 |
| 7 | 1.159916000 | -1.212872000 | -1.756477000 |
| 7 | 3.000822000 | -0.649884000 | 0.393432000 |
| 6 | -0.890547000 | -1.384541000 | 1.611117000 |
| 1 | -0.665525000 | -0.803317000 | 2.511144000 |
| 1 | -1.418916000 | -2.293168000 | 1.924554000 |
| 6 | -1.760182000 | -0.540298000 | 0.707670000 |
| 6 | -3.136672000 | -0.659030000 | 0.696191000 |
| 1 | -3.598924000 | -1.415279000 | 1.318073000 |
| 6 | -3.918382000 | 0.201470000 | -0.124371000 |
| 6 | -3.198350000 | 1.149566000 | -0.903806000 |
| 1 | -3.704087000 | 1.842949000 | -1.563318000 |
| 6 | -1.819583000 | 1.182614000 | -0.831235000 |
| 1 | -1.257340000 | 1.894127000 | -1.429215000 |
| 6 | 1.486436000 | -1.963979000 | 1.905628000 |
| 1 | 1.372500000 | -2.946824000 | 2.384761000 |
| 1 | 1.422265000 | -1.200109000 | 2.683636000 |
| 6 | 2.852785000 | -1.886014000 | 1.222460000 |
| 1 | 3.630394000 | -1.909500000 | 1.993238000 |
| 1 | 3.017067000 | -2.761168000 | 0.593397000 |
| 6 | 3.519309000 | -0.946689000 | -0.967454000 |
| 1 | 4.483742000 | -1.472199000 | -0.906459000 |
| 1 | 3.692589000 | 0.014485000 | -1.459910000 |
| 6 | 2.539485000 | -1.783016000 | -1.786761000 |
| 1 | 2.898006000 | -1.836037000 | -2.820530000 |
| 1 | 2.506835000 | -2.808847000 | -1.418230000 |
| 6 | 0.132344000 | -2.248291000 | -1.491689000 |
| 1 | 0.226754000 | -3.080055000 | -2.204745000 |
| 1 | -0.840273000 | -1.779328000 | -1.652772000 |
| 6 | 0.230075000 | -2.789510000 | -0.064773000 |
| 1 | -0.670511000 | -3.373297000 | 0.154854000 |
| 1 | 1.073249000 | -3.475659000 | 0.025274000 |
| 6 | 3.886137000 | 0.320023000 | 1.065411000 |
| 1 | 4.913286000 | -0.067220000 | 1.129770000 |
| 1 | 3.514091000 | 0.510762000 | 2.073330000 |
| 1 | 3.892474000 | 1.258974000 | 0.506832000 |
| 6 | 0.858916000 | -0.513578000 | -3.021759000 |
| 1 | 0.802295000 | -1.225715000 | -3.857381000 |
| 1 | 1.644125000 | 0.215819000 | -3.229083000 |
| 1 | -0.095985000 | 0.010256000 | -2.931329000 |
| 7 | 1.644421000 | 1.865019000 | -1.033344000 |
| 7 | 0.990963000 | 1.323897000 | 1.767376000 |
| 6 | 1.959908000 | 2.858679000 | -1.533330000 |
| 6 | 0.872556000 | 1.993833000 | 2.703003000 |
| 6 | 2.359146000 | 4.104629000 | -2.160943000 |
| 1 | 2.888875000 | 3.893692000 | -3.095518000 |
| 1 | 1.470414000 | 4.707366000 | -2.374643000 |
| 1 | 3.019058000 | 4.659424000 | -1.486059000 |
| 6 | 0.726681000 | 2.822446000 | 3.886777000 |
| 1 | 1.713423000 | 3.141206000 | 4.237808000 |
| 1 | 0.125185000 | 3.705391000 | 3.647936000 |
| 1 | 0.229266000 | 2.249198000 | 4.675883000 |
| 7 | -5.270797000 | 0.116380000 | -0.163971000 |
| 6 | -5.965545000 | -0.908999000 | 0.609234000 |
| 1 | -7.037957000 | -0.811095000 | 0.441758000 |
| 1 | -5.656465000 | -1.916959000 | 0.303863000 |
| 1 | -5.770960000 | -0.795271000 | 1.682684000 |
| 6 | -6.037017000 | 0.996078000 | -1.041861000 |
| 1 | -5.790246000 | 0.822128000 | -2.097410000 |
| 1 | -7.099097000 | 0.799315000 | -0.897553000 |
| 1 | -5.846363000 | 2.050096000 | -0.8075010 |



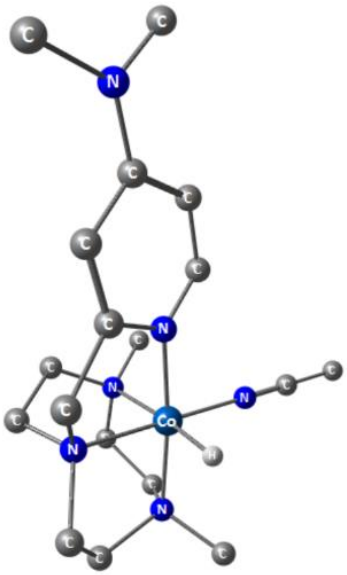
**$1^{NMe2}$-$Co^{I}$ (triplet, 1 AC, G = -2416.53622568)**

| | | | |
|---|---|---|---|
| 27 | -1.088577000 | 0.277778000 | -0.399716000 |
| 7 | -0.494808000 | -1.848985000 | -0.470453000 |
| 7 | 1.030727000 | 0.446742000 | -0.467389000 |
| 7 | -1.340253000 | -0.191035000 | 1.737783000 |
| 7 | -3.115142000 | -0.673069000 | -0.511175000 |
| 6 | 0.798949000 | -1.858333000 | -1.168120000 |
| 1 | 0.601302000 | -1.714914000 | -2.236743000 |
| 1 | 1.322247000 | -2.819286000 | -1.053714000 |
| 6 | 1.677668000 | -0.720028000 | -0.693224000 |
| 6 | 3.045261000 | -0.876683000 | -0.538855000 |
| 1 | 3.482559000 | -1.848936000 | -0.730857000 |
| 6 | 3.846597000 | 0.224225000 | -0.133805000 |
| 6 | 3.158310000 | 1.447435000 | 0.085379000 |
| 1 | 3.681476000 | 2.344855000 | 0.391410000 |
| 6 | 1.785292000 | 1.496291000 | -0.089650000 |
| 1 | 1.249335000 | 2.426564000 | 0.082366000 |
| 6 | -1.569981000 | -2.495349000 | -1.245658000 |
| 1 | -1.462668000 | -3.592842000 | -1.264175000 |
| 1 | -1.483360000 | -2.133183000 | -2.274501000 |
| 6 | -2.955444000 | -2.136102000 | -0.700041000 |
| 1 | -3.713394000 | -2.518457000 | -1.396155000 |
| 1 | -3.130905000 | -2.646549000 | 0.248793000 |
| 6 | -3.665563000 | -0.317795000 | 0.811235000 |
| 1 | -4.644801000 | -0.798656000 | 0.983254000 |
| 1 | -3.824190000 | 0.764840000 | 0.807694000 |
| 6 | -2.722779000 | -0.692957000 | 1.956234000 |
| 1 | -3.131046000 | -0.287781000 | 2.891278000 |
| 1 | -2.694873000 | -1.777076000 | 2.082613000 |
| 6 | -0.318206000 | -1.231545000 | 1.964471000 |
| 1 | -0.415821000 | -1.677843000 | 2.968992000 |
| 1 | 0.655000000 | -0.737376000 | 1.915988000 |
| 6 | -0.385076000 | -2.354650000 | 0.920974000 |
| 1 | 0.509660000 | -2.981786000 | 1.027807000 |
| 1 | -1.240148000 | -3.001395000 | 1.125609000 |
| 6 | -3.922211000 | -0.090147000 | -1.588252000 |
| 1 | -4.954728000 | -0.480055000 | -1.586568000 |
| 1 | -3.462273000 | -0.323924000 | -2.553311000 |
| 1 | -3.955329000 | 0.996518000 | -1.474684000 |
| 6 | -1.073248000 | 0.985608000 | 2.573443000 |
| 1 | -1.093040000 | 0.738130000 | 3.648745000 |
| 1 | -1.830078000 | 1.749313000 | 2.375924000 |
| 1 | -0.091478000 | 1.396885000 | 2.323152000 |
| 7 | -1.607607000 | 2.112033000 | -0.525704000 |
| 6 | -1.924374000 | 3.233557000 | -0.603791000 |
| 6 | -2.321386000 | 4.632401000 | -0. 684330000 |
| 1 | -2.452191000 | 5.044971000 | 0.322686000 |
| 1 | -1.554994000 | 5.217767000 | -1.204906000 |
| 1 | -3.267593000 | 4.730168000 | -1.228564000 |
| 7 | 5.192837000 | 0.110129000 | 0.041178000 |
| 6 | 5.868323000 | -1.141532000 | -0.280806000 |
| 1 | 6.927591000 | -1.043291000 | -0.042278000 |
| 1 | 5.460539000 | -1.972120000 | 0.307558000 |
| 1 | 5.772805000 | -1.392193000 | -1.346697000 |
| 6 | 5.987754000 | 1.289363000 | 0.364126000 |
| 1 | 7.029934000 | 0.991698000 | 0.482138000 |
| 1 | 5.929587000 | 2.047420000 | -0.429552000 |
| 1 | 5.652869000 | 1.745268000 | 1.303369000 |



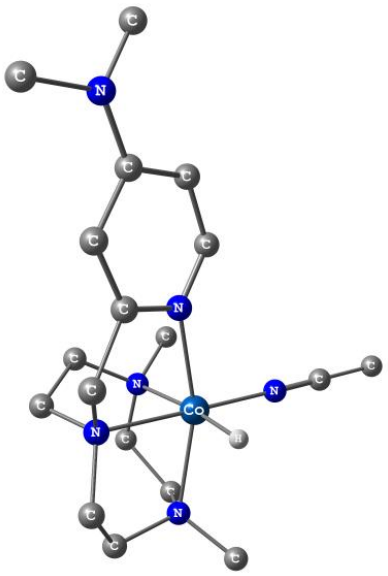
**$1^{NMe2}$-$Co^{III}$-H (singlet, 1 AC, G = -2416.99074165)**

| | | | |
|---|---|---|---|
| 27 | -1.033340000 | 0.065622000 | -0.402948000 |
| 7 | -0.647207000 | -1.838950000 | -0.345120000 |
| 7 | 0.898473000 | 0.264750000 | -0.330207000 |
| 7 | -1.292672000 | -0.025943000 | 1.676238000 |
| 7 | -2.962899000 | -0.412711000 | -0.541630000 |
| 6 | 0.678307000 | -2.018275000 | -1.006448000 |
| 1 | 0.518542000 | -1.958488000 | -2.086947000 |
| 1 | 1.103899000 | -2.997815000 | -0.772322000 |
| 6 | 1.570470000 | -0.888332000 | -0.583270000 |
| 6 | 2.941930000 | -0.995024000 | -0.497316000 |
| 1 | 3.399798000 | -1.955029000 | -0.698574000 |
| 6 | 3.721729000 | 0.144743000 | -0.154266000 |
| 6 | 2.999643000 | 1.348151000 | 0.082467000 |
| 1 | 3.504944000 | 2.268251000 | 0.344937000 |
| 6 | 1.623974000 | 1.356810000 | -0.011840000 |
| 1 | 1.069318000 | 2.267663000 | 0.176708000 |
| 6 | -1.748327000 | -2.497228000 | -1.111417000 |
| 1 | -1.719037000 | -3.583454000 | -0.968274000 |
| 1 | -1.587292000 | -2.272130000 | -2.166029000 |
| 6 | -3.069236000 | -1.917019000 | -0.639306000 |
| 1 | -3.871050000 | -2.183256000 | -1.332480000 |
| 1 | -3.344884000 | -2.315499000 | 0.336034000 |
| 6 | -3.578585000 | 0.092757000 | 0.723851000 |
| 1 | -4.604386000 | -0.284512000 | 0.817720000 |
| 1 | -3.618601000 | 1.180963000 | 0.645113000 |
| 6 | -2.741785000 | -0.322258000 | 1.922723000 |
| 1 | -3.085528000 | 0.213826000 | 2.812394000 |
| 1 | -2.857717000 | -1.385561000 | 2.133444000 |
| 6 | -0.419580000 | -1.165326000 | 2.060446000 |
| 1 | -0.643236000 | -1.500361000 | 3.081943000 |
| 1 | 0.609839000 | -0.804677000 | 2.041468000 |
| 6 | -0.606342000 | -2.322053000 | 1.087976000 |
| 1 | 0.205090000 | -3.044973000 | 1.202262000 |
| 1 | -1.537135000 | -2.850227000 | 1.290835000 |
| 6 | -3.657000000 | 0.195332000 | -1.707256000 |
| 1 | -4.726502000 | -0.042723000 | -1.661074000 |
| 1 | -3.232452000 | -0.209653000 | -2.626439000 |
| 1 | -3.525315000 | 1.276860000 | -1.692576000 |
| 6 | -0.895232000 | 1.185924000 | 2.423614000 |
| 1 | -0.974211000 | 1.007109000 | 3.504071000 |
| 1 | -1.551459000 | 2.013758000 | 2.150058000 |
| 1 | 0.135347000 | 1.447055000 | 2.180464000 |
| 7 | -1.359178000 | 1.924983000 | -0.538744000 |
| 6 | -1.538654000 | 3.060514000 | -0.636480000 |
| 6 | -1.771664000 | 4.487393000 | -0.747257000 |
| 1 | -1.886051000 | 4.917885000 | 0.252967000 |
| 1 | -0.923385000 | 4.960402000 | -1.252276000 |
| 1 | -2.683655000 | 4.664901000 | -1.326528000 |
| 1 | -0.907170000 | 0.025150000 | -1.857497000 |
| 7 | 5.069805000 | 0.085152000 | -0.054338000 |
| 6 | 5.833782000 | 1.280128000 | 0.296090000 |
| 1 | 5.536851000 | 1.664946000 | 1.279356000 |
| 1 | 6.892384000 | 1.024178000 | 0.330717000 |
| 1 | 5.692526000 | 2.073454000 | -0.448314000 |
| 6 | 5.770535000 | -1.172605000 | -0.300345000 |
| 1 | 6.839218000 | -1.014222000 | -0.158780000 |
| 1 | 5.439697000 | -1.951801000 | 0.397339000 |
| 1 | 5.603752000 | -1.526556000 | -1.325307000 |



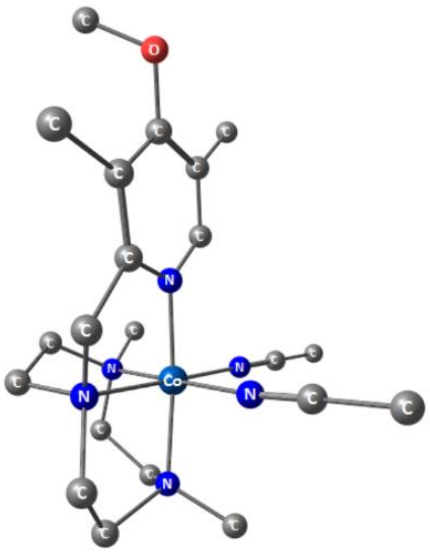
**$1^{NMe2}$-$Co^{II}$-H (doublet, 1 AC, G = -2417.11512138)**

| | | | |
|---|---|---|---|
| 27 | -1.111304000 | 0.172086000 | -0.454551000 |
| 7 | -0.504014000 | -1.808004000 | -0.316202000 |
| 7 | 1.067333000 | 0.423889000 | -0.364922000 |
| 7 | -1.337260000 | 0.047259000 | 1.614900000 |
| 7 | -3.152946000 | -0.754260000 | -0.473678000 |
| 6 | 0.797081000 | -1.892495000 | -1.012825000 |
| 1 | 0.599971000 | -1.818666000 | -2.086987000 |
| 1 | 1.289570000 | -2.855572000 | -0.822835000 |
| 6 | 1.697482000 | -0.744709000 | -0.606394000 |
| 6 | 3.072268000 | -0.900158000 | -0.522049000 |
| 1 | 3.499008000 | -1.878848000 | -0.704446000 |
| 6 | 3.892424000 | 0.213544000 | -0.197453000 |
| 6 | 3.214019000 | 1.436618000 | 0.053432000 |
| 1 | 3.750354000 | 2.336977000 | 0.325448000 |
| 6 | 1.833070000 | 1.479472000 | -0.043338000 |
| 1 | 1.303647000 | 2.409053000 | 0.152806000 |
| 6 | -1.556254000 | -2.604339000 | -0.992634000 |
| 1 | -1.392956000 | -3.682162000 | -0.845100000 |
| 1 | -1.483324000 | -2.388883000 | -2.060616000 |
| 6 | -2.950967000 | -2.224154000 | -0.482832000 |
| 1 | -3.698971000 | -2.709709000 | -1.122076000 |
| 1 | -3.109597000 | -2.617933000 | 0.522635000 |
| 6 | -3.697589000 | -0.241235000 | 0.796127000 |
| 1 | -4.655746000 | -0.723617000 | 1.054227000 |
| 1 | -3.891705000 | 0.825660000 | 0.651553000 |
| 6 | -2.718672000 | -0.438455000 | 1.947357000 |
| 1 | -3.091486000 | 0.090152000 | 2.831464000 |
| 1 | -2.661872000 | -1.493109000 | 2.220529000 |
| 6 | -0.315012000 | -0.952532000 | 2.026164000 |
| 1 | -0.468701000 | -1.251187000 | 3.073539000 |
| 1 | 0.657346000 | -0.464861000 | 1.955295000 |
| 6 | -0.362552000 | -2.183301000 | 1.126153000 |
| 1 | 0.546449000 | -2.776674000 | 1.274212000 |
| 1 | -1.200953000 | -2.824116000 | 1.400589000 |
| 6 | -3.974895000 | -0.324662000 | -1.609578000 |
| 1 | -5.008558000 | -0.700602000 | -1.529002000 |
| 1 | -3.536679000 | -0.699742000 | -2.537872000 |
| 1 | -3.997477000 | 0.767754000 | -1.654306000 |
| 6 | -1.076392000 | 1.322037000 | 2.315649000 |
| 1 | -1.068242000 | 1.170763000 | 3.404638000 |
| 1 | -1.857015000 | 2.041255000 | 2.063340000 |
| 1 | -0.110454000 | 1.720650000 | 2.000787000 |
| 7 | -1.643023000 | 2.006562000 | -0.593360000 |
| 6 | -1.944190000 | 3.121863000 | -0.685150000 |
| 6 | -2.320934000 | 4.521934000 | -0.796839000 |
| 1 | -2.456033000 | 4.951253000 | 0.201564000 |
| 1 | -1.537258000 | 5.078405000 | -1.321726000 |
| 1 | -3.258421000 | 4.613272000 | -1.355425000 |
| 1 | -1.007821000 | 0.124152000 | -1.987136000 |
| 7 | 5.249655000 | 0.113490000 | -0.126037000 |
| 6 | 6.036862000 | 1.243787000 | 0.355033000 |
| 1 | 5.786029000 | 1.501747000 | 1.393863000 |
| 1 | 7.094461000 | 0.982811000 | 0.308130000 |
| 1 | 5.875211000 | 2.128809000 | -0.270660000 |
| 6 | 5.894283000 | -1.187974000 | -0.261722000 |
| 1 | 6.975623000 | -1.049043000 | -0.243239000 |
| 1 | 5.614088000 | -1.869359000 | 0.554554000 |
| 1 | 5.628290000 | -1.658937000 | -1.214389000 |



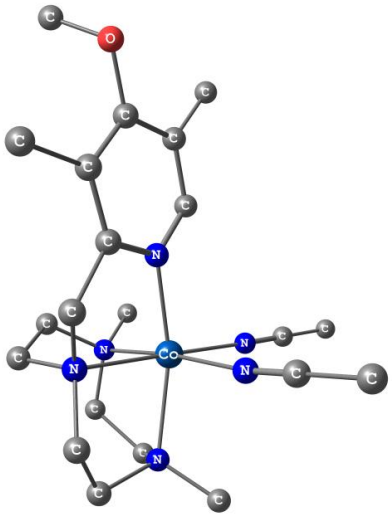
**$1^{DMM}$-$Co^{III}$ (singlet, 2 AC, G = -2608.23672420)**

| | | | |
|---|---|---|---|
| 27 | 1.030930000 | 0.012118000 | -0.006373000 |
| 7 | 0.631225000 | -1.887704000 | 0.083695000 |
| 7 | -0.918918000 | 0.215296000 | -0.033510000 |
| 7 | 1.187008000 | -0.194979000 | -1.980812000 |
| 7 | 2.968787000 | -0.467455000 | 0.109440000 |
| 6 | -0.678209000 | -2.028732000 | 0.792833000 |
| 1 | -0.499513000 | -1.984464000 | 1.870348000 |
| 1 | -1.111171000 | -3.004649000 | 0.567977000 |
| 6 | -1.570952000 | -0.893289000 | 0.384538000 |
| 6 | -2.961553000 | -0.943571000 | 0.487487000 |
| 6 | -3.669105000 | 0.213022000 | 0.116717000 |
| 6 | -2.995359000 | 1.380554000 | -0.282701000 |
| 6 | -1.608460000 | 1.329137000 | -0.333445000 |
| 1 | -1.037196000 | 2.199421000 | -0.628570000 |
| 6 | 1.760748000 | -2.506135000 | 0.850178000 |
| 1 | 1.710347000 | -3.596390000 | 0.766758000 |
| 1 | 1.641688000 | -2.227605000 | 1.896659000 |
| 6 | 3.064875000 | -1.969777000 | 0.292283000 |
| 1 | 3.887583000 | -2.193707000 | 0.974119000 |
| 1 | 3.305813000 | -2.427100000 | -0.665502000 |
| 6 | 3.536883000 | -0.038134000 | -1.204509000 |
| 1 | 4.544585000 | -0.450872000 | -1.323305000 |
| 1 | 3.607772000 | 1.050201000 | -1.187418000 |
| 6 | 2.629999000 | -0.507280000 | -2.318704000 |
| 1 | 2.889700000 | -0.007369000 | -3.253695000 |
| 1 | 2.725803000 | -1.577670000 | -2.489627000 |
| 6 | 0.297905000 | -1.351211000 | -2.316782000 |
| 1 | 0.513971000 | -1.692758000 | -3.334226000 |
| 1 | -0.730817000 | -0.994098000 | -2.285829000 |
| 6 | 0.532972000 | -2.461506000 | -1.315324000 |
| 1 | -0.282818000 | -3.185438000 | -1.347416000 |
| 1 | 1.453053000 | -3.001912000 | -1.527662000 |
| 6 | 3.722168000 | 0.203332000 | 1.206340000 |
| 1 | 4.787784000 | -0.013073000 | 1.076159000 |
| 1 | 3.392279000 | -0.185378000 | 2.168136000 |
| 1 | 3.559959000 | 1.279530000 | 1.163242000 |
| 6 | 0.756933000 | 0.982384000 | -2.787106000 |
| 1 | 0.780205000 | 0.697838000 | -3.844042000 |
| 1 | 1.441927000 | 1.812031000 | -2.622380000 |
| 1 | -0.257369000 | 1.269919000 | -2.518551000 |
| 7 | 1.392591000 | 1.892823000 | -0.075095000 |
| 7 | 0.882692000 | 0.219105000 | 1.901089000 |
| 6 | 1.592599000 | 3.026737000 | -0.027338000 |
| 6 | 0.741559000 | 0.456378000 | 3.019646000 |
| 6 | 1.843519000 | 4.451290000 | 0.012369000 |
| 1 | 2.341386000 | 4.757205000 | -0.913633000 |
| 1 | 0.891936000 | 4.983841000 | 0.111521000 |
| 1 | 2.485048000 | 4.683701000 | 0.868590000 |
| 6 | 0.582487000 | 0.735601000 | 4.430678000 |
| 1 | 1.569770000 | 0.859230000 | 4.887988000 |
| 1 | 0.000886000 | 1.654447000 | 4.556868000 |
| 1 | 0.058513000 | -0.098588000 | 4.908445000 |
| 6 | -3.652810000 | -2.177921000 | 1.002347000 |
| 1 | -4.694867000 | -1.963835000 | 1.247212000 |
| 1 | -3.632567000 | -2.983135000 | 0.257650000 |
| 1 | -3.160817000 | -2.550659000 | 1.907094000 |
| 6 | -3.739564000 | 2.636553000 | -0.637583000 |
| 1 | -3.041699000 | 3.428129000 | -0.925078000 |
| 1 | -4.429937000 | 2.464258000 | -1.470787000 |
| 1 | -4.336597000 | 2.990590000 | 0.210551000 |
| 8 | -5.029630000 | 0.250156000 | 0.201404000 |
| 6 | -5.726134000 | -0.392070000 | -0.890794000 |
| 1 | -5.506700000 | 0.123154000 | -1.832348000 |
| 1 | -5.443947000 | -1.446459000 | -0.970661000 |
| 1 | -6.788756000 | -0.308535000 | -0.658178000 |



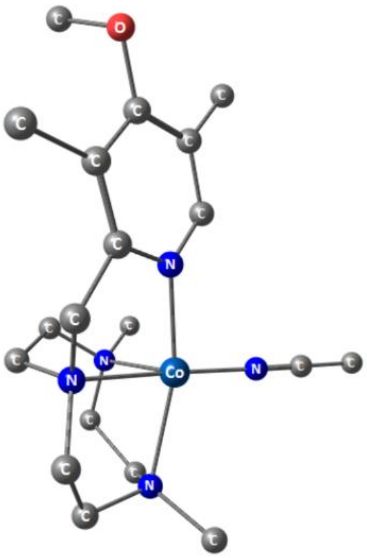
**$1^{DMM}$-$Co^{II}$ (quartet, 2 AC, G = -2608.41620473)**

| | | | |
|---|---|---|---|
| 27 | 1.057685000 | 0.121501000 | -0.028316000 |
| 7 | 0.480708000 | -1.918572000 | 0.400494000 |
| 7 | -1.050750000 | 0.292837000 | 0.032789000 |
| 7 | 1.261977000 | -0.660448000 | -2.042685000 |
| 7 | 3.072425000 | -0.696732000 | 0.197365000 |
| 6 | -0.809877000 | -1.855551000 | 1.118254000 |
| 1 | -0.609259000 | -1.621656000 | 2.169491000 |
| 1 | -1.313943000 | -2.826988000 | 1.093962000 |
| 6 | -1.695510000 | -0.766169000 | 0.552395000 |
| 6 | -3.094510000 | -0.828285000 | 0.615946000 |
| 6 | -3.803951000 | 0.260585000 | 0.083262000 |
| 6 | -3.138057000 | 1.376195000 | -0.453108000 |
| 6 | -1.747835000 | 1.334146000 | -0.446253000 |
| 1 | -1.167176000 | 2.161625000 | -0.843166000 |
| 6 | 1.583354000 | -2.415772000 | 1.260937000 |
| 1 | 1.489791000 | -3.495481000 | 1.443847000 |
| 1 | 1.499345000 | -1.901240000 | 2.220359000 |
| 6 | 2.950109000 | -2.120239000 | 0.641383000 |
| 1 | 3.724687000 | -2.344104000 | 1.382478000 |
| 1 | 3.137948000 | -2.779024000 | -0.206859000 |
| 6 | 3.609096000 | -0.581908000 | -1.184118000 |
| 1 | 4.583787000 | -1.085364000 | -1.261459000 |
| 1 | 3.765535000 | 0.483262000 | -1.376764000 |
| 6 | 2.654766000 | -1.164827000 | -2.223569000 |
| 1 | 3.018437000 | -0.904687000 | -3.223669000 |
| 1 | 2.649902000 | -2.254389000 | -2.171426000 |
| 6 | 0.255536000 | -1.748506000 | -2.094851000 |
| 1 | 0.369583000 | -2.339853000 | -3.014930000 |
| 1 | -0.727861000 | -1.274214000 | -2.123253000 |
| 6 | 0.363113000 | -2.673413000 | -0.882438000 |
| 1 | -0.517318000 | -3.324221000 | -0.853719000 |
| 1 | 1.229412000 | -3.327942000 | -0.981819000 |
| 6 | 3.924719000 | 0.065094000 | 1.130308000 |
| 1 | 4.961805000 | -0.298245000 | 1.097311000 |
| 1 | 3.540960000 | -0.046571000 | 2.145713000 |
| 1 | 3.906430000 | 1.123849000 | 0.861180000 |
| 6 | 0.946873000 | 0.376195000 | -3.044958000 |
| 1 | 0.917206000 | -0.053329000 | -4.056547000 |
| 1 | 1.711400000 | 1.154664000 | -3.012105000 |
| 1 | -0.023674000 | 0.822971000 | -2.815524000 |
| 7 | 1.636335000 | 2.089835000 | -0.433525000 |
| 7 | 0.979108000 | 0.732501000 | 2.068656000 |
| 6 | 1.920973000 | 3.193623000 | -0.626744000 |
| 6 | 0.838387000 | 1.132271000 | 3.144982000 |
| 6 | 2.278795000 | 4.577698000 | -0.874014000 |
| 1 | 2.893661000 | 4.642978000 | -1.777402000 |
| 1 | 1.369108000 | 5.171364000 | -1.010528000 |
| 1 | 2.842487000 | 4.969186000 | -0.021034000 |
| 6 | 0.668853000 | 1.626537000 | 4.499975000 |
| 1 | 1.600178000 | 1.491342000 | 5.059475000 |
| 1 | 0.413058000 | 2.690676000 | 4.474136000 |
| 1 | -0.135395000 | 1.073217000 | 4.995437000 |
| 6 | -3.801432000 | -2.003198000 | 1.239650000 |
| 1 | -4.868734000 | -1.800653000 | 1.347575000 |
| 1 | -3.684307000 | -2.907651000 | 0.629825000 |
| 1 | -3.395086000 | -2.223745000 | 2.232878000 |
| 6 | -3.886691000 | 2.561361000 | -0.996119000 |
| 1 | -3.188349000 | 3.337265000 | -1.324381000 |
| 1 | -4.514150000 | 2.282805000 | -1.850713000 |
| 1 | -4.549437000 | 2.990905000 | -0.236015000 |
| 8 | -5.174314000 | 0.276736000 | 0.129106000 |
| 6 | -5.814265000 | -0.393858000 | -0.975661000 |
| 1 | -5.541878000 | 0.082115000 | -1.924453000 |
| 1 | -5.536021000 | -1.453268000 | -1.002460000 |
| 1 | -6.888393000 | -0.297841000 | -0.806989000 |



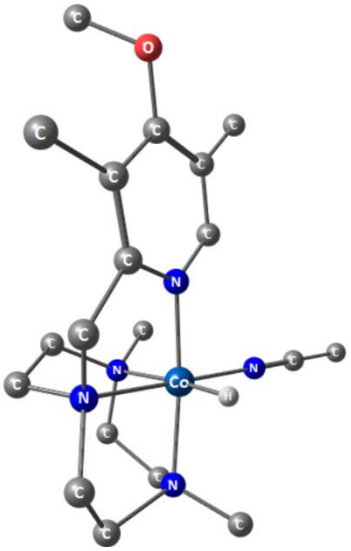
**$1^{DMM}$-$Co^{I}$ (triplet, 1 AC, G = -2475.72746346)**

| | | | |
|---|---|---|---|
| 27 | -1.142852000 | 0.243789000 | -0.400136000 |
| 7 | -0.583464000 | -1.877800000 | -0.395760000 |
| 7 | 0.960189000 | 0.373877000 | -0.523591000 |
| 7 | -1.342426000 | -0.112207000 | 1.759844000 |
| 7 | -3.184559000 | -0.661694000 | -0.415428000 |
| 6 | 0.690803000 | -1.950913000 | -1.127293000 |
| 1 | 0.470637000 | -1.888768000 | -2.199936000 |
| 1 | 1.193046000 | -2.910840000 | -0.954299000 |
| 6 | 1.596286000 | -0.791543000 | -0.758663000 |
| 6 | 2.991705000 | -0.919241000 | -0.690637000 |
| 6 | 3.719615000 | 0.226633000 | -0.330336000 |
| 6 | 3.074724000 | 1.451481000 | -0.094120000 |
| 6 | 1.687391000 | 1.460504000 | -0.214804000 |
| 1 | 1.127830000 | 2.377156000 | -0.047170000 |
| 6 | -1.690872000 | -2.540769000 | -1.110697000 |
| 1 | -1.600311000 | -3.639506000 | -1.083505000 |
| 1 | -1.629346000 | -2.224765000 | -2.156348000 |
| 6 | -3.053673000 | -2.134577000 | -0.541768000 |
| 1 | -3.838019000 | -2.535151000 | -1.197061000 |
| 1 | -3.208904000 | -2.598274000 | 0.434127000 |
| 6 | -3.694596000 | -0.238431000 | 0.903355000 |
| 1 | -4.676244000 | -0.694566000 | 1.121545000 |
| 1 | -3.835194000 | 0.845628000 | 0.855211000 |
| 6 | -2.726970000 | -0.578427000 | 2.038289000 |
| 1 | -3.101807000 | -0.123588000 | 2.964270000 |
| 1 | -2.713575000 | -1.655977000 | 2.214301000 |
| 6 | -0.332950000 | -1.160201000 | 2.007603000 |
| 1 | -0.415101000 | -1.562276000 | 3.031858000 |
| 1 | 0.647302000 | -0.686438000 | 1.917629000 |
| 6 | -0.442765000 | -2.324728000 | 1.014236000 |
| 1 | 0.445943000 | -2.959371000 | 1.124349000 |
| 1 | -1.300768000 | -2.949662000 | 1.268254000 |
| 6 | -4.009417000 | -0.113784000 | -1.497746000 |
| 1 | -5.048083000 | -0.483615000 | -1.450966000 |
| 1 | -3.579814000 | -0.401949000 | -2.462069000 |
| 1 | -4.019783000 | 0.977513000 | -1.435591000 |
| 6 | -1.032962000 | 1.097663000 | 2.531777000 |
| 1 | -1.027871000 | 0.900787000 | 3.617412000 |
| 1 | -1.782002000 | 1.864697000 | 2.318271000 |
| 1 | -0.051718000 | 1.479247000 | 2.236607000 |
| 7 | -1.619437000 | 2.089779000 | -0.604236000 |
| 6 | -1.894862000 | 3.216659000 | -0.733059000 |
| 6 | -2.236682000 | 4.624464000 | -0.879460000 |
| 1 | -2.358237000 | 5.086154000 | 0.107060000 |
| 1 | -1.444172000 | 5.154690000 | -1.419486000 |
| 1 | -3.174721000 | 4.732822000 | -1.435493000 |
| 6 | 3.843519000 | 2.694072000 | 0.263439000 |
| 1 | 3.161618000 | 3.537895000 | 0.409236000 |
| 1 | 4.421806000 | 2.558449000 | 1.184787000 |
| 1 | 4.556276000 | 2.960217000 | -0.526224000 |
| 6 | 3.685513000 | -2.221986000 | -1.000772000 |
| 1 | 3.487372000 | -2.976292000 | -0.229128000 |
| 1 | 3.341957000 | -2.635225000 | -1.955476000 |
| 1 | 4.766212000 | -2.078357000 | -1.065231000 |
| 8 | 5.092402000 | 0.180170000 | -0.245399000 |
| 6 | 5.581672000 | -0.290383000 | 1.023991000 |
| 1 | 5.234397000 | 0.359474000 | 1.835928000 |
| 1 | 5.252459000 | -1.318573000 | 1.213600000 |
| 1 | 6.671602000 | -0.257819000 | 0.964593000 |



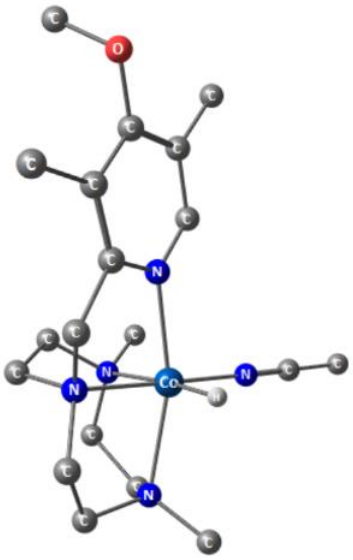
**$1^{DMM}$-$Co^{III}$-H (singlet, 1 AC, G = -2476.18052056)**

| | | | |
|---|---|---|---|
| 27 | -1.086293000 | 0.035737000 | -0.386452000 |
| 7 | -0.690057000 | -1.858287000 | -0.254948000 |
| 7 | 0.850002000 | 0.243950000 | -0.362420000 |
| 7 | -1.312223000 | 0.037582000 | 1.695286000 |
| 7 | -3.013678000 | -0.452667000 | -0.476789000 |
| 6 | 0.623832000 | -2.069673000 | -0.929109000 |
| 1 | 0.448893000 | -2.102490000 | -2.009139000 |
| 1 | 1.056245000 | -3.025709000 | -0.625534000 |
| 6 | 1.516732000 | -0.904834000 | -0.612657000 |
| 6 | 2.911703000 | -0.975685000 | -0.620152000 |
| 6 | 3.609474000 | 0.207229000 | -0.323880000 |
| 6 | 2.927132000 | 1.410584000 | -0.079668000 |
| 6 | 1.538226000 | 1.371911000 | -0.116788000 |
| 1 | 0.958782000 | 2.267762000 | 0.065487000 |
| 6 | -1.800926000 | -2.555028000 | -0.973886000 |
| 1 | -1.762493000 | -3.633670000 | -0.784276000 |
| 1 | -1.659068000 | -2.373939000 | -2.039585000 |
| 6 | -3.116012000 | -1.960201000 | -0.505586000 |
| 1 | -3.927277000 | -2.259852000 | -1.173677000 |
| 1 | -3.376143000 | -2.315467000 | 0.490321000 |
| 6 | -3.613657000 | 0.106832000 | 0.773849000 |
| 1 | -4.635480000 | -0.271660000 | 0.899129000 |
| 1 | -3.661232000 | 1.190100000 | 0.646437000 |
| 6 | -2.756923000 | -0.250868000 | 1.977389000 |
| 1 | -3.088124000 | 0.324961000 | 2.846643000 |
| 1 | -2.865782000 | -1.303673000 | 2.238354000 |
| 6 | -0.429335000 | -1.081335000 | 2.116388000 |
| 1 | -0.637439000 | -1.372167000 | 3.154426000 |
| 1 | 0.598682000 | -0.718787000 | 2.068008000 |
| 6 | -0.626564000 | -2.278867000 | 1.198079000 |
| 1 | 0.188170000 | -2.994346000 | 1.331388000 |
| 1 | -1.553410000 | -2.799218000 | 1.436027000 |
| 6 | -3.725675000 | 0.098531000 | -1.660223000 |
| 1 | -4.792670000 | -0.144364000 | -1.589732000 |
| 1 | -3.309250000 | -0.345512000 | -2.564984000 |
| 1 | -3.601956000 | 1.180246000 | -1.697359000 |
| 6 | -0.907812000 | 1.282830000 | 2.382455000 |
| 1 | -0.970342000 | 1.151144000 | 3.470553000 |
| 1 | -1.571209000 | 2.095573000 | 2.082425000 |
| 1 | 0.118300000 | 1.536026000 | 2.112956000 |
| 7 | -1.429257000 | 1.885105000 | -0.601954000 |
| 6 | -1.621799000 | 3.012156000 | -0.756229000 |
| 6 | -1.869448000 | 4.428536000 | -0.942124000 |
| 1 | -1.982508000 | 4.912026000 | 0.033677000 |
| 1 | -1.028493000 | 4.880796000 | -1.477514000 |
| 1 | -2.786364000 | 4.564953000 | -1.524773000 |
| 1 | -0.979683000 | -0.066715000 | -1.839966000 |
| 6 | 3.662626000 | 2.689470000 | 0.207603000 |
| 1 | 2.956839000 | 3.504199000 | 0.394398000 |
| 1 | 4.310528000 | 2.585944000 | 1.085190000 |
| 1 | 4.303222000 | 2.973094000 | -0.635545000 |
| 6 | 3.624403000 | -2.259024000 | -0.955736000 |
| 1 | 3.579923000 | -2.970668000 | -0.121821000 |
| 1 | 3.171867000 | -2.743731000 | -1.826971000 |
| 1 | 4.675275000 | -2.068029000 | -1.183204000 |
| 8 | 4.976973000 | 0.227032000 | -0.325499000 |
| 6 | 5.591245000 | -0.298709000 | 0.870279000 |
| 1 | 5.304762000 | 0.303265000 | 1.739953000 |
| 1 | 5.306271000 | -1.343269000 | 1.033433000 |
| 1 | 6.668434000 | -0.230886000 | 0.709205000 |

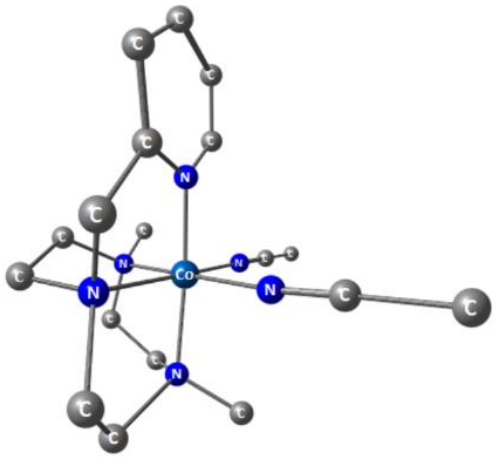


**$1^{DMM}$-$Co^{II}$-H (doublet, 1 AC, G =-2476.30633094)**

| | | | |
|---|---|---|---|
| 27 | -1.155828000 | 0.147198000 | -0.437995000 |
| 7 | -0.598672000 | -1.819477000 | -0.207897000 |
| 7 | 1.035245000 | 0.340862000 | -0.309699000 |
| 7 | -1.437116000 | 0.127259000 | 1.629394000 |
| 7 | -3.226099000 | -0.730363000 | -0.460826000 |
| 6 | 0.710221000 | -1.987301000 | -0.877540000 |
| 1 | 0.535783000 | -2.009358000 | -1.958814000 |
| 1 | 1.163471000 | -2.944500000 | -0.595424000 |
| 6 | 1.638496000 | -0.831070000 | -0.564610000 |
| 6 | 3.035300000 | -0.970784000 | -0.595540000 |
| 6 | 3.792676000 | 0.181106000 | -0.329347000 |
| 6 | 3.174818000 | 1.416270000 | -0.072157000 |
| 6 | 1.781563000 | 1.428209000 | -0.078542000 |
| 1 | 1.239928000 | 2.351685000 | 0.112121000 |
| 6 | -1.657329000 | -2.629786000 | -0.863124000 |
| 1 | -1.513804000 | -3.701177000 | -0.660572000 |
| 1 | -1.562949000 | -2.467099000 | -1.938526000 |
| 6 | -3.053386000 | -2.201905000 | -0.397871000 |
| 1 | -3.797711000 | -2.703741000 | -1.028790000 |
| 1 | -3.237987000 | -2.545775000 | 0.621270000 |
| 6 | -3.783965000 | -0.149538000 | 0.772751000 |
| 1 | -4.758748000 | -0.597256000 | 1.030890000 |
| 1 | -3.948177000 | 0.914571000 | 0.578574000 |
| 6 | -2.833632000 | -0.319086000 | 1.952001000 |
| 1 | -3.213884000 | 0.252366000 | 2.805729000 |
| 1 | -2.802638000 | -1.361950000 | 2.270066000 |
| 6 | -0.440688000 | -0.869012000 | 2.104714000 |
| 1 | -0.621916000 | -1.122777000 | 3.159391000 |
| 1 | 0.539914000 | -0.397787000 | 2.036021000 |
| 6 | -0.485983000 | -2.134459000 | 1.254552000 |
| 1 | 0.414538000 | -2.728858000 | 1.442129000 |
| 1 | -1.334796000 | -2.756677000 | 1.540060000 |
| 6 | -4.013715000 | -0.335701000 | -1.632611000 |
| 1 | -5.056824000 | -0.686284000 | -1.558854000 |
| 1 | -3.564069000 | -0.760562000 | -2.533696000 |
| 1 | -4.012148000 | 0.753972000 | -1.725833000 |
| 6 | -1.169414000 | 1.427647000 | 2.279110000 |
| 1 | -1.186131000 | 1.323597000 | 3.373483000 |
| 1 | -1.932808000 | 2.147252000 | 1.979609000 |
| 1 | -0.190840000 | 1.797632000 | 1.968178000 |
| 7 | -1.638769000 | 1.977931000 | -0.664965000 |
| 6 | -1.915692000 | 3.094358000 | -0.804249000 |
| 6 | -2.261572000 | 4.496538000 | -0.972739000 |
| 1 | -2.398306000 | 4.965526000 | 0.007458000 |
| 1 | -1.460613000 | 5.016430000 | -1.508851000 |
| 1 | -3.190981000 | 4.586178000 | -1.544902000 |
| 1 | -1.010233000 | 0.032237000 | -1.964969000 |
| 6 | 3.973837000 | 2.664986000 | 0.181049000 |
| 1 | 3.307825000 | 3.514574000 | 0.362238000 |
| 1 | 4.631276000 | 2.554186000 | 1.050975000 |
| 1 | 4.613657000 | 2.905804000 | -0.676359000 |
| 6 | 3.690958000 | -2.288822000 | -0.917399000 |
| 1 | 3.543152000 | -3.015682000 | -0.108748000 |
| 1 | 3.271594000 | -2.727111000 | -1.829920000 |
| 1 | 4.765019000 | -2.161130000 | -1.066518000 |
| 8 | 5.166203000 | 0.130352000 | -0.375773000 |
| 6 | 5.788359000 | -0.264167000 | 0.861320000 |
| 1 | 5.532743000 | 0.435891000 | 1.665070000 |
| 1 | 5.482046000 | -1.277102000 | 1.147488000 |
| 1 | 6.865092000 | -0.242629000 | 0.681429000 |

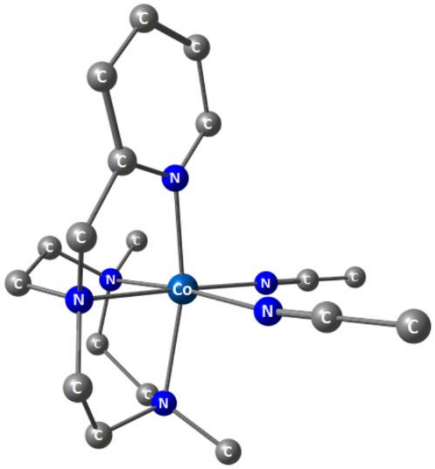


**$1^{H}$-$Co^{III}$ (singlet, 2 AC, G = -2415.06655455)**



| | | | |
|---|---|---|---|
| 27 | 0.313907000 | 0.026196000 | 0.008207000 |
| 7 | -0.116330000 | -1.602919000 | 0.984772000 |
| 7 | -1.616099000 | 0.088617000 | -0.350416000 |
| 7 | 0.721998000 | -1.124559000 | -1.565788000 |
| 7 | 2.213535000 | -0.225698000 | 0.575792000 |
| 6 | -1.509684000 | -1.441964000 | 1.503640000 |
| 1 | -1.473592000 | -0.840712000 | 2.415039000 |
| 1 | -1.934022000 | -2.415273000 | 1.760005000 |
| 6 | -2.324197000 | -0.723183000 | 0.470465000 |
| 6 | -3.707442000 | -0.814480000 | 0.379198000 |
| 1 | -4.241807000 | -1.488584000 | 1.040306000 |
| 6 | -4.375209000 | -0.029778000 | -0.560116000 |
| 1 | -5.455658000 | -0.084676000 | -0.649916000 |
| 6 | -3.637937000 | 0.826793000 | -1.378590000 |
| 1 | -4.117374000 | 1.461808000 | -2.115414000 |
| 6 | -2.255625000 | 0.861154000 | -1.246414000 |
| 1 | -1.645864000 | 1.508893000 | -1.861833000 |
| 6 | 0.895509000 | -1.697553000 | 2.085915000 |
| 1 | 0.848076000 | -2.688624000 | 2.547949000 |
| 1 | 0.639606000 | -0.948816000 | 2.834961000 |
| 6 | 2.269018000 | -1.428561000 | 1.499525000 |
| 1 | 2.984899000 | -1.230445000 | 2.299736000 |
| 1 | 2.644080000 | -2.283516000 | 0.938681000 |
| 6 | 2.954536000 | -0.479967000 | -0.698243000 |
| 1 | 3.960474000 | -0.848234000 | -0.469461000 |
| 1 | 3.045550000 | 0.474825000 | -1.217852000 |
| 6 | 2.192880000 | -1.485436000 | -1.531389000 |
| 1 | 2.576767000 | -1.500917000 | -2.552982000 |
| 1 | 2.293695000 | -2.494149000 | -1.134142000 |
| 6 | -0.130287000 | -2.342798000 | -1.383504000 |
| 1 | 0.212746000 | -3.130449000 | -2.062150000 |
| 1 | -1.150136000 | -2.074757000 | -1.657865000 |
| 6 | -0.037199000 | -2.797817000 | 0.057159000 |
| 1 | -0.845348000 | -3.490264000 | 0.296656000 |
| 1 | 0.902816000 | -3.311990000 | 0.250331000 |
| 6 | 2.830000000 | 0.943378000 | 1.265585000 |
| 1 | 3.901810000 | 0.749388000 | 1.378827000 |
| 1 | 2.381630000 | 1.065308000 | 2.249946000 |
| 1 | 2.681947000 | 1.845273000 | 0.673721000 |
| 6 | 0.411839000 | -0.523929000 | -2.893632000 |
| 1 | 0.554343000 | -1.293930000 | -3.658886000 |
| 1 | 1.087410000 | 0.306530000 | -3.088313000 |
| 1 | -0.621723000 | -0.185187000 | -2.918876000 |
| 7 | 0.704875000 | 1.640299000 | -0.944803000 |
| 7 | -0.074829000 | 1.138876000 | 1.527757000 |
| 6 | 0.923504000 | 2.652949000 | -1.449701000 |
| 6 | -0.356536000 | 1.893283000 | 2.351793000 |
| 6 | 1.208371000 | 3.913941000 | -2.098875000 |
| 1 | 1.733746000 | 3.724830000 | -3.040912000 |
| 1 | 0.269668000 | 4.440218000 | -2.300804000 |
| 1 | 1.837637000 | 4.524930000 | -1.443393000 |
| 6 | -0.692849000 | 2.826877000 | 3.404848000 |
| 1 | 0.225450000 | 3.160974000 | 3.898968000 |
| 1 | -1.213558000 | 3.688747000 | 2.975263000 |
| 1 | -1.342937000 | 2.331741000 | 4.133651000 |

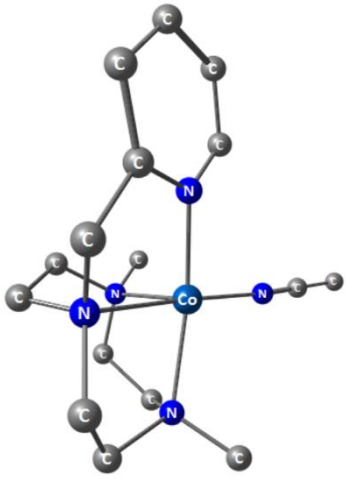
**$1^{H}$-$Co^{II}$ (quartet, 2 AC, G = -2415.24743197)**



| | | | |
|---|---|---|---|
| 27 | 0.329407000 | 0.107484000 | -0.056942000 |
| 7 | -0.430698000 | -1.544786000 | 1.127993000 |
| 7 | -1.754920000 | 0.271845000 | -0.410712000 |
| 7 | 0.759657000 | -1.475170000 | -1.466128000 |
| 7 | 2.234115000 | -0.521218000 | 0.817724000 |
| 6 | -1.797466000 | -1.164521000 | 1.538013000 |
| 1 | -1.719080000 | -0.457277000 | 2.370023000 |
| 1 | -2.369306000 | -2.029860000 | 1.893823000 |
| 6 | -2.522635000 | -0.476998000 | 0.405280000 |
| 6 | -3.902491000 | -0.562197000 | 0.228713000 |
| 1 | -4.493443000 | -1.183931000 | 0.894010000 |
| 6 | -4.497144000 | 0.154617000 | -0.810384000 |
| 1 | -5.570187000 | 0.100023000 | -0.969414000 |
| 6 | -3.695401000 | 0.935711000 | -1.645335000 |
| 1 | -4.117628000 | 1.506897000 | -2.465564000 |
| 6 | -2.324128000 | 0.964264000 | -1.410237000 |
| 1 | -1.652937000 | 1.547956000 | -2.032605000 |
| 6 | 0.508670000 | -1.614842000 | 2.275273000 |
| 1 | 0.321490000 | -2.508123000 | 2.887323000 |
| 1 | 0.325221000 | -0.734531000 | 2.895401000 |
| 6 | 1.963318000 | -1.613189000 | 1.803576000 |
| 1 | 2.613075000 | -1.493573000 | 2.676704000 |
| 1 | 2.224025000 | -2.572340000 | 1.355615000 |
| 6 | 2.964639000 | -1.014545000 | -0.379463000 |
| 1 | 3.910079000 | -1.492897000 | -0.084863000 |
| 1 | 3.206933000 | -0.138650000 | -0.987604000 |
| 6 | 2.130358000 | -2.000456000 | -1.193156000 |
| 1 | 2.645598000 | -2.207403000 | -2.137422000 |
| 1 | 2.048591000 | -2.954133000 | -0.671125000 |
| 6 | -0.292364000 | -2.485682000 | -1.197607000 |
| 1 | -0.080652000 | -3.419189000 | -1.738476000 |
| 1 | -1.228742000 | -2.080448000 | -1.586887000 |
| 6 | -0.425194000 | -2.785152000 | 0.296748000 |
| 1 | -1.349534000 | -3.348568000 | 0.462537000 |
| 1 | 0.390834000 | -3.425335000 | 0.633356000 |
| 6 | 2.991267000 | 0.574197000 | 1.453137000 |
| 1 | 3.996711000 | 0.237510000 | 1.743947000 |
| 1 | 2.458127000 | 0.913218000 | 2.343109000 |
| 1 | 3.082043000 | 1.410404000 | 0.755938000 |
| 6 | 0.655823000 | -0.993548000 | -2.858543000 |
| 1 | 0.732661000 | -1.830483000 | -3.567119000 |
| 1 | 1.461036000 | -0.283925000 | -3.057785000 |
| 1 | -0.303376000 | -0.490017000 | -3.001762000 |
| 7 | 1.107935000 | 1.693029000 | -1.173604000 |
| 7 | -0.008870000 | 1.581428000 | 1.506689000 |
| 6 | 1.528637000 | 2.590351000 | -1.768948000 |
| 6 | -0.279654000 | 2.425578000 | 2.249683000 |
| 6 | 2.065700000 | 3.712117000 | -2.515836000 |
| 1 | 2.675876000 | 3.341647000 | -3.345888000 |
| 1 | 1.243565000 | 4.317807000 | -2.910459000 |
| 1 | 2.685107000 | 4.327938000 | -1.855566000 |
| 6 | -0.617194000 | 3.481420000 | 3.187449000 |
| 1 | 0.281409000 | 3.794414000 | 3.728846000 |
| 1 | -1.029093000 | 4.337739000 | 2.643721000 |
| 1 | -1.361367000 | 3.114433000 | 3.901707000 |

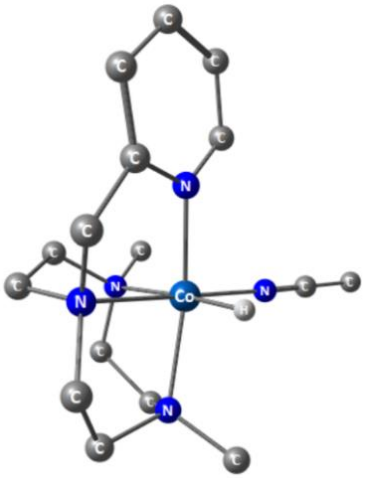
**$1^{H}$-$Co^{I}$ (triplet, 1 AC, G = -2282.56161631)**

| | | | |
|---|---|---|---|
| 27 | -0.313518000 | 0.217564000 | -0.306267000 |
| 7 | 0.304170000 | -1.852056000 | -0.485401000 |
| 7 | 1.773310000 | 0.455120000 | -0.317638000 |
| 7 | -0.696920000 | -0.339326000 | 1.706063000 |
| 7 | -2.279779000 | -0.611775000 | -0.663133000 |
| 6 | 1.648056000 | -1.838991000 | -1.097712000 |
| 1 | 1.525078000 | -1.730340000 | -2.180775000 |
| 1 | 2.182030000 | -2.779985000 | -0.920882000 |
| 6 | 2.464138000 | -0.666478000 | -0.607366000 |
| 6 | 3.853501000 | -0.708974000 | -0.510735000 |
| 1 | 4.380572000 | -1.629640000 | -0.741087000 |
| 6 | 4.540005000 | 0.439252000 | -0.115731000 |
| 1 | 5.622915000 | 0.428295000 | -0.033538000 |
| 6 | 3.817728000 | 1.598263000 | 0.177120000 |
| 1 | 4.313254000 | 2.511523000 | 0.489267000 |
| 6 | 2.431806000 | 1.562431000 | 0.066642000 |
| 1 | 1.821413000 | 2.431517000 | 0.289765000 |
| 6 | -0.721753000 | -2.424906000 | -1.394736000 |
| 1 | -0.617917000 | -3.515861000 | -1.476410000 |
| 1 | -0.547699000 | -1.990413000 | -2.382855000 |
| 6 | -2.134441000 | -2.075162000 | -0.932712000 |
| 1 | -2.844550000 | -2.382498000 | -1.707631000 |
| 1 | -2.396733000 | -2.633863000 | -0.034127000 |
| 6 | -2.953839000 | -0.341489000 | 0.634482000 |
| 1 | -3.939707000 | -0.826723000 | 0.667816000 |
| 1 | -3.106738000 | 0.739870000 | 0.696126000 |
| 6 | -2.108484000 | -0.818432000 | 1.814848000 |
| 1 | -2.553864000 | -0.452918000 | 2.746158000 |
| 1 | -2.106497000 | -1.907081000 | 1.875230000 |
| 6 | 0.292159000 | -1.410925000 | 1.982015000 |
| 1 | 0.083289000 | -1.891663000 | 2.947789000 |
| 1 | 1.270532000 | -0.929978000 | 2.052921000 |
| 6 | 0.300064000 | -2.466862000 | 0.874608000 |
| 1 | 1.181284000 | -3.104576000 | 0.999493000 |
| 1 | -0.572113000 | -3.116254000 | 0.959952000 |
| 6 | -2.992883000 | 0.050943000 | -1.772399000 |
| 1 | -4.015707000 | -0.339383000 | -1.871396000 |
| 1 | -2.449847000 | -0.127553000 | -2.704410000 |
| 1 | -3.036897000 | 1.126459000 | -1.589125000 |
| 6 | -0.466736000 | 0.817545000 | 2.597582000 |
| 1 | -0.537877000 | 0.516422000 | 3.651790000 |
| 1 | -1.216679000 | 1.584356000 | 2.392486000 |
| 1 | 0.526751000 | 1.231434000 | 2.406988000 |
| 7 | -0.882242000 | 2.195587000 | -0.397281000 |
| 6 | -1.123606000 | 3.325101000 | -0.452986000 |
| 6 | -1.430158000 | 4.740372000 | -0.521084000 |
| 1 | -1.539265000 | 5.139363000 | 0.492706000 |
| 1 | -0.618406000 | 5.266285000 | -1.033937000 |
| 1 | -2.364742000 | 4.886007000 | -1.072420000 |



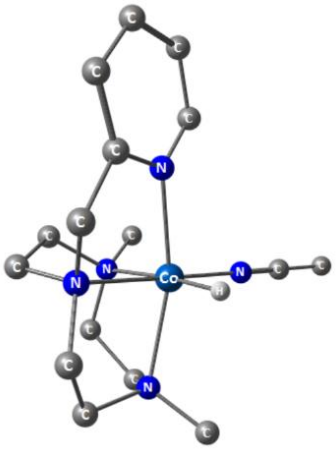
**$1^{H}$-$Co^{III}$-H (singlet, 1 AC, G = -2283.01093911)**

| | | | |
|---|---|---|---|
| 27 | -0.325072000 | 0.156241000 | -0.349586000 |
| 7 | 0.296062000 | -1.885215000 | -0.394142000 |
| 7 | 1.712193000 | 0.416067000 | -0.340477000 |
| 7 | -0.621850000 | -0.189284000 | 1.674039000 |
| 7 | -2.233018000 | -0.650243000 | -0.632932000 |
| 6 | 1.633894000 | -1.898615000 | -1.021592000 |
| 1 | 1.498890000 | -1.840173000 | -2.106575000 |
| 1 | 2.172286000 | -2.826346000 | -0.799458000 |
| 6 | 2.431167000 | -0.696421000 | -0.587557000 |
| 6 | 3.820568000 | -0.696186000 | -0.494778000 |
| 1 | 4.370149000 | -1.612200000 | -0.687121000 |
| 6 | 4.475631000 | 0.486820000 | -0.153738000 |
| 1 | 5.558353000 | 0.510097000 | -0.073984000 |
| 6 | 3.721416000 | 1.637119000 | 0.087323000 |
| 1 | 4.190425000 | 2.577683000 | 0.356010000 |
| 6 | 2.337016000 | 1.560728000 | -0.014480000 |
| 1 | 1.704555000 | 2.421324000 | 0.172565000 |
| 6 | -0.731019000 | -2.552805000 | -1.233527000 |
| 1 | -0.631507000 | -3.644727000 | -1.183969000 |
| 1 | -0.562554000 | -2.233664000 | -2.263826000 |
| 6 | -2.129897000 | -2.138426000 | -0.790648000 |
| 1 | -2.857943000 | -2.477176000 | -1.533159000 |
| 1 | -2.396942000 | -2.614305000 | 0.152668000 |
| 6 | -2.899441000 | -0.273626000 | 0.651189000 |
| 1 | -3.881436000 | -0.759571000 | 0.720086000 |
| 1 | -3.057630000 | 0.807195000 | 0.623965000 |
| 6 | -2.041060000 | -0.653628000 | 1.850202000 |
| 1 | -2.463455000 | -0.204832000 | 2.754126000 |
| 1 | -2.039762000 | -1.732449000 | 2.005399000 |
| 6 | 0.359271000 | -1.255326000 | 2.025311000 |
| 1 | 0.151471000 | -1.642272000 | 3.031405000 |
| 1 | 1.345005000 | -0.786110000 | 2.043080000 |
| 6 | 0.324581000 | -2.396527000 | 1.012066000 |
| 1 | 1.200454000 | -3.035878000 | 1.159381000 |
| 1 | -0.554008000 | -3.022834000 | 1.166844000 |
| 6 | -2.970384000 | -0.063277000 | -1.777120000 |
| 1 | -4.012601000 | -0.407382000 | -1.769670000 |
| 1 | -2.491553000 | -0.373374000 | -2.707240000 |
| 1 | -2.947959000 | 1.025575000 | -1.706935000 |
| 6 | -0.374256000 | 1.010102000 | 2.508184000 |
| 1 | -0.434721000 | 0.747971000 | 3.572181000 |
| 1 | -1.125380000 | 1.767907000 | 2.281154000 |
| 1 | 0.618401000 | 1.409564000 | 2.290884000 |
| 7 | -0.867094000 | 2.117346000 | -0.394208000 |
| 6 | -1.129498000 | 3.240114000 | -0.472054000 |
| 6 | -1.458391000 | 4.648239000 | -0.565858000 |
| 1 | -1.592513000 | 5.061598000 | 0.438968000 |
| 1 | -0.647241000 | 5.178814000 | -1.074992000 |
| 1 | -2.384981000 | 4.767514000 | -1.136929000 |
| 1 | -0.172518000 | 0.309145000 | -1.809519000 |

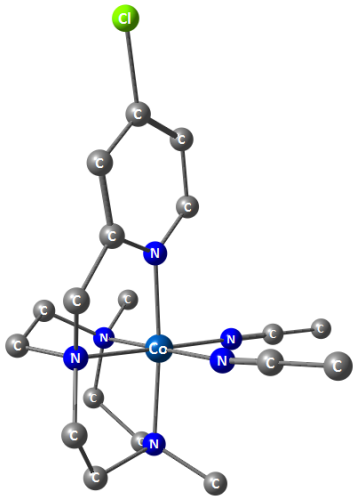


**$1^{H}$-$Co^{II}$-H (doublet, 1 AC, G =-2283.13791102)**

| | | | |
|---|---|---|---|
| 27 | -0.346231000 | 0.176819000 | -0.436612000 |
| 7 | 0.286082000 | -1.789337000 | -0.349285000 |
| 7 | 1.833226000 | 0.462648000 | -0.296258000 |
| 7 | -0.617821000 | -0.011312000 | 1.620813000 |
| 7 | -2.375099000 | -0.772222000 | -0.529842000 |
| 6 | 1.600241000 | -1.837659000 | -1.024121000 |
| 1 | 1.422672000 | -1.750027000 | -2.100889000 |
| 1 | 2.108816000 | -2.793420000 | -0.841653000 |
| 6 | 2.475743000 | -0.683463000 | -0.589553000 |
| 6 | 3.866522000 | -0.783916000 | -0.534223000 |
| 1 | 4.350495000 | -1.729475000 | -0.761099000 |
| 6 | 4.611871000 | 0.342724000 | -0.183205000 |
| 1 | 5.695839000 | 0.290570000 | -0.133112000 |
| 6 | 3.942363000 | 1.533521000 | 0.107196000 |
| 1 | 4.481890000 | 2.433562000 | 0.385487000 |
| 6 | 2.550201000 | 1.543689000 | 0.041094000 |
| 1 | 1.982180000 | 2.442111000 | 0.267957000 |
| 6 | -0.740835000 | -2.581513000 | -1.071480000 |
| 1 | -0.561867000 | -3.659976000 | -0.951866000 |
| 1 | -0.649146000 | -2.332859000 | -2.130672000 |
| 6 | -2.151755000 | -2.238066000 | -0.581067000 |
| 1 | -2.877273000 | -2.712848000 | -1.253300000 |
| 1 | -2.328166000 | -2.667121000 | 0.406971000 |
| 6 | -2.954710000 | -0.307736000 | 0.742998000 |
| 1 | -3.911071000 | -0.811193000 | 0.964563000 |
| 1 | -3.160982000 | 0.760527000 | 0.628379000 |
| 6 | -1.997993000 | -0.528514000 | 1.908219000 |
| 1 | -2.397273000 | -0.035087000 | 2.801081000 |
| 1 | -1.930117000 | -1.590774000 | 2.147818000 |
| 6 | 0.411951000 | -1.007247000 | 2.023519000 |
| 1 | 0.240912000 | -1.341307000 | 3.057258000 |
| 1 | 1.377737000 | -0.502348000 | 1.990828000 |
| 6 | 0.404272000 | -2.209132000 | 1.084267000 |
| 1 | 1.319707000 | -2.792248000 | 1.231897000 |
| 1 | -0.429184000 | -2.871755000 | 1.318973000 |
| 6 | -3.178006000 | -0.317550000 | -1.669843000 |
| 1 | -4.207833000 | -0.709098000 | -1.623463000 |
| 1 | -2.714522000 | -0.657331000 | -2.599455000 |
| 1 | -3.214671000 | 0.775293000 | -1.680533000 |
| 6 | -0.393602000 | 1.245982000 | 2.364774000 |
| 1 | -0.402062000 | 1.061230000 | 3.448485000 |
| 1 | -1.183870000 | 1.957226000 | 2.120338000 |
| 1 | 0.569617000 | 1.673027000 | 2.080036000 |
| 7 | -0.896562000 | 2.005031000 | -0.539484000 |
| 6 | -1.221171000 | 3.114841000 | -0.613066000 |
| 6 | -1.630650000 | 4.507097000 | -0.702916000 |
| 1 | -1.774283000 | 4.917799000 | 0.302064000 |
| 1 | -0.861292000 | 5.089765000 | -1.220384000 |
| 1 | -2.570924000 | 4.584156000 | -1.258964000 |
| 1 | -0.202546000 | 0.175500000 | -1.965397000 |



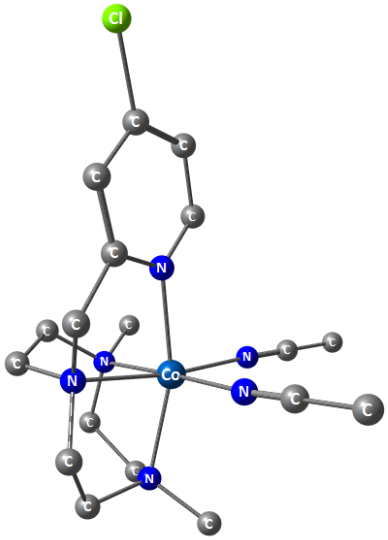
**$1^{Cl}$-$Co^{III}$ (singlet, 1 AC, G = -2874.70945412)**




| | | | |
|---|---|---|---|
| 27 | 0.762771000 | 0.026005000 | 0.002540000 |
| 7 | 0.377640000 | -1.585071000 | 1.026528000 |
| 7 | -1.191746000 | 0.121545000 | -0.201541000 |
| 7 | 1.021733000 | -1.148869000 | -1.587971000 |
| 7 | 2.693489000 | -0.259134000 | 0.418240000 |
| 6 | -0.965358000 | -1.391368000 | 1.655529000 |
| 1 | -0.845787000 | -0.775467000 | 2.550043000 |
| 1 | -1.384452000 | -2.351891000 | 1.962302000 |
| 6 | -1.846426000 | -0.671985000 | 0.678707000 |
| 6 | -3.231715000 | -0.755105000 | 0.696840000 |
| 1 | -3.727287000 | -1.414433000 | 1.400339000 |
| 6 | -3.944577000 | 0.030825000 | -0.206234000 |
| 6 | -3.276555000 | 0.874893000 | -1.091696000 |
| 1 | -3.805934000 | 1.504053000 | -1.797510000 |
| 6 | -1.889583000 | 0.890366000 | -1.054607000 |
| 1 | -1.327661000 | 1.527200000 | -1.724877000 |
| 6 | 1.473335000 | -1.687418000 | 2.044816000 |
| 1 | 1.442234000 | -2.671154000 | 2.523557000 |
| 1 | 1.296720000 | -0.922855000 | 2.800638000 |
| 6 | 2.797694000 | -1.458681000 | 1.341386000 |
| 1 | 3.585993000 | -1.276697000 | 2.074235000 |
| 1 | 3.095602000 | -2.326669000 | 0.755518000 |
| 6 | 3.324008000 | -0.534812000 | -0.909612000 |
| 1 | 4.341671000 | -0.911901000 | -0.761535000 |
| 1 | 3.380353000 | 0.414100000 | -1.444557000 |
| 6 | 2.482742000 | -1.537232000 | -1.665581000 |
| 1 | 2.783002000 | -1.569421000 | -2.714336000 |
| 1 | 2.597966000 | -2.543451000 | -1.267049000 |
| 6 | 0.166603000 | -2.348419000 | -1.325622000 |
| 1 | 0.443872000 | -3.149170000 | -2.018683000 |
| 1 | -0.866905000 | -2.068050000 | -1.526385000 |
| 6 | 0.362096000 | -2.791119000 | 0.108573000 |
| 1 | -0.439352000 | -3.465654000 | 0.414689000 |
| 1 | 1.302402000 | -3.323925000 | 0.236422000 |
| 6 | 3.383485000 | 0.901535000 | 1.051065000 |
| 1 | 4.456354000 | 0.685464000 | 1.087763000 |
| 1 | 3.010470000 | 1.039764000 | 2.064382000 |
| 1 | 3.212493000 | 1.802105000 | 0.463384000 |
| 6 | 0.620446000 | -0.555210000 | -2.894892000 |
| 1 | 0.689898000 | -1.336460000 | -3.658938000 |
| 1 | 1.293936000 | 0.260683000 | -3.150047000 |
| 1 | -0.406056000 | -0.197874000 | -2.845265000 |
| 7 | 1.108439000 | 1.624931000 | -0.992084000 |
| 7 | 0.510575000 | 1.160768000 | 1.533636000 |
| 6 | 1.301771000 | 2.631399000 | -1.519138000 |
| 6 | 0.283935000 | 1.927726000 | 2.363092000 |
| 6 | 1.552832000 | 3.885286000 | -2.195300000 |
| 1 | 2.077208000 | 3.689814000 | -3.136594000 |
| 1 | 0.600333000 | 4.384290000 | -2.401944000 |
| 1 | 2.170907000 | 4.524400000 | -1.556235000 |
| 6 | 0.008289000 | 2.877243000 | 3.419341000 |
| 1 | 0.929592000 | 3.409037000 | 3.678973000 |
| 1 | -0.745040000 | 3.593554000 | 3.075637000 |
| 1 | -0.367427000 | 2.342315000 | 4.297746000 |
| 17 | -5.685233000 | -0.041211000 | -0.223995000 |

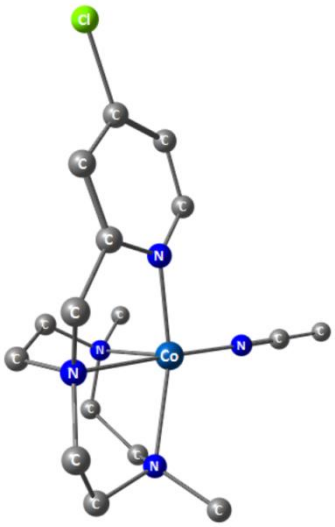
**$1^{Cl}$-$Co^{II}$ (quartet, 2 AC, G = -2874.89472499)**

| | | | |
|---|---|---|---|
| 27 | 0.833041000 | 0.178862000 | 0.012751000 |
| 7 | 0.270148000 | -1.656758000 | 1.006618000 |
| 7 | -1.310832000 | 0.204388000 | -0.208901000 |
| 7 | 1.158087000 | -1.186767000 | -1.695017000 |
| 7 | 2.822750000 | -0.477862000 | 0.520619000 |
| 6 | -1.057596000 | -1.407046000 | 1.597872000 |
| 1 | -0.924644000 | -0.793180000 | 2.494190000 |
| 1 | -1.547549000 | -2.338728000 | 1.904807000 |
| 6 | -1.936568000 | -0.644393000 | 0.629940000 |
| 6 | -3.322834000 | -0.785750000 | 0.633623000 |
| 1 | -3.801398000 | -1.487410000 | 1.307997000 |
| 6 | -4.059593000 | -0.005801000 | -0.253692000 |
| 6 | -3.423318000 | 0.881945000 | -1.119274000 |
| 1 | -3.975622000 | 1.496906000 | -1.820447000 |
| 6 | -2.035634000 | 0.946725000 | -1.058192000 |
| 1 | -1.483395000 | 1.613345000 | -1.712174000 |
| 6 | 1.338067000 | -1.832661000 | 2.022350000 |
| 1 | 1.258443000 | -2.809860000 | 2.518358000 |
| 1 | 1.199064000 | -1.055747000 | 2.777341000 |
| 6 | 2.724701000 | -1.691726000 | 1.388961000 |
| 1 | 3.472189000 | -1.637467000 | 2.187493000 |
| 1 | 2.970299000 | -2.572967000 | 0.795706000 |
| 6 | 3.447101000 | -0.768854000 | -0.794026000 |
| 1 | 4.437325000 | -1.228119000 | -0.660468000 |
| 1 | 3.585940000 | 0.191395000 | -1.298912000 |
| 6 | 2.566268000 | -1.680789000 | -1.639592000 |
| 1 | 2.980569000 | -1.741213000 | -2.651726000 |
| 1 | 2.572442000 | -2.696423000 | -1.241961000 |
| 6 | 0.184579000 | -2.277417000 | -1.439334000 |
| 1 | 0.375090000 | -3.128557000 | -2.109171000 |
| 1 | -0.806531000 | -1.887526000 | -1.678558000 |
| 6 | 0.232379000 | -2.770158000 | 0.009662000 |
| 1 | -0.642745000 | -3.402167000 | 0.194388000 |
| 1 | 1.108176000 | -3.399952000 | 0.165871000 |
| 6 | 3.571484000 | 0.594041000 | 1.209626000 |
| 1 | 4.625671000 | 0.311306000 | 1.338275000 |
| 1 | 3.128667000 | 0.771975000 | 2.191178000 |
| 1 | 3.516651000 | 1.515167000 | 0.623488000 |
| 6 | 0.880926000 | -0.568036000 | -3.005073000 |
| 1 | 0.917553000 | -1.320090000 | -3.806630000 |
| 1 | 1.626396000 | 0.202716000 | -3.207781000 |
| 1 | -0.109358000 | -0.107502000 | -2.991348000 |
| 7 | 1.179978000 | 1.882775000 | -1.140534000 |
| 7 | 0.495653000 | 1.363990000 | 1.779491000 |
| 6 | 1.387846000 | 2.865297000 | -1.713305000 |
| 6 | 0.272009000 | 2.065175000 | 2.671615000 |
| 6 | 1.647976000 | 4.091675000 | -2.442343000 |
| 1 | 2.153335000 | 3.858469000 | -3.385171000 |
| 1 | 0.702107000 | 4.601755000 | -2.652035000 |
| 1 | 2.286386000 | 4.746606000 | -1.840483000 |
| 6 | -0.006812000 | 2.932983000 | 3.800925000 |
| 1 | 0.933263000 | 3.322925000 | 4.204295000 |
| 1 | -0.637965000 | 3.767168000 | 3.478365000 |
| 1 | -0.526394000 | 2.364063000 | 4.578916000 |
| 17 | -5.803673000 | -0.150928000 | -0.287204000 |



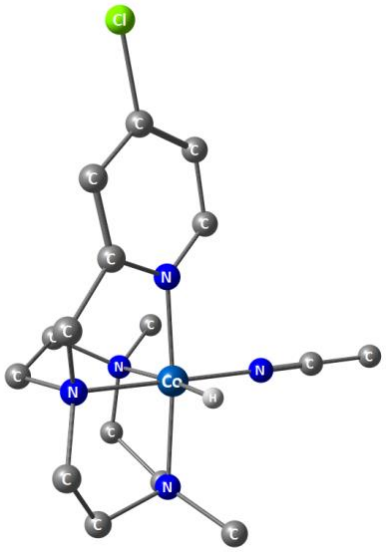
**$1^{Cl}$-$Co^{I}$ (triplet, 1 AC, G = -2742.20956267)**

| | | | |
|---|---|---|---|
| 27 | -0.826952000 | 0.268576000 | -0.404372000 |
| 7 | -0.271617000 | -1.863466000 | -0.512588000 |
| 7 | 1.249497000 | 0.424612000 | -0.457661000 |
| 7 | -1.063673000 | -0.227024000 | 1.727161000 |
| 7 | -2.862208000 | -0.624356000 | -0.517676000 |
| 6 | 1.019110000 | -1.867359000 | -1.213410000 |
| 1 | 0.823491000 | -1.706248000 | -2.279979000 |
| 1 | 1.545677000 | -2.827469000 | -1.112918000 |
| 6 | 1.894279000 | -0.736007000 | -0.721515000 |
| 6 | 3.270880000 | -0.878163000 | -0.569167000 |
| 1 | 3.749975000 | -1.829639000 | -0.774631000 |
| 6 | 4.001410000 | 0.229459000 | -0.142206000 |
| 6 | 3.359018000 | 1.437438000 | 0.121476000 |
| 1 | 3.901971000 | 2.315047000 | 0.454602000 |
| 6 | 1.979021000 | 1.481308000 | -0.054499000 |
| 1 | 1.428471000 | 2.396966000 | 0.139064000 |
| 6 | -1.363550000 | -2.467586000 | -1.299015000 |
| 1 | -1.282006000 | -3.566128000 | -1.342909000 |
| 1 | -1.272310000 | -2.082978000 | -2.319220000 |
| 6 | -2.737148000 | -2.087765000 | -0.737062000 |
| 1 | -3.508090000 | -2.437531000 | -1.435574000 |
| 1 | -2.917820000 | -2.612894000 | 0.202630000 |
| 6 | -3.398903000 | -0.282503000 | 0.814940000 |
| 1 | -4.386451000 | -0.746555000 | 0.982340000 |
| 1 | -3.535026000 | 0.803004000 | 0.832288000 |
| 6 | -2.457639000 | -0.699359000 | 1.946383000 |
| 1 | -2.848795000 | -0.300743000 | 2.891166000 |
| 1 | -2.454710000 | -1.785740000 | 2.053637000 |
| 6 | -0.067886000 | -1.298026000 | 1.932192000 |
| 1 | -0.176771000 | -1.760417000 | 2.927713000 |
| 1 | 0.918090000 | -0.828466000 | 1.895165000 |
| 6 | -0.164513000 | -2.399380000 | 0.867746000 |
| 1 | 0.717070000 | -3.047476000 | 0.955864000 |
| 1 | -1.031990000 | -3.031534000 | 1.064558000 |
| 6 | -3.662652000 | -0.003116000 | -1.579693000 |
| 1 | -4.701091000 | -0.375408000 | -1.581563000 |
| 1 | -3.210144000 | -0.224019000 | -2.551239000 |
| 1 | -3.676395000 | 1.081034000 | -1.441910000 |
| 6 | -0.762734000 | 0.927932000 | 2.582525000 |
| 1 | -0.778599000 | 0.659610000 | 3.652450000 |
| 1 | -1.504411000 | 1.711432000 | 2.406616000 |
| 1 | 0.225541000 | 1.322238000 | 2.330970000 |
| 7 | -1.306246000 | 2.138296000 | -0.477026000 |
| 6 | -1.576659000 | 3.271256000 | -0.523280000 |
| 6 | -1.913063000 | 4.686770000 | -0.568792000 |
| 1 | -2.020324000 | 5.079242000 | 0.448652000 |
| 1 | -1.123753000 | 5.247893000 | -1.081144000 |
| 1 | -2.857071000 | 4.834902000 | -1.104792000 |
| 17 | 5.739358000 | 0.096147000 | 0.072412000 |



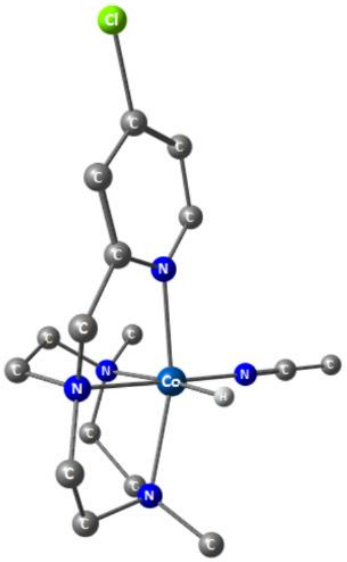
**$1^{Cl}$-$Co^{III}$-H (singlet, 1 AC, G =-2742.65635751)**

| | | | |
|---|---|---|---|
| 27 | -0.779647000 | 0.073063000 | -0.389673000 |
| 7 | -0.403811000 | -1.833986000 | -0.381121000 |
| 7 | 1.159104000 | 0.264446000 | -0.287741000 |
| 7 | -1.080183000 | -0.073558000 | 1.676353000 |
| 7 | -2.702418000 | -0.387968000 | -0.584512000 |
| 6 | 0.929794000 | -2.005104000 | -1.023974000 |
| 1 | 0.793222000 | -1.930661000 | -2.107163000 |
| 1 | 1.357011000 | -2.984984000 | -0.795635000 |
| 6 | 1.816307000 | -0.882381000 | -0.578727000 |
| 6 | 3.200140000 | -0.978283000 | -0.507130000 |
| 1 | 3.694329000 | -1.916760000 | -0.731862000 |
| 6 | 3.914225000 | 0.160450000 | -0.142472000 |
| 6 | 3.248900000 | 1.350741000 | 0.142338000 |
| 1 | 3.780141000 | 2.251668000 | 0.426186000 |
| 6 | 1.862474000 | 1.355575000 | 0.059362000 |
| 1 | 1.299928000 | 2.253438000 | 0.279581000 |
| 6 | -1.493507000 | -2.464925000 | -1.188128000 |
| 1 | -1.471792000 | -3.554389000 | -1.072979000 |
| 1 | -1.310312000 | -2.212351000 | -2.232689000 |
| 6 | -2.818429000 | -1.888908000 | -0.725418000 |
| 1 | -3.608171000 | -2.128092000 | -1.441645000 |
| 1 | -3.116153000 | -2.311751000 | 0.233119000 |
| 6 | -3.345095000 | 0.086524000 | 0.680356000 |
| 1 | -4.373942000 | -0.288745000 | 0.738964000 |
| 1 | -3.378747000 | 1.176463000 | 0.631301000 |
| 6 | -2.537145000 | -0.366970000 | 1.884512000 |
| 1 | -2.895383000 | 0.147443000 | 2.780969000 |
| 1 | -2.663519000 | -1.434654000 | 2.064463000 |
| 6 | -0.222878000 | -1.229872000 | 2.048055000 |
| 1 | -0.473517000 | -1.592203000 | 3.053550000 |
| 1 | 0.809403000 | -0.876233000 | 2.067017000 |
| 6 | -0.394006000 | -2.357995000 | 1.039726000 |
| 1 | 0.411514000 | -3.087828000 | 1.149967000 |
| 1 | -1.331193000 | -2.886668000 | 1.207630000 |
| 6 | -3.366974000 | 0.255726000 | -1.749420000 |
| 1 | -4.437608000 | 0.020370000 | -1.731937000 |
| 1 | -2.923642000 | -0.126401000 | -2.669413000 |
| 1 | -3.232103000 | 1.335670000 | -1.701178000 |
| 6 | -0.693042000 | 1.114208000 | 2.468072000 |
| 1 | -0.798182000 | 0.903174000 | 3.540167000 |
| 1 | -1.338631000 | 1.953153000 | 2.204113000 |
| 1 | 0.344489000 | 1.376957000 | 2.258030000 |
| 7 | -1.096594000 | 1.937920000 | -0.484131000 |
| 6 | -1.274091000 | 3.075542000 | -0.557310000 |
| 6 | -1.503589000 | 4.504638000 | -0.637531000 |
| 1 | -1.619316000 | 4.913143000 | 0.371740000 |
| 1 | -0.652765000 | 4.985946000 | -1.130421000 |
| 1 | -2.413856000 | 4.696235000 | -1.215150000 |
| 1 | -0.626558000 | 0.071590000 | -1.841319000 |
| 17 | 5.656155000 | 0.091293000 | -0.038826000 |



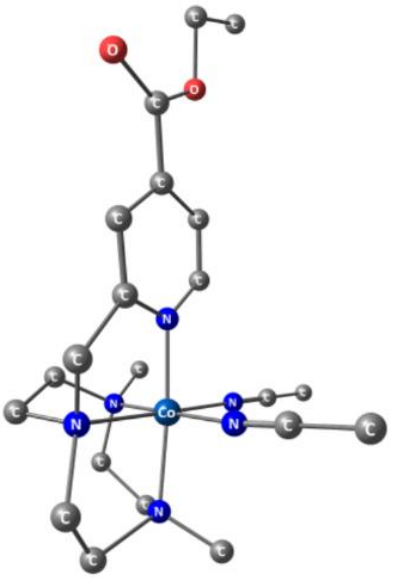
**$1^{Cl}$-$Co^{II}$-H (doublet, 1 AC, G =-2742.78488613)**

| | | | |
|---|---|---|---|
| 27 | -0.845576000 | 0.180802000 | -0.434444000 |
| 7 | -0.266296000 | -1.798663000 | -0.342163000 |
| 7 | 1.343643000 | 0.407825000 | -0.271824000 |
| 7 | -1.144312000 | 0.000354000 | 1.620347000 |
| 7 | -2.897836000 | -0.713620000 | -0.548365000 |
| 6 | 1.051473000 | -1.886042000 | -1.004670000 |
| 1 | 0.889239000 | -1.791512000 | -2.083197000 |
| 1 | 1.532246000 | -2.854805000 | -0.817201000 |
| 6 | 1.953372000 | -0.755461000 | -0.563050000 |
| 6 | 3.338906000 | -0.905802000 | -0.501424000 |
| 1 | 3.801043000 | -1.861075000 | -0.726282000 |
| 6 | 4.096662000 | 0.205465000 | -0.142158000 |
| 6 | 3.481559000 | 1.420756000 | 0.149688000 |
| 1 | 4.050480000 | 2.299260000 | 0.432668000 |
| 6 | 2.091143000 | 1.464266000 | 0.071638000 |
| 1 | 1.555178000 | 2.381941000 | 0.297469000 |
| 6 | -1.306580000 | -2.563698000 | -1.076239000 |
| 1 | -1.155551000 | -3.646193000 | -0.955985000 |
| 1 | -1.197950000 | -2.315750000 | -2.133967000 |
| 6 | -2.712278000 | -2.184633000 | -0.598451000 |
| 1 | -3.443522000 | -2.640478000 | -1.277548000 |
| 1 | -2.907975000 | -2.609690000 | 0.387556000 |
| 6 | -3.478593000 | -0.234700000 | 0.718674000 |
| 1 | -4.450112000 | -0.712905000 | 0.929534000 |
| 1 | -3.654923000 | 0.838717000 | 0.602550000 |
| 6 | -2.540146000 | -0.481166000 | 1.893469000 |
| 1 | -2.935133000 | 0.022168000 | 2.782622000 |
| 1 | -2.502365000 | -1.544800000 | 2.133267000 |
| 6 | -0.144816000 | -1.021763000 | 2.033118000 |
| 1 | -0.335045000 | -1.352258000 | 3.064576000 |
| 1 | 0.833991000 | -0.541896000 | 2.011504000 |
| 6 | -0.173725000 | -2.222599000 | 1.092817000 |
| 1 | 0.724502000 | -2.829382000 | 1.249428000 |
| 1 | -1.026655000 | -2.863265000 | 1.317907000 |
| 6 | -3.676415000 | -0.237815000 | -1.696571000 |
| 1 | -4.715926000 | -0.604069000 | -1.661996000 |
| 1 | -3.211113000 | -0.587825000 | -2.621447000 |
| 1 | -3.686275000 | 0.855597000 | -1.705697000 |
| 6 | -0.896183000 | 1.252138000 | 2.366348000 |
| 1 | -0.919595000 | 1.067864000 | 3.449888000 |
| 1 | -1.666342000 | 1.982407000 | 2.113993000 |
| 1 | 0.080000000 | 1.655366000 | 2.091129000 |
| 7 | -1.340491000 | 2.023573000 | -0.542426000 |
| 6 | -1.624727000 | 3.144092000 | -0.618942000 |
| 6 | -1.981831000 | 4.550271000 | -0.713466000 |
| 1 | -2.113742000 | 4.968555000 | 0.289984000 |
| 1 | -1.189123000 | 5.102025000 | -1.229628000 |
| 1 | -2.916452000 | 4.660590000 | -1.273401000 |
| 1 | -0.683178000 | 0.176662000 | -1.960560000 |
| 17 | 5.843821000 | 0.068644000 | -0.050049000 |



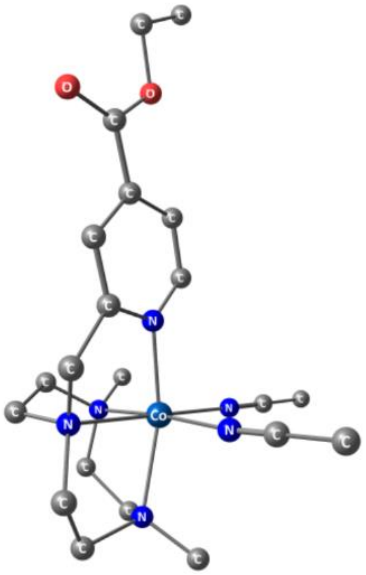
**$1^{CO2Et}$-$Co^{III}$ (singlet, 2 AC, G = -2682.31692582)**

| | | | |
|---|---|---|---|
| 27 | 1.438630000 | 0.072086000 | -0.009891000 |
| 7 | 1.339694000 | -1.851071000 | 0.282544000 |
| 7 | -0.522518000 | -0.037240000 | -0.099256000 |
| 7 | 1.710461000 | -0.323003000 | -1.942166000 |
| 7 | 3.417392000 | -0.065374000 | 0.213062000 |
| 6 | 0.038930000 | -2.121217000 | 0.970137000 |
| 1 | 0.162463000 | -1.926609000 | 2.038174000 |
| 1 | -0.242827000 | -3.169458000 | 0.850998000 |
| 6 | -1.000661000 | -1.190909000 | 0.422446000 |
| 6 | -2.364368000 | -1.436474000 | 0.500926000 |
| 1 | -2.723542000 | -2.373916000 | 0.909773000 |
| 6 | -3.255033000 | -0.457187000 | 0.059415000 |
| 6 | -2.749615000 | 0.739526000 | -0.455235000 |
| 1 | -3.402773000 | 1.529535000 | -0.803557000 |
| 6 | -1.373984000 | 0.913868000 | -0.519041000 |
| 1 | -0.943445000 | 1.825076000 | -0.911551000 |
| 6 | 2.517598000 | -2.191032000 | 1.145600000 |
| 1 | 2.652761000 | -3.276581000 | 1.175909000 |
| 1 | 2.299974000 | -1.836916000 | 2.152726000 |
| 6 | 3.747094000 | -1.498935000 | 0.585081000 |
| 1 | 4.544205000 | -1.497129000 | 1.331085000 |
| 1 | 4.133241000 | -2.007524000 | -0.296396000 |
| 6 | 3.968272000 | 0.292646000 | -1.131030000 |
| 1 | 5.032367000 | 0.036823000 | -1.171673000 |
| 1 | 3.865826000 | 1.372838000 | -1.245230000 |
| 6 | 3.196838000 | -0.443362000 | -2.202229000 |
| 1 | 3.418208000 | -0.022804000 | -3.185056000 |
| 1 | 3.461099000 | -1.498495000 | -2.236680000 |
| 6 | 1.027284000 | -1.635249000 | -2.170026000 |
| 1 | 1.340404000 | -2.042918000 | -3.136398000 |
| 1 | -0.045333000 | -1.446772000 | -2.208569000 |
| 6 | 1.392201000 | -2.580047000 | -1.045101000 |
| 1 | 0.704022000 | -3.425974000 | -1.015063000 |
| 1 | 2.394948000 | -2.982682000 | -1.171590000 |
| 6 | 4.007119000 | 0.846772000 | 1.234396000 |
| 1 | 5.097847000 | 0.788026000 | 1.157771000 |
| 1 | 3.699467000 | 0.529279000 | 2.229051000 |
| 1 | 3.683883000 | 1.870293000 | 1.051166000 |
| 6 | 1.142977000 | 0.681971000 | -2.885346000 |
| 1 | 1.251669000 | 0.292916000 | -3.902811000 |
| 1 | 1.689709000 | 1.618867000 | -2.796547000 |
| 1 | 0.086810000 | 0.838865000 | -2.675294000 |
| 7 | 1.502911000 | 1.965656000 | -0.283875000 |
| 7 | 1.177379000 | 0.451457000 | 1.858415000 |
| 6 | 1.527305000 | 3.114630000 | -0.369794000 |
| 6 | 0.932124000 | 0.773347000 | 2.937226000 |
| 6 | 1.564322000 | 4.555291000 | -0.495983000 |
| 1 | 1.594196000 | 4.825291000 | -1.556703000 |
| 1 | 0.670099000 | 4.984225000 | -0.032384000 |
| 1 | 2.458200000 | 4.939024000 | 0.006824000 |
| 6 | 0.634357000 | 1.154446000 | 4.300902000 |
| 1 | 1.542444000 | 1.536177000 | 4.778763000 |
| 1 | -0.136331000 | 1.932384000 | 4.300315000 |
| 1 | 0.271387000 | 0.278139000 | 4.848127000 |
| 6 | -4.728527000 | -0.726584000 | 0.166561000 |
| 8 | -5.182132000 | -1.771604000 | 0.601202000 |
| 8 | -5.459228000 | 0.302405000 | -0.258956000 |
| 6 | -6.912199000 | 0.163473000 | -0.187145000 |
| 1 | -7.178682000 | -0.056613000 | 0.850144000 |
| 1 | -7.200351000 | -0.683939000 | -0.815460000 |
| 6 | -7.516417000 | 1.463679000 | -0.667231000 |
| 1 | -7.231760000 | 1.674969000 | -1.703895000 |
| 1 | -7.204447000 | 2.302267000 | -0.034883000 |
| 1 | -8.608782000 | 1.385708000 | -0.620255000 |



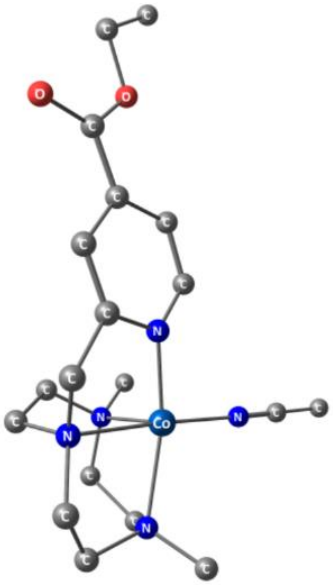
**$1^{CO2Et}$-$Co^{II}$ (quartet, 1 AC, G = -2682.50288535)**

| | | | |
|---|---|---|---|
| 27 | 1.457257000 | 0.174648000 | -0.044151000 |
| 7 | 1.155424000 | -1.887808000 | 0.552926000 |
| 7 | -0.664453000 | 0.078921000 | 0.066710000 |
| 7 | 1.694401000 | -0.725284000 | -1.999478000 |
| 7 | 3.560616000 | -0.364213000 | 0.166338000 |
| 6 | -0.108395000 | -1.921556000 | 1.315883000 |
| 1 | 0.091385000 | -1.545940000 | 2.325070000 |
| 1 | -0.496292000 | -2.942310000 | 1.414153000 |
| 6 | -1.141002000 | -1.021042000 | 0.680162000 |
| 6 | -2.508039000 | -1.272533000 | 0.757262000 |
| 1 | -2.872305000 | -2.170073000 | 1.244770000 |
| 6 | -3.399750000 | -0.355002000 | 0.196114000 |
| 6 | -2.894462000 | 0.789318000 | -0.429625000 |
| 1 | -3.549289000 | 1.525370000 | -0.879181000 |
| 6 | -1.515825000 | 0.963444000 | -0.473003000 |
| 1 | -1.072131000 | 1.829719000 | -0.952684000 |
| 6 | 2.340281000 | -2.177849000 | 1.400222000 |
| 1 | 2.391061000 | -3.244550000 | 1.658991000 |
| 1 | 2.222124000 | -1.610054000 | 2.325745000 |
| 6 | 3.636993000 | -1.757823000 | 0.706159000 |
| 1 | 4.457594000 | -1.830717000 | 1.427497000 |
| 1 | 3.878982000 | -2.442457000 | -0.107047000 |
| 6 | 4.035417000 | -0.279435000 | -1.239757000 |
| 1 | 5.066854000 | -0.652007000 | -1.321995000 |
| 1 | 4.038790000 | 0.780144000 | -1.510336000 |
| 6 | 3.136986000 | -1.058687000 | -2.196819000 |
| 1 | 3.435024000 | -0.831332000 | -3.226127000 |
| 1 | 3.274241000 | -2.132663000 | -2.066945000 |
| 6 | 0.841414000 | -1.937341000 | -1.939403000 |
| 1 | 1.014342000 | -2.576391000 | -2.817103000 |
| 1 | -0.196379000 | -1.598698000 | -1.974581000 |
| 6 | 1.092282000 | -2.747798000 | -0.666500000 |
| 1 | 0.294953000 | -3.490777000 | -0.557667000 |
| 1 | 2.026371000 | -3.304709000 | -0.744044000 |
| 6 | 4.333850000 | 0.562462000 | 1.015100000 |
| 1 | 5.406667000 | 0.325957000 | 0.974046000 |
| 1 | 3.990079000 | 0.479569000 | 2.047500000 |
| 1 | 4.180171000 | 1.588402000 | 0.672386000 |
| 6 | 1.219610000 | 0.173679000 | -3.070992000 |
| 1 | 1.218834000 | -0.344338000 | -4.040437000 |
| 1 | 1.876675000 | 1.043102000 | -3.132987000 |
| 1 | 0.205512000 | 0.511047000 | -2.843579000 |
| 7 | 1.751114000 | 2.167223000 | -0.634349000 |
| 7 | 1.343228000 | 0.937843000 | 1.983041000 |
| 6 | 1.888133000 | 3.274538000 | -0.937083000 |
| 6 | 1.202325000 | 1.398181000 | 3.034681000 |
| 6 | 2.064040000 | 4.661868000 | -1.322863000 |
| 1 | 2.395664000 | 4.713449000 | -2.364845000 |
| 1 | 1.113911000 | 5.195304000 | -1.215942000 |
| 1 | 2.816308000 | 5.128299000 | -0.678432000 |
| 6 | 1.033353000 | 1.967582000 | 4.359320000 |
| 1 | 1.975750000 | 2.415513000 | 4.690409000 |
| 1 | 0.255652000 | 2.737821000 | 4.332370000 |
| 1 | 0.738894000 | 1.180924000 | 5.061424000 |
| 6 | -4.870141000 | -0.635805000 | 0.279812000 |
| 8 | -5.333183000 | -1.643485000 | 0.789030000 |
| 8 | -5.600688000 | 0.339306000 | -0.264719000 |
| 6 | -7.051172000 | 0.180716000 | -0.246466000 |
| 1 | -7.297377000 | -0.756125000 | -0.753893000 |
| 1 | -7.371518000 | 0.112933000 | 0.797100000 |
| 6 | -7.644334000 | 1.381911000 | -0.948683000 |
| 1 | -7.301816000 | 1.440805000 | -1.987817000 |
| 1 | -7.378739000 | 2.312266000 | -0.434294000 |
| 1 | -8.736666000 | 1.290715000 | -0.951376000 |



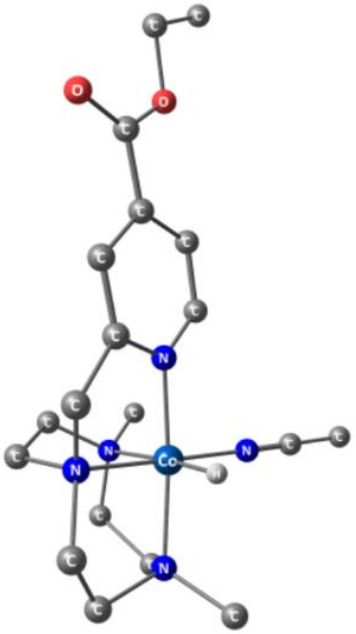
**$1^{CO2Et}$-$Co^{I}$ (triplet, 2 AC, G =-2549.81967923)**

| | | | |
|---|---|---|---|
| 27 | -1.531621000 | 0.216905000 | -0.433821000 |
| 7 | -1.294563000 | -1.938151000 | -0.392421000 |
| 7 | 0.434596000 | 0.163338000 | -0.661156000 |
| 7 | -1.661896000 | -0.006346000 | 1.724811000 |
| 7 | -3.652505000 | -0.337438000 | -0.326928000 |
| 6 | -0.075563000 | -2.144417000 | -1.196952000 |
| 1 | -0.357471000 | -2.021662000 | -2.249579000 |
| 1 | 0.336826000 | -3.155134000 | -1.071992000 |
| 6 | 0.952980000 | -1.099203000 | -0.842616000 |
| 6 | 2.293496000 | -1.379988000 | -0.704779000 |
| 1 | 2.645336000 | -2.398849000 | -0.831574000 |
| 6 | 3.212309000 | -0.346641000 | -0.392668000 |
| 6 | 2.679946000 | 0.955946000 | -0.232102000 |
| 1 | 3.324118000 | 1.795649000 | 0.003884000 |
| 6 | 1.323059000 | 1.160732000 | -0.372470000 |
| 1 | 0.892978000 | 2.149410000 | -0.247403000 |
| 6 | -2.521826000 | -2.453371000 | -1.027848000 |
| 1 | -2.594894000 | -3.549964000 | -0.958399000 |
| 1 | -2.470051000 | -2.184562000 | -2.087178000 |
| 6 | -3.767776000 | -1.820780000 | -0.403583000 |
| 1 | -4.645432000 | -2.101904000 | -0.998097000 |
| 1 | -3.935658000 | -2.220419000 | 0.597424000 |
| 6 | -4.049049000 | 0.200542000 | 0.992710000 |
| 1 | -5.074046000 | -0.105256000 | 1.256883000 |
| 1 | -4.035146000 | 1.291030000 | 0.909358000 |
| 6 | -3.087933000 | -0.246268000 | 2.094379000 |
| 1 | -3.331462000 | 0.293195000 | 3.017073000 |
| 1 | -3.227182000 | -1.306454000 | 2.312016000 |
| 6 | -0.804973000 | -1.192399000 | 1.965333000 |
| 1 | -0.901131000 | -1.539943000 | 3.005764000 |
| 1 | 0.228542000 | -0.870089000 | 1.818542000 |
| 6 | -1.127614000 | -2.361060000 | 1.022063000 |
| 1 | -0.321026000 | -3.100471000 | 1.101625000 |
| 1 | -2.040354000 | -2.863196000 | 1.346190000 |
| 6 | -4.418925000 | 0.297134000 | -1.411994000 |
| 1 | -5.495973000 | 0.088942000 | -1.317834000 |
| 1 | -4.068065000 | -0.088773000 | -2.373564000 |
| 1 | -4.262414000 | 1.377983000 | -1.390912000 |
| 6 | -1.127608000 | 1.163431000 | 2.440917000 |
| 1 | -1.084051000 | 0.982634000 | 3.526212000 |
| 1 | -1.769724000 | 2.026724000 | 2.251866000 |
| 1 | -0.122156000 | 1.387242000 | 2.075840000 |
| 7 | -1.831520000 | 2.233039000 | -0.597655000 |
| 6 | -1.974312000 | 3.379926000 | -0.681558000 |
| 6 | -2.159946000 | 4.818204000 | -0.771816000 |
| 1 | -2.253889000 | 5.240560000 | 0.234147000 |
| 1 | -1.301351000 | 5.274395000 | -1.275058000 |
| 1 | -3.069261000 | 5.039087000 | -1.340426000 |
| 6 | 4.630616000 | -0.664346000 | -0.241405000 |
| 8 | 5.115153000 | -1.790574000 | -0.373988000 |
| 8 | 5.385000000 | 0.419378000 | 0.068703000 |
| 6 | 6.805947000 | 0.199465000 | 0.242236000 |
| 1 | 6.952671000 | -0.525583000 | 1.049180000 |
| 1 | 7.211223000 | -0.225635000 | -0.681530000 |
| 6 | 7.439351000 | 1.535396000 | 0.569759000 |
| 1 | 7.024069000 | 1.954728000 | 1.493407000 |
| 1 | 7.287387000 | 2.255202000 | -0.242666000 |
| 1 | 8.518264000 | 1.399337000 | 0.710032000 |



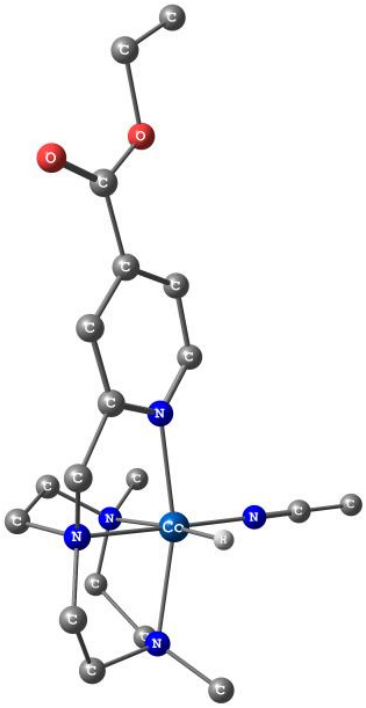
**$1^{CO2Et}$-$Co^{III}$-H (singlet, 1 AC, G =-2550.26472066)**

| | | | |
|---|---|---|---|
| 27 | -1.523433000 | 0.101333000 | -0.388582000 |
| 7 | -1.405713000 | -1.837208000 | -0.290891000 |
| 7 | 0.422540000 | 0.033666000 | -0.347008000 |
| 7 | -1.781063000 | 0.098165000 | 1.687643000 |
| 7 | -3.495921000 | -0.102844000 | -0.514611000 |
| 6 | -0.129250000 | -2.215741000 | -0.959936000 |
| 1 | -0.292909000 | -2.172927000 | -2.040876000 |
| 1 | 0.170890000 | -3.233325000 | -0.695498000 |
| 6 | 0.913016000 | -1.203789000 | -0.596266000 |
| 6 | 2.274436000 | -1.470186000 | -0.555067000 |
| 1 | 2.636871000 | -2.474731000 | -0.740916000 |
| 6 | 3.161057000 | -0.428467000 | -0.274043000 |
| 6 | 2.648150000 | 0.849629000 | -0.035536000 |
| 1 | 3.294951000 | 1.689215000 | 0.186556000 |
| 6 | 1.272378000 | 1.039024000 | -0.076692000 |
| 1 | 0.836282000 | 2.010900000 | 0.112125000 |
| 6 | -2.596427000 | -2.351730000 | -1.034764000 |
| 1 | -2.718540000 | -3.427164000 | -0.863980000 |
| 1 | -2.415569000 | -2.176427000 | -2.095580000 |
| 6 | -3.815401000 | -1.579547000 | -0.568104000 |
| 1 | -4.654735000 | -1.746954000 | -1.247446000 |
| 1 | -4.133631000 | -1.906635000 | 0.420348000 |
| 6 | -4.032793000 | 0.518977000 | 0.735568000 |
| 1 | -5.100042000 | 0.287542000 | 0.836733000 |
| 1 | -3.924214000 | 1.599665000 | 0.626127000 |
| 6 | -3.258300000 | 0.022138000 | 1.945273000 |
| 1 | -3.513888000 | 0.628491000 | 2.819073000 |
| 1 | -3.528797000 | -1.005772000 | 2.187541000 |
| 6 | -1.075931000 | -1.143734000 | 2.100132000 |
| 1 | -1.343709000 | -1.420650000 | 3.128094000 |
| 1 | -0.006111000 | -0.929681000 | 2.078635000 |
| 6 | -1.417426000 | -2.287819000 | 1.155274000 |
| 1 | -0.703837000 | -3.105051000 | 1.283631000 |
| 1 | -2.406292000 | -2.688379000 | 1.373826000 |
| 6 | -4.100137000 | 0.563131000 | -1.699548000 |
| 1 | -5.192040000 | 0.478058000 | -1.646918000 |
| 1 | -3.738287000 | 0.076058000 | -2.605547000 |
| 1 | -3.818388000 | 1.615378000 | -1.715388000 |
| 6 | -1.211398000 | 1.259685000 | 2.405295000 |
| 1 | -1.313959000 | 1.120026000 | 3.489139000 |
| 1 | -1.742251000 | 2.165793000 | 2.109690000 |
| 1 | -0.153709000 | 1.364344000 | 2.160159000 |
| 7 | -1.586986000 | 1.983619000 | -0.565827000 |
| 6 | -1.598644000 | 3.130417000 | -0.691276000 |
| 6 | -1.614981000 | 4.572181000 | -0.840306000 |
| 1 | -1.637277000 | 5.042346000 | 0.148158000 |
| 1 | -0.716902000 | 4.894428000 | -1.377253000 |
| 1 | -2.503721000 | 4.870888000 | -1.405805000 |
| 1 | -1.414626000 | 0.010838000 | -1.841836000 |
| 6 | 4.629554000 | -0.728872000 | -0.235654000 |
| 8 | 5.088529000 | -1.841221000 | -0.437056000 |
| 8 | 5.359440000 | 0.352114000 | 0.041589000 |
| 6 | 6.807889000 | 0.179395000 | 0.106486000 |
| 1 | 7.144184000 | -0.220475000 | -0.854060000 |
| 1 | 7.026434000 | -0.551370000 | 0.890086000 |
| 6 | 7.412571000 | 1.532856000 | 0.404708000 |
| 1 | 7.059615000 | 1.921946000 | 1.366228000 |
| 1 | 7.169992000 | 2.255756000 | -0.382008000 |
| 1 | 8.502957000 | 1.431659000 | 0.454003000 |



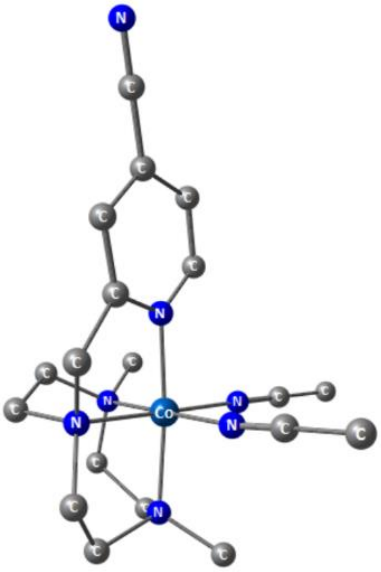
**$1^{CO2Et}$-$Co^{II}$-H (doublet, 1 AC, G =-2550.39253824)**

| | | | |
|---|---|---|---|
| 27 | -1.584181000 | 0.199110000 | -0.435054000 |
| 7 | -1.261193000 | -1.831021000 | -0.250656000 |
| 7 | 0.607674000 | 0.157318000 | -0.294579000 |
| 7 | -1.893411000 | 0.154040000 | 1.626443000 |
| 7 | -3.732114000 | -0.428636000 | -0.507720000 |
| 6 | 0.031368000 | -2.117677000 | -0.906678000 |
| 1 | -0.127010000 | -2.072571000 | -1.989151000 |
| 1 | 0.391503000 | -3.124644000 | -0.659923000 |
| 6 | 1.070489000 | -1.082153000 | -0.542649000 |
| 6 | 2.431367000 | -1.378147000 | -0.517020000 |
| 1 | 2.777205000 | -2.389624000 | -0.701536000 |
| 6 | 3.344074000 | -0.352728000 | -0.253394000 |
| 6 | 2.858549000 | 0.937712000 | -0.012030000 |
| 1 | 3.526768000 | 1.764003000 | 0.198851000 |
| 6 | 1.481501000 | 1.139914000 | -0.038029000 |
| 1 | 1.056913000 | 2.121105000 | 0.154142000 |
| 6 | -2.394606000 | -2.489713000 | -0.949771000 |
| 1 | -2.383379000 | -3.576005000 | -0.779588000 |
| 1 | -2.260069000 | -2.305981000 | -2.017457000 |
| 6 | -3.737631000 | -1.911512000 | -0.490546000 |
| 1 | -4.525817000 | -2.300354000 | -1.147214000 |
| 1 | -3.976979000 | -2.264415000 | 0.513972000 |
| 6 | -4.240544000 | 0.179505000 | 0.735133000 |
| 1 | -5.265913000 | -0.156288000 | 0.964491000 |
| 1 | -4.273270000 | 1.260559000 | 0.570147000 |
| 6 | -3.337182000 | -0.133810000 | 1.920948000 |
| 1 | -3.659907000 | 0.454510000 | 2.786710000 |
| 1 | -3.434573000 | -1.181844000 | 2.206693000 |
| 6 | -1.028158000 | -0.965098000 | 2.086296000 |
| 1 | -1.252254000 | -1.220763000 | 3.132116000 |
| 1 | 0.002892000 | -0.612866000 | 2.042557000 |
| 6 | -1.216424000 | -2.194765000 | 1.203288000 |
| 1 | -0.403571000 | -2.905288000 | 1.387895000 |
| 1 | -2.144544000 | -2.707060000 | 1.459022000 |
| 6 | -4.448747000 | 0.092801000 | -1.676478000 |
| 1 | -5.527579000 | -0.129188000 | -1.623715000 |
| 1 | -4.041615000 | -0.358374000 | -2.584790000 |
| 1 | -4.311979000 | 1.176031000 | -1.735819000 |
| 6 | -1.485889000 | 1.397568000 | 2.312983000 |
| 1 | -1.529497000 | 1.268707000 | 3.403905000 |
| 1 | -2.156465000 | 2.208453000 | 2.024336000 |
| 1 | -0.466412000 | 1.658793000 | 2.023295000 |
| 7 | -1.848731000 | 2.081722000 | -0.620035000 |
| 6 | -2.002857000 | 3.224692000 | -0.729302000 |
| 6 | -2.203099000 | 4.658949000 | -0.858242000 |
| 1 | -2.302086000 | 5.110081000 | 0.134795000 |
| 1 | -1.349235000 | 5.111497000 | -1.373117000 |
| 1 | -3.113322000 | 4.857899000 | -1.433736000 |
| 1 | -1.427870000 | 0.104934000 | -1.958573000 |
| 6 | 4.804336000 | -0.678959000 | -0.233584000 |
| 8 | 5.248172000 | -1.798616000 | -0.436060000 |
| 8 | 5.561094000 | 0.390666000 | 0.030308000 |
| 6 | 7.004656000 | 0.191919000 | 0.075951000 |
| 1 | 7.324657000 | -0.207516000 | -0.890580000 |
| 1 | 7.222694000 | -0.546775000 | 0.852484000 |
| 6 | 7.636010000 | 1.533652000 | 0.374698000 |
| 1 | 7.298422000 | 1.923536000 | 1.341447000 |
| 1 | 7.397033000 | 2.264783000 | -0.405574000 |
| 1 | 8.725147000 | 1.415424000 | 0.412784000 |



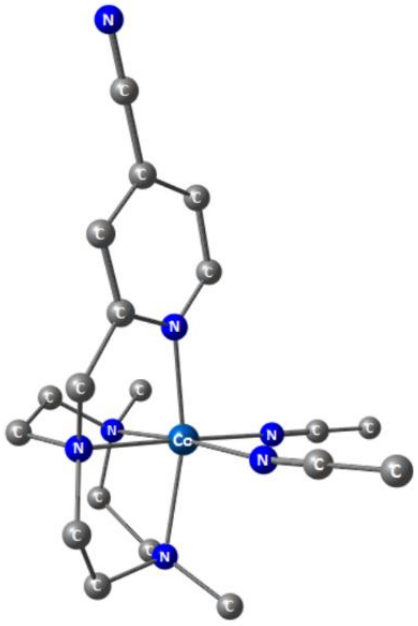
**$1^{CN}$-$Co^{III}$ (singlet, 2 AC, G = -2507.34225562)**

| | | | |
|---|---|---|---|
| 27 | 0.676697000 | 0.023798000 | 0.000872000 |
| 7 | 0.278643000 | -1.576507000 | 1.036684000 |
| 7 | -1.281010000 | 0.137188000 | -0.200305000 |
| 7 | 0.923334000 | -1.164871000 | -1.581937000 |
| 7 | 2.604326000 | -0.275992000 | 0.416367000 |
| 6 | -1.061016000 | -1.365806000 | 1.666292000 |
| 1 | -0.935645000 | -0.742557000 | 2.555042000 |
| 1 | -1.488617000 | -2.319566000 | 1.982310000 |
| 6 | -1.937592000 | -0.648475000 | 0.685211000 |
| 6 | -3.323088000 | -0.727797000 | 0.696019000 |
| 1 | -3.825558000 | -1.381935000 | 1.399117000 |
| 6 | -4.039896000 | 0.051703000 | -0.219030000 |
| 6 | -3.355229000 | 0.891765000 | -1.105555000 |
| 1 | -3.881213000 | 1.515768000 | -1.818081000 |
| 6 | -1.968185000 | 0.905028000 | -1.061895000 |
| 1 | -1.398355000 | 1.533717000 | -1.732748000 |
| 6 | 1.374661000 | -1.682106000 | 2.054636000 |
| 1 | 1.334759000 | -2.662402000 | 2.539689000 |
| 1 | 1.206096000 | -0.911027000 | 2.805698000 |
| 6 | 2.699518000 | -1.470624000 | 1.347235000 |
| 1 | 3.491178000 | -1.290892000 | 2.076943000 |
| 1 | 2.987766000 | -2.345439000 | 0.766845000 |
| 6 | 3.231199000 | -0.565395000 | -0.910452000 |
| 1 | 4.245768000 | -0.949815000 | -0.760239000 |
| 1 | 3.294773000 | 0.379477000 | -1.451694000 |
| 6 | 2.380966000 | -1.566395000 | -1.657891000 |
| 1 | 2.679603000 | -1.609395000 | -2.706689000 |
| 1 | 2.487376000 | -2.570273000 | -1.251284000 |
| 6 | 0.058403000 | -2.355238000 | -1.310149000 |
| 1 | 0.328572000 | -3.163441000 | -1.997254000 |
| 1 | -0.972949000 | -2.068296000 | -1.513351000 |
| 6 | 0.250475000 | -2.789157000 | 0.127206000 |
| 1 | -0.557647000 | -3.453255000 | 0.438475000 |
| 1 | 1.185268000 | -3.330512000 | 0.258839000 |
| 6 | 3.305043000 | 0.882412000 | 1.041817000 |
| 1 | 4.376022000 | 0.657124000 | 1.076930000 |
| 1 | 2.935917000 | 1.028380000 | 2.055430000 |
| 1 | 3.140389000 | 1.781408000 | 0.450068000 |
| 6 | 0.526032000 | -0.577872000 | -2.893224000 |
| 1 | 0.590528000 | -1.365347000 | -3.651220000 |
| 1 | 1.204640000 | 0.231861000 | -3.154143000 |
| 1 | -0.498530000 | -0.214306000 | -2.846721000 |
| 7 | 1.036723000 | 1.612346000 | -1.005011000 |
| 7 | 0.437386000 | 1.171111000 | 1.523898000 |
| 6 | 1.242706000 | 2.612614000 | -1.539076000 |
| 6 | 0.227453000 | 1.946898000 | 2.349535000 |
| 6 | 1.511094000 | 3.858199000 | -2.223562000 |
| 1 | 2.034982000 | 3.649207000 | -3.162236000 |
| 1 | 0.565586000 | 4.368004000 | -2.435884000 |
| 1 | 2.135931000 | 4.493771000 | -1.587529000 |
| 6 | -0.022988000 | 2.907340000 | 3.401923000 |
| 1 | 0.932154000 | 3.257495000 | 3.806787000 |
| 1 | -0.582577000 | 3.755512000 | 2.994323000 |
| 1 | -0.606411000 | 2.430248000 | 4.196160000 |
| 6 | -5.473181000 | -0.012116000 | -0.247125000 |
| 7 | -6.633529000 | -0.062692000 | -0.270929000 |



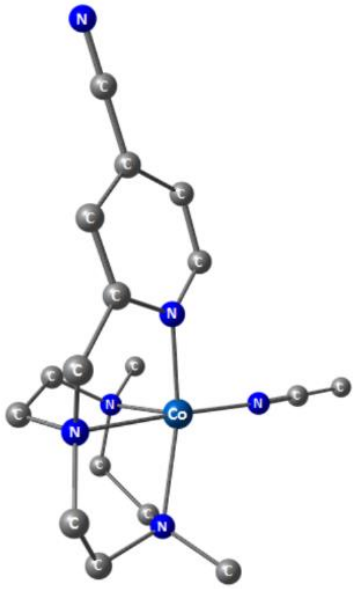
**$1^{CN}$-$Co^{II}$ (quartet, 2 AC, G = -2507.52934363)**

| | | | |
|---|---|---|---|
| 27 | 0.696974000 | 0.104985000 | -0.062203000 |
| 7 | 0.060924000 | -1.566758000 | 1.160782000 |
| 7 | -1.441612000 | 0.255480000 | -0.215251000 |
| 7 | 1.010532000 | -1.449256000 | -1.526754000 |
| 7 | 2.676551000 | -0.507835000 | 0.620807000 |
| 6 | -1.263512000 | -1.214865000 | 1.707685000 |
| 1 | -1.116325000 | -0.523130000 | 2.543320000 |
| 1 | -1.789244000 | -2.094719000 | 2.096778000 |
| 6 | -2.105723000 | -0.513139000 | 0.668453000 |
| 6 | -3.494246000 | -0.612740000 | 0.646956000 |
| 1 | -4.011400000 | -1.247919000 | 1.357557000 |
| 6 | -4.198527000 | 0.121412000 | -0.315254000 |
| 6 | -3.503210000 | 0.929285000 | -1.225385000 |
| 1 | -4.022612000 | 1.506771000 | -1.981145000 |
| 6 | -2.116651000 | 0.959962000 | -1.134817000 |
| 1 | -1.524005000 | 1.559091000 | -1.818117000 |
| 6 | 1.105192000 | -1.636310000 | 2.215853000 |
| 1 | 0.982976000 | -2.535774000 | 2.834828000 |
| 1 | 0.972410000 | -0.761820000 | 2.856956000 |
| 6 | 2.508958000 | -1.617531000 | 1.609985000 |
| 1 | 3.238764000 | -1.506775000 | 2.418814000 |
| 1 | 2.731016000 | -2.566774000 | 1.121172000 |
| 6 | 3.302906000 | -0.975645000 | -0.643029000 |
| 1 | 4.275037000 | -1.447962000 | -0.440136000 |
| 1 | 3.481702000 | -0.088861000 | -1.256899000 |
| 6 | 2.407969000 | -1.959828000 | -1.391217000 |
| 1 | 2.834200000 | -2.144595000 | -2.383121000 |
| 1 | 2.385812000 | -2.922999000 | -0.880705000 |
| 6 | -0.000146000 | -2.478099000 | -1.178654000 |
| 1 | 0.174465000 | -3.401565000 | -1.748886000 |
| 1 | -0.973392000 | -2.082225000 | -1.477012000 |
| 6 | 0.004749000 | -2.798220000 | 0.316899000 |
| 1 | -0.894793000 | -3.374110000 | 0.558073000 |
| 1 | 0.855604000 | -3.430800000 | 0.570624000 |
| 6 | 3.472191000 | 0.590459000 | 1.202364000 |
| 1 | 4.503766000 | 0.264299000 | 1.396921000 |
| 1 | 3.016375000 | 0.909666000 | 2.141310000 |
| 1 | 3.488497000 | 1.436676000 | 0.511600000 |
| 6 | 0.772139000 | -0.950295000 | -2.896841000 |
| 1 | 0.798786000 | -1.776542000 | -3.621258000 |
| 1 | 1.544190000 | -0.224232000 | -3.157063000 |
| 1 | -0.204862000 | -0.462939000 | -2.944570000 |
| 7 | 1.352553000 | 1.716582000 | -1.217563000 |
| 7 | 0.472872000 | 1.551861000 | 1.536905000 |
| 6 | 1.697680000 | 2.622248000 | -1.847769000 |
| 6 | 0.272777000 | 2.407736000 | 2.288655000 |
| 6 | 2.140174000 | 3.752752000 | -2.641492000 |
| 1 | 2.698332000 | 3.392912000 | -3.511878000 |
| 1 | 1.270738000 | 4.326263000 | -2.978855000 |
| 1 | 2.785910000 | 4.395994000 | -2.035041000 |
| 6 | 0.026256000 | 3.480170000 | 3.235532000 |
| 1 | 0.980013000 | 3.893356000 | 3.579167000 |
| 1 | -0.557319000 | 4.270026000 | 2.751660000 |
| 1 | -0.531316000 | 3.092112000 | 4.093995000 |
| 6 | -5.630032000 | 0.040009000 | -0.371289000 |
| 7 | -6.789716000 | -0.024671000 | -0.415844000 |



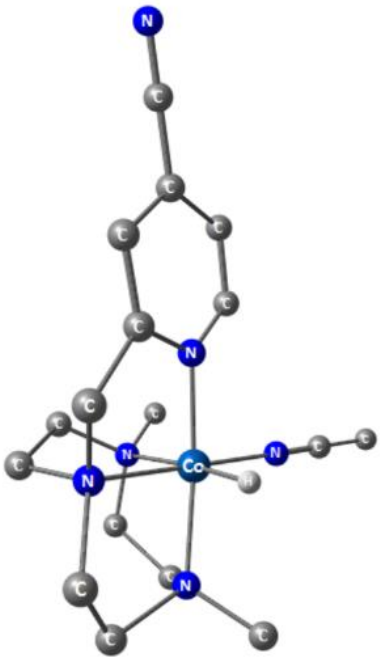
**$1^{CN}$-$Co^{I}$ (triplet, 1 AC, G = -2374.85144465)**

| | | | |
|---|---|---|---|
| 27 | -0.700565000 | 0.188029000 | -0.439089000 |
| 7 | -0.181409000 | -1.920005000 | -0.473958000 |
| 7 | 1.263687000 | 0.402090000 | -0.530015000 |
| 7 | -0.914557000 | -0.167902000 | 1.701057000 |
| 7 | -2.727407000 | -0.628916000 | -0.477556000 |
| 6 | 1.099898000 | -1.925059000 | -1.203544000 |
| 1 | 0.868669000 | -1.791936000 | -2.267107000 |
| 1 | 1.636146000 | -2.877098000 | -1.089894000 |
| 6 | 1.957330000 | -0.770610000 | -0.744348000 |
| 6 | 3.314875000 | -0.880833000 | -0.558680000 |
| 1 | 3.806656000 | -1.835122000 | -0.719807000 |
| 6 | 4.066584000 | 0.259670000 | -0.156166000 |
| 6 | 3.355557000 | 1.474034000 | 0.046754000 |
| 1 | 3.875682000 | 2.376244000 | 0.352027000 |
| 6 | 1.993571000 | 1.496016000 | -0.148431000 |
| 1 | 1.427661000 | 2.409484000 | 0.001357000 |
| 6 | -1.294132000 | -2.545903000 | -1.213420000 |
| 1 | -1.231818000 | -3.645123000 | -1.201410000 |
| 1 | -1.213347000 | -2.214068000 | -2.252583000 |
| 6 | -2.646376000 | -2.108921000 | -0.643544000 |
| 1 | -3.442142000 | -2.457602000 | -1.312194000 |
| 1 | -2.823128000 | -2.587251000 | 0.320801000 |
| 6 | -3.263766000 | -0.230705000 | 0.843365000 |
| 1 | -4.250574000 | -0.684700000 | 1.024770000 |
| 1 | -3.392793000 | 0.854978000 | 0.819742000 |
| 6 | -2.311721000 | -0.613263000 | 1.975460000 |
| 1 | -2.671804000 | -0.165166000 | 2.908619000 |
| 1 | -2.317037000 | -1.693285000 | 2.130770000 |
| 6 | 0.075513000 | -1.245457000 | 1.939029000 |
| 1 | -0.029586000 | -1.654060000 | 2.955829000 |
| 1 | 1.065072000 | -0.789400000 | 1.865752000 |
| 6 | -0.048940000 | -2.394366000 | 0.927495000 |
| 1 | 0.832341000 | -3.040048000 | 1.025476000 |
| 1 | -0.915764000 | -3.012140000 | 1.167240000 |
| 6 | -3.513348000 | -0.028467000 | -1.569205000 |
| 1 | -4.554940000 | -0.384323000 | -1.555167000 |
| 1 | -3.060867000 | -0.296845000 | -2.528327000 |
| 1 | -3.508035000 | 1.059426000 | -1.470727000 |
| 6 | -0.580825000 | 1.021650000 | 2.502325000 |
| 1 | -0.569397000 | 0.787707000 | 3.577979000 |
| 1 | -1.323757000 | 1.800985000 | 2.317568000 |
| 1 | 0.402376000 | 1.397013000 | 2.208572000 |
| 7 | -1.238480000 | 2.172431000 | -0.500830000 |
| 6 | -1.491397000 | 3.302481000 | -0.527464000 |
| 6 | -1.806052000 | 4.720591000 | -0.548867000 |
| 1 | -2.318223000 | 4.998997000 | 0.378044000 |
| 1 | -0.883108000 | 5.302411000 | -0.640185000 |
| 1 | -2.457308000 | 4.942401000 | -1.400548000 |
| 6 | 5.461285000 | 0.183148000 | 0.040588000 |
| 7 | 6.620443000 | 0.119116000 | 0.205694000 |



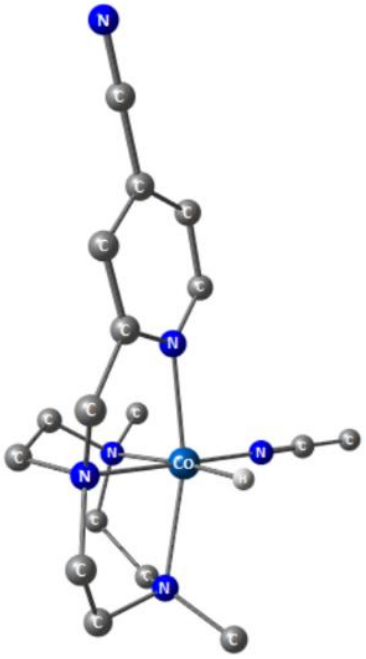
**$1^{CN}$-$Co^{III}$-H (singlet, 1 AC, G = -2375.28967822)**

| | | | |
|---|---|---|---|
| 27 | -0.685400000 | 0.072684000 | -0.387177000 |
| 7 | -0.308151000 | -1.833745000 | -0.381683000 |
| 7 | 1.251711000 | 0.268136000 | -0.289483000 |
| 7 | -0.986813000 | -0.076589000 | 1.677313000 |
| 7 | -2.606961000 | -0.389709000 | -0.584494000 |
| 6 | 1.024918000 | -2.002548000 | -1.025466000 |
| 1 | 0.887842000 | -1.929992000 | -2.108831000 |
| 1 | 1.455703000 | -2.980633000 | -0.796349000 |
| 6 | 1.909364000 | -0.877896000 | -0.584230000 |
| 6 | 3.293127000 | -0.966366000 | -0.517542000 |
| 1 | 3.792048000 | -1.901965000 | -0.743137000 |
| 6 | 4.015559000 | 0.176510000 | -0.154734000 |
| 6 | 3.333796000 | 1.365600000 | 0.132131000 |
| 1 | 3.863745000 | 2.267566000 | 0.414596000 |
| 6 | 1.947788000 | 1.364986000 | 0.055163000 |
| 1 | 1.379065000 | 2.257977000 | 0.277616000 |
| 6 | -1.397016000 | -2.464977000 | -1.190085000 |
| 1 | -1.373728000 | -3.554463000 | -1.076063000 |
| 1 | -1.213743000 | -2.210855000 | -2.234228000 |
| 6 | -2.722236000 | -1.890794000 | -0.726971000 |
| 1 | -3.511642000 | -2.129343000 | -1.443721000 |
| 1 | -3.020129000 | -2.314884000 | 0.230911000 |
| 6 | -3.251395000 | 0.083106000 | 0.680270000 |
| 1 | -4.279755000 | -0.293568000 | 0.737288000 |
| 1 | -3.286359000 | 1.173017000 | 0.632236000 |
| 6 | -2.443989000 | -0.371055000 | 1.884422000 |
| 1 | -2.802588000 | 0.142456000 | 2.781170000 |
| 1 | -2.569627000 | -1.438939000 | 2.063485000 |
| 6 | -0.129075000 | -1.233048000 | 2.048612000 |
| 1 | -0.381161000 | -1.596840000 | 3.053122000 |
| 1 | 0.903046000 | -0.878791000 | 2.070403000 |
| 6 | -0.297956000 | -2.360030000 | 1.038651000 |
| 1 | 0.508691000 | -3.088685000 | 1.147833000 |
| 1 | -1.234372000 | -2.890371000 | 1.205207000 |
| 6 | -3.270857000 | 0.254199000 | -1.749903000 |
| 1 | -4.341049000 | 0.017065000 | -1.733526000 |
| 1 | -2.825880000 | -0.126819000 | -2.669542000 |
| 1 | -3.137800000 | 1.334234000 | -1.700673000 |
| 6 | -0.601187000 | 1.110559000 | 2.471197000 |
| 1 | -0.706747000 | 0.897210000 | 3.542706000 |
| 1 | -1.247604000 | 1.949109000 | 2.208292000 |
| 1 | 0.436302000 | 1.374797000 | 2.262535000 |
| 7 | -1.006963000 | 1.937131000 | -0.479867000 |
| 6 | -1.187234000 | 3.074256000 | -0.553623000 |
| 6 | -1.416797000 | 4.503184000 | -0.635744000 |
| 1 | -1.933527000 | 4.842801000 | 0.267831000 |
| 1 | -0.456542000 | 5.022028000 | -0.722977000 |
| 1 | -2.031625000 | 4.726113000 | -1.513764000 |
| 6 | 5.446784000 | 0.126482000 | -0.072956000 |
| 7 | 6.606390000 | 0.086707000 | -0.006780000 |
| 1 | -0.532848000 | 0.072787000 | -1.838811000 |



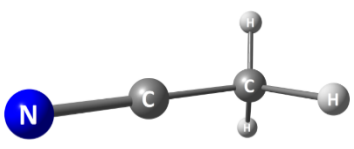
**$1^{CN}$-$Co^{II}$-H (doublet, 1 AC, G = -2375.42027709)**

| | | | |
|---|---|---|---|
| 27 | -0.737710000 | 0.179188000 | -0.428785000 |
| 7 | -0.170472000 | -1.805728000 | -0.343353000 |
| 7 | 1.432341000 | 0.400425000 | -0.266185000 |
| 7 | -1.046867000 | -0.008975000 | 1.623222000 |
| 7 | -2.793501000 | -0.703237000 | -0.555519000 |
| 6 | 1.148658000 | -1.893540000 | -1.001605000 |
| 1 | 0.990159000 | -1.802103000 | -2.081083000 |
| 1 | 1.631955000 | -2.860183000 | -0.810336000 |
| 6 | 2.047012000 | -0.760009000 | -0.563519000 |
| 6 | 3.432026000 | -0.895862000 | -0.510058000 |
| 1 | 3.904341000 | -1.846036000 | -0.735502000 |
| 6 | 4.196056000 | 0.224234000 | -0.155810000 |
| 6 | 3.556910000 | 1.437389000 | 0.136736000 |
| 1 | 4.122120000 | 2.319811000 | 0.414794000 |
| 6 | 2.168000000 | 1.468646000 | 0.069933000 |
| 1 | 1.620675000 | 2.378407000 | 0.297864000 |
| 6 | -1.212154000 | -2.561248000 | -1.085147000 |
| 1 | -1.068399000 | -3.645083000 | -0.968755000 |
| 1 | -1.097731000 | -2.309398000 | -2.141310000 |
| 6 | -2.617217000 | -2.175274000 | -0.611290000 |
| 1 | -3.348624000 | -2.623357000 | -1.295258000 |
| 1 | -2.819297000 | -2.603327000 | 0.372105000 |
| 6 | -3.378045000 | -0.227139000 | 0.711042000 |
| 1 | -4.353014000 | -0.701229000 | 0.914631000 |
| 1 | -3.548041000 | 0.847732000 | 0.599261000 |
| 6 | -2.446343000 | -0.484397000 | 1.888706000 |
| 1 | -2.842008000 | 0.017097000 | 2.778526000 |
| 1 | -2.415206000 | -1.549288000 | 2.123693000 |
| 6 | -0.054102000 | -1.038129000 | 2.035298000 |
| 1 | -0.249655000 | -1.371653000 | 3.064708000 |
| 1 | 0.927458000 | -0.563271000 | 2.019978000 |
| 6 | -0.085782000 | -2.235344000 | 1.090308000 |
| 1 | 0.808475000 | -2.847596000 | 1.248289000 |
| 1 | -0.943227000 | -2.871957000 | 1.309549000 |
| 6 | -3.565014000 | -0.217927000 | -1.704838000 |
| 1 | -4.606553000 | -0.578551000 | -1.675394000 |
| 1 | -3.098199000 | -0.566704000 | -2.629384000 |
| 1 | -3.568781000 | 0.875499000 | -1.709136000 |
| 6 | -0.795661000 | 1.238368000 | 2.375753000 |
| 1 | -0.824878000 | 1.049339000 | 3.458277000 |
| 1 | -1.560993000 | 1.973513000 | 2.123027000 |
| 1 | 0.183791000 | 1.638045000 | 2.107036000 |
| 7 | -1.228509000 | 2.026126000 | -0.533576000 |
| 6 | -1.516326000 | 3.145604000 | -0.610153000 |
| 6 | -1.880218000 | 4.549835000 | -0.705311000 |
| 1 | -2.357551000 | 4.874153000 | 0.225336000 |
| 1 | -0.984980000 | 5.156074000 | -0.878813000 |
| 1 | -2.578223000 | 4.698150000 | -1.535994000 |
| 6 | 5.624537000 | 0.126039000 | -0.085133000 |
| 7 | 6.783375000 | 0.046883000 | -0.026776000 |
| 1 | -0.574033000 | 0.177901000 | -1.953077000 |



**Acetonitrile (singlet, G = -132.801268035)**

| | | | |
|---|---|---|---|
| 1 | 1.551127000 | 0.906689000 | -0.488670000 |
| 1 | 1.552336000 | -0.876499000 | -0.539241000 |
| 6 | 1.179713000 | 0.000242000 | -0.000082000 |
| 1 | 1.549409000 | -0.028716000 | 1.029910000 |
| 6 | -0.276633000 | -0.001032000 | -0.000324000 |
| 7 | -1.438765000 | 0.000467000 | 0.000063000 |

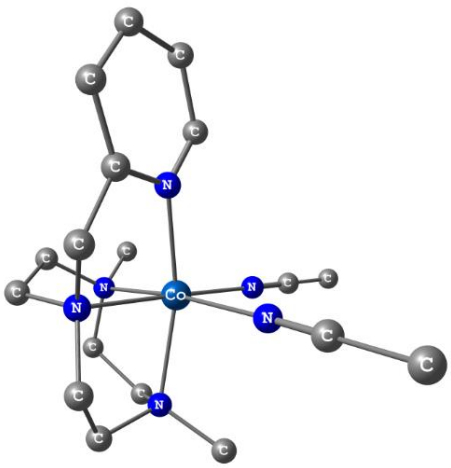


**Cartesian coordinates of optimized geometries in water**

To generate the reaction energy profiles of $\mathbf{1}^{H}$ and $\mathbf{1}^{COOEt}$, geometries were optimized at the B3LYP (SMD/water)/6-31+G* level of theory. The electronic energies have been obtained through a single point calculation at the B3LYP-$D_3$(SMD/water)/aug-cc-pVTZ(-$d^{H}$, -$f^{C,N,O}$, -$g^{Co}$). In parenthesis, there are indicated the ground spin states, the number of coordinating acetonitrile molecules (n AC where n = 1, 2) and the associated free energy values ($G = E_{elec} + \Delta G_{corr}$) in Hartrees. Irrelevant hydrogen atoms are omitted for clarity in the inserted figures.

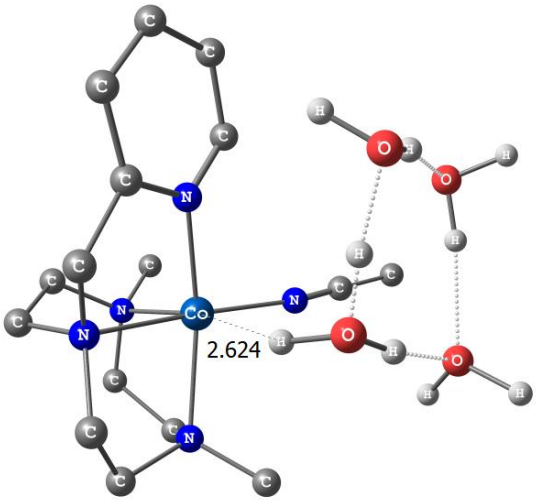
**$1^{H}$-$Co^{II}$ (quartet, 2 AC, G = -2415.13426349)**

| | | | |
|---|---|---|---|
| 27 | 0.328957000 | 0.129131000 | -0.071897000 |
| 7 | -0.511718000 | -1.495656000 | 1.105147000 |
| 7 | -1.760598000 | 0.435803000 | -0.373112000 |
| 7 | 0.610109000 | -1.457287000 | -1.525883000 |
| 7 | 2.212635000 | -0.653380000 | 0.731604000 |
| 6 | -1.837547000 | -1.021604000 | 1.559030000 |
| 1 | -1.683055000 | -0.312664000 | 2.379016000 |
| 1 | -2.453313000 | -1.843609000 | 1.944126000 |
| 6 | -2.550734000 | -0.293103000 | 0.442282000 |
| 6 | -3.933936000 | -0.328114000 | 0.274282000 |
| 1 | -4.543040000 | -0.931052000 | 0.940653000 |
| 6 | -4.508512000 | 0.411033000 | -0.761810000 |
| 1 | -5.583704000 | 0.394731000 | -0.915022000 |
| 6 | -3.683991000 | 1.162372000 | -1.602457000 |
| 1 | -4.089649000 | 1.746373000 | -2.422056000 |
| 6 | -2.310918000 | 1.143350000 | -1.373318000 |
| 1 | -1.620590000 | 1.704180000 | -1.996632000 |
| 6 | 0.455984000 | -1.652027000 | 2.223086000 |
| 1 | 0.223209000 | -2.538109000 | 2.830278000 |
| 1 | 0.358586000 | -0.770273000 | 2.860517000 |
| 6 | 1.895057000 | -1.745296000 | 1.706748000 |
| 1 | 2.577656000 | -1.691795000 | 2.561729000 |
| 1 | 2.072480000 | -2.712018000 | 1.234332000 |
| 6 | 2.871799000 | -1.165868000 | -0.500468000 |
| 1 | 3.796514000 | -1.706633000 | -0.250026000 |
| 1 | 3.145985000 | -0.292461000 | -1.099589000 |
| 6 | 1.951200000 | -2.079719000 | -1.308118000 |
| 1 | 2.424827000 | -2.298991000 | -2.271552000 |
| 1 | 1.825035000 | -3.038643000 | -0.803826000 |
| 6 | -0.505842000 | -2.394360000 | -1.243780000 |
| 1 | -0.385397000 | -3.328737000 | -1.810950000 |
| 1 | -1.420792000 | -1.910392000 | -1.592281000 |
| 6 | -0.618534000 | -2.717311000 | 0.249218000 |
| 1 | -1.576139000 | -3.218743000 | 0.427607000 |
| 1 | 0.158201000 | -3.422422000 | 0.548004000 |
| 6 | 3.056991000 | 0.382736000 | 1.360283000 |
| 1 | 4.057712000 | -0.011046000 | 1.589310000 |
| 1 | 2.585158000 | 0.721713000 | 2.284360000 |
| 1 | 3.151652000 | 1.234578000 | 0.681999000 |
| 6 | 0.499449000 | -0.926951000 | -2.901262000 |
| 1 | 0.500875000 | -1.742525000 | -3.638538000 |
| 1 | 1.343212000 | -0.263296000 | -3.101089000 |
| 1 | -0.426269000 | -0.353704000 | -2.998740000 |
| 7 | 1.180252000 | 1.673516000 | -1.196874000 |
| 7 | 0.149034000 | 1.560310000 | 1.565064000 |
| 6 | 1.647103000 | 2.521705000 | -1.829692000 |
| 6 | 0.009239000 | 2.234937000 | 2.494992000 |
| 6 | 2.229884000 | 3.589517000 | -2.620195000 |
| 1 | 2.814175000 | 3.162801000 | -3.441606000 |
| 1 | 1.431249000 | 4.217224000 | -3.028768000 |
| 1 | 2.881704000 | 4.199713000 | -1.986579000 |
| 6 | -0.163812000 | 3.078716000 | 3.663841000 |
| 1 | 0.803386000 | 3.231292000 | 4.153570000 |
| 1 | -0.573358000 | 4.047603000 | 3.360798000 |
| 1 | -0.853423000 | 2.597138000 | 4.364580000 |



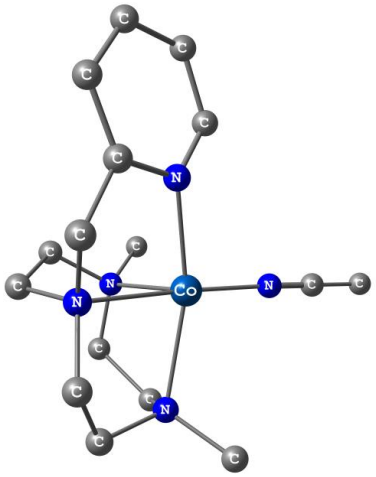
**$1^{H}$-$Co^{II}$_$H_3O^+$_$3H_2O$ (quartet, 1 AC, G = -2588.63200740)**

| | | | |
|---|---|---|---|
| 27 | 0.527129000 | -0.191195000 | 0.112568000 |
| 7 | 1.517117000 | 1.355686000 | -1.058971000 |
| 7 | -0.796771000 | 1.378490000 | 0.387814000 |
| 7 | 2.061941000 | 0.200457000 | 1.500969000 |
| 7 | 2.004237000 | -1.467207000 | -0.821415000 |
| 6 | 0.473090000 | 2.330408000 | -1.446375000 |
| 1 | -0.030528000 | 1.951975000 | -2.342849000 |
| 1 | 0.902701000 | 3.305714000 | -1.703818000 |
| 6 | -0.574457000 | 2.474737000 | -0.365766000 |
| 6 | -1.317252000 | 3.640395000 | -0.183781000 |
| 1 | -1.116623000 | 4.508519000 | -0.803864000 |
| 6 | -2.303704000 | 3.667588000 | 0.803463000 |
| 1 | -2.891537000 | 4.566647000 | 0.963655000 |
| 6 | -2.518492000 | 2.530942000 | 1.588488000 |
| 1 | -3.270739000 | 2.513935000 | 2.370062000 |
| 6 | -1.739944000 | 1.404460000 | 1.347343000 |
| 1 | -1.861144000 | 0.492660000 | 1.922734000 |
| 6 | 2.054652000 | 0.605837000 | -2.225408000 |
| 1 | 2.715249000 | 1.236776000 | -2.836650000 |
| 1 | 1.203180000 | 0.315417000 | -2.845880000 |
| 6 | 2.805855000 | -0.652673000 | -1.787072000 |
| 1 | 3.038828000 | -1.249648000 | -2.675606000 |
| 1 | 3.763156000 | -0.393017000 | -1.333552000 |
| 6 | 2.795303000 | -1.899547000 | 0.362754000 |
| 1 | 3.682497000 | -2.470449000 | 0.053436000 |
| 1 | 2.152320000 | -2.562747000 | 0.949245000 |
| 6 | 3.220713000 | -0.704218000 | 1.218076000 |
| 1 | 3.649663000 | -1.068317000 | 2.157665000 |
| 1 | 4.005446000 | -0.133975000 | 0.719684000 |
| 6 | 2.375129000 | 1.638597000 | 1.283810000 |
| 1 | 3.267047000 | 1.934215000 | 1.853701000 |
| 1 | 1.525763000 | 2.207973000 | 1.670018000 |
| 6 | 2.582563000 | 1.958699000 | -0.200054000 |
| 1 | 2.597004000 | 3.046490000 | -0.325779000 |
| 1 | 3.552721000 | 1.594189000 | -0.540179000 |
| 6 | 1.381701000 | -2.623840000 | -1.497289000 |
| 1 | 2.142645000 | -3.304997000 | -1.903928000 |
| 1 | 0.751989000 | -2.261394000 | -2.313593000 |
| 1 | 0.762072000 | -3.169944000 | -0.782871000 |
| 8 | -3.943328000 | -1.331592000 | 0.294032000 |
| 1 | -3.436529000 | -1.976889000 | -0.246453000 |
| 6 | 1.538059000 | -0.023727000 | 2.867716000 |
| 1 | 2.266922000 | 0.298107000 | 3.624040000 |
| 1 | 1.326216000 | -1.087403000 | 2.998605000 |
| 1 | 0.608826000 | 0.538452000 | 2.995107000 |
| 7 | -0.571927000 | -1.691415000 | 0.945459000 |
| 6 | -1.182698000 | -2.465369000 | 1.549905000 |
| 6 | -1.946499000 | -3.442364000 | 2.298663000 |
| 1 | -2.494893000 | -4.084822000 | 1.602423000 |
| 1 | -1.265754000 | -4.051787000 | 2.901989000 |
| 1 | -2.655462000 | -2.926604000 | 2.953951000 |
| 1 | -0.886043000 | -0.270569000 | -2.096441000 |
| 8 | -1.724456000 | -0.576524000 | -2.495867000 |
| 1 | -1.889319000 | -1.517239000 | -2.129230000 |
| 1 | -2.514343000 | 0.035492000 | -2.085146000 |
| 1 | -3.329165000 | 1.508193000 | -1.079027000 |
| 8 | -3.630134000 | 0.683329000 | -1.500250000 |
| 1 | -3.838748000 | 0.053480000 | -0.753922000 |
| 1 | -1.525551000 | -3.375867000 | -1.157276000 |
| 8 | -2.316066000 | -2.896909000 | -1.465206000 |
| 1 | -2.735401000 | -3.481632000 | -2.121766000 |
| 1 | -4.859387000 | -1.656739000 | 0.276662000 |



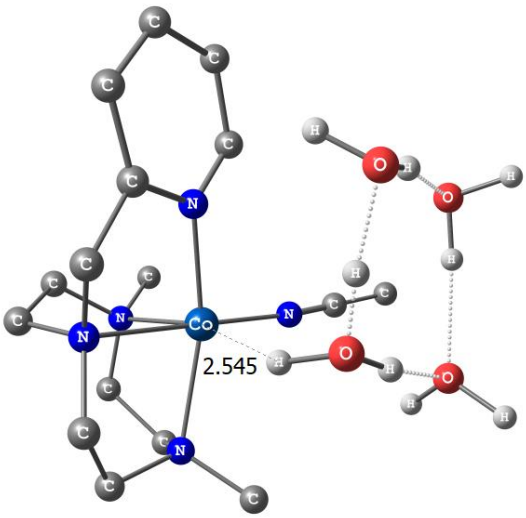
**$1^{H}$-$Co^{I}$ (triplet, 1 AC, G = -2282.46188308)**

| | | | |
|---|---|---|---|
| 27 | -0.335572000 | 0.227927000 | -0.451784000 |
| 7 | 0.456261000 | -1.840469000 | -0.444013000 |
| 7 | 1.714335000 | 0.612409000 | -0.524958000 |
| 7 | -0.512485000 | -0.180246000 | 1.710437000 |
| 7 | -2.259313000 | -0.900430000 | -0.501124000 |
| 6 | 1.739748000 | -1.722501000 | -1.156267000 |
| 1 | 1.517904000 | -1.607392000 | -2.223758000 |
| 1 | 2.366104000 | -2.619444000 | -1.040081000 |
| 6 | 2.485934000 | -0.488502000 | -0.695943000 |
| 6 | 3.860352000 | -0.471307000 | -0.469330000 |
| 1 | 4.438694000 | -1.380921000 | -0.604647000 |
| 6 | 4.470706000 | 0.718143000 | -0.058594000 |
| 1 | 5.540223000 | 0.753499000 | 0.128355000 |
| 6 | 3.675761000 | 1.854564000 | 0.115127000 |
| 1 | 4.101323000 | 2.800323000 | 0.436935000 |
| 6 | 2.307862000 | 1.754817000 | -0.128704000 |
| 1 | 1.645937000 | 2.607422000 | -0.004149000 |
| 6 | -0.562859000 | -2.608687000 | -1.185807000 |
| 1 | -0.357190000 | -3.692015000 | -1.173301000 |
| 1 | -0.520642000 | -2.270226000 | -2.225855000 |
| 6 | -1.974038000 | -2.353448000 | -0.638324000 |
| 1 | -2.698640000 | -2.825680000 | -1.314703000 |
| 1 | -2.102558000 | -2.845121000 | 0.328293000 |
| 6 | -2.826771000 | -0.532107000 | 0.812949000 |
| 1 | -3.768747000 | -1.071718000 | 1.014575000 |
| 1 | -3.058477000 | 0.536751000 | 0.767442000 |
| 6 | -1.848817000 | -0.787001000 | 1.963783000 |
| 1 | -2.282607000 | -0.383591000 | 2.888326000 |
| 1 | -1.732065000 | -1.860205000 | 2.129700000 |
| 6 | 0.598920000 | -1.119146000 | 1.967888000 |
| 1 | 0.548698000 | -1.533780000 | 2.989271000 |
| 1 | 1.525082000 | -0.543292000 | 1.894131000 |
| 6 | 0.630725000 | -2.282970000 | 0.964517000 |
| 1 | 1.583972000 | -2.815371000 | 1.083031000 |
| 1 | -0.152307000 | -3.004501000 | 1.205074000 |
| 6 | -3.111087000 | -0.423757000 | -1.598672000 |
| 1 | -4.113687000 | -0.884043000 | -1.575493000 |
| 1 | -2.635368000 | -0.665436000 | -2.554292000 |
| 1 | -3.218466000 | 0.662594000 | -1.533464000 |
| 6 | -0.340642000 | 1.059679000 | 2.478663000 |
| 1 | -0.321176000 | 0.873249000 | 3.566017000 |
| 1 | -1.165368000 | 1.740551000 | 2.251768000 |
| 1 | 0.593788000 | 1.545120000 | 2.182909000 |
| 7 | -1.076508000 | 2.006547000 | -0.559000000 |
| 6 | -1.569763000 | 3.063975000 | -0.564668000 |
| 6 | -2.185105000 | 4.383188000 | -0.559583000 |
| 1 | -2.235157000 | 4.768806000 | 0.464897000 |
| 1 | -1.598403000 | 5.078314000 | -1.170376000 |
| 1 | -3.202009000 | 4.327733000 | -0.964045000 |



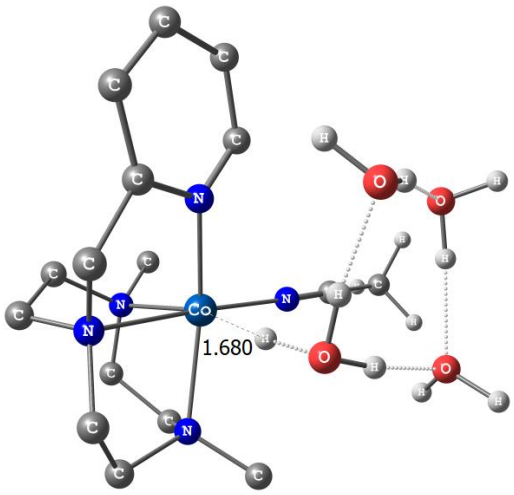
**$1^{H}$-$Co^{I}$_$H_3O^+$_$3H_2O$ (triplet, 1 AC, G = -2588.74409774)**

| | | | |
|---|---|---|---|
| 27 | 0.440872000 | -0.225040000 | 0.073481000 |
| 7 | 1.410149000 | 1.416253000 | -1.084347000 |
| 7 | -0.939439000 | 1.290335000 | 0.349283000 |
| 7 | 1.926949000 | 0.368904000 | 1.564871000 |
| 7 | 2.154167000 | -1.341136000 | -0.765323000 |
| 6 | 0.288255000 | 2.267574000 | -1.506917000 |
| 1 | -0.192698000 | 1.790170000 | -2.368903000 |
| 1 | 0.619118000 | 3.264799000 | -1.833262000 |
| 6 | -0.754085000 | 2.393541000 | -0.413786000 |
| 6 | -1.514635000 | 3.549206000 | -0.237086000 |
| 1 | -1.329932000 | 4.414860000 | -0.866972000 |
| 6 | -2.503807000 | 3.572439000 | 0.750181000 |
| 1 | -3.109637000 | 4.461035000 | 0.902501000 |
| 6 | -2.691443000 | 2.434133000 | 1.540173000 |
| 1 | -3.443689000 | 2.405236000 | 2.322611000 |
| 6 | -1.885986000 | 1.322403000 | 1.308230000 |
| 1 | -1.991654000 | 0.413849000 | 1.893570000 |
| 6 | 2.081749000 | 0.717349000 | -2.198171000 |
| 1 | 2.728718000 | 1.392851000 | -2.782390000 |
| 1 | 1.301948000 | 0.348292000 | -2.870835000 |
| 6 | 2.917605000 | -0.469275000 | -1.698715000 |
| 1 | 3.259331000 | -1.044914000 | -2.568863000 |
| 1 | 3.820947000 | -0.109930000 | -1.202226000 |
| 6 | 2.901377000 | -1.664010000 | 0.470104000 |
| 1 | 3.862145000 | -2.158653000 | 0.244972000 |
| 1 | 2.286073000 | -2.370707000 | 1.035724000 |
| 6 | 3.165893000 | -0.424113000 | 1.330602000 |
| 1 | 3.599255000 | -0.747083000 | 2.286044000 |
| 1 | 3.918974000 | 0.210757000 | 0.859138000 |
| 6 | 2.105664000 | 1.813474000 | 1.305898000 |
| 1 | 2.938232000 | 2.229175000 | 1.898490000 |
| 1 | 1.188309000 | 2.308515000 | 1.635601000 |
| 6 | 2.353077000 | 2.123027000 | -0.177920000 |
| 1 | 2.279614000 | 3.209491000 | -0.321179000 |
| 1 | 3.373641000 | 1.847874000 | -0.452084000 |
| 6 | 1.694141000 | -2.563010000 | -1.440430000 |
| 1 | 2.535853000 | -3.196529000 | -1.768816000 |
| 1 | 1.097415000 | -2.292575000 | -2.317165000 |
| 1 | 1.067943000 | -3.142242000 | -0.756573000 |
| 6 | 1.403084000 | 0.144565000 | 2.919441000 |
| 1 | 2.080332000 | 0.541455000 | 3.694459000 |
| 1 | 1.269087000 | -0.927995000 | 3.081445000 |
| 1 | 0.427307000 | 0.629296000 | 3.016663000 |
| 7 | -0.461179000 | -1.654718000 | 1.009256000 |
| 6 | -1.031429000 | -2.455359000 | 1.636001000 |
| 6 | -1.755347000 | -3.446160000 | 2.417673000 |
| 1 | -2.255905000 | -4.155319000 | 1.749314000 |
| 1 | -1.062627000 | -3.996411000 | 3.063977000 |
| 1 | -2.510363000 | -2.955511000 | 3.041720000 |
| 1 | -0.664591000 | -0.489797000 | -2.203841000 |
| 8 | -1.494880000 | -0.831766000 | -2.600268000 |
| 1 | -1.645206000 | -1.753091000 | -2.174978000 |
| 1 | -2.290479000 | -0.221391000 | -2.227420000 |
| 1 | -3.142593000 | 1.255782000 | -1.233041000 |
| 8 | -3.447595000 | 0.441213000 | -1.670719000 |
| 1 | -3.673997000 | -0.189643000 | -0.930465000 |
| 1 | -1.192216000 | -3.385585000 | -0.941885000 |
| 8 | -1.994600000 | -3.079294000 | -1.401835000 |
| 1 | -2.244822000 | -3.800862000 | -2.005973000 |
| 1 | -4.718278000 | -1.918271000 | 0.035388000 |
| 8 | -3.830564000 | -1.539021000 | 0.151581000 |
| 1 | -3.227185000 | -2.172076000 | -0.296646000 |



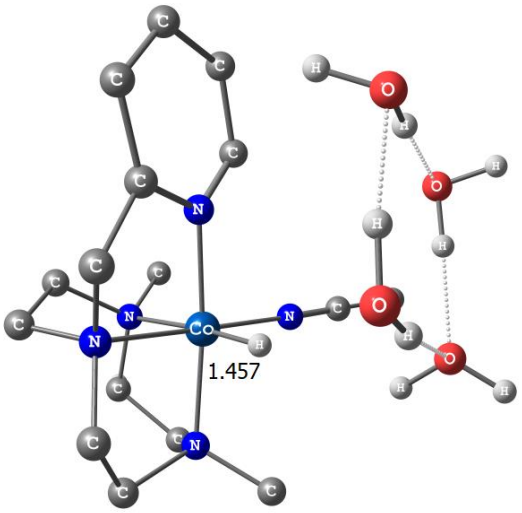
**$1^{H}$-TS1 (triplet, 1 AC, G = -2588.73580303, Imaginary frequency: -927.25 a.u.)**

| | | | |
|---|---|---|---|
| 27 | 0.439922000 | -0.173072000 | 0.109826000 |
| 7 | 1.527271000 | 1.296642000 | -1.081516000 |
| 7 | -0.844249000 | 1.420434000 | 0.304722000 |
| 7 | 2.057566000 | 0.181819000 | 1.534895000 |
| 7 | 1.892272000 | -1.531962000 | -0.788836000 |
| 6 | 0.519148000 | 2.292545000 | -1.496642000 |
| 1 | -0.004858000 | 1.894992000 | -2.373040000 |
| 1 | 0.976498000 | 3.245808000 | -1.791686000 |
| 6 | -0.520836000 | 2.511531000 | -0.421217000 |
| 6 | -1.166655000 | 3.730814000 | -0.225655000 |
| 1 | -0.886475000 | 4.591329000 | -0.825571000 |
| 6 | -2.164524000 | 3.820664000 | 0.747518000 |
| 1 | -2.680343000 | 4.761475000 | 0.916836000 |
| 6 | -2.483201000 | 2.690624000 | 1.504628000 |
| 1 | -3.248300000 | 2.719462000 | 2.273631000 |
| 6 | -1.797383000 | 1.507045000 | 1.249198000 |
| 1 | -2.008508000 | 0.594321000 | 1.796925000 |
| 6 | 2.048217000 | 0.511542000 | -2.226706000 |
| 1 | 2.746772000 | 1.101454000 | -2.838961000 |
| 1 | 1.191152000 | 0.246126000 | -2.849298000 |
| 6 | 2.736980000 | -0.773044000 | -1.760898000 |
| 1 | 2.951873000 | -1.393142000 | -2.638534000 |
| 1 | 3.702355000 | -0.547627000 | -1.305224000 |
| 6 | 2.662585000 | -1.956096000 | 0.415213000 |
| 1 | 3.514655000 | -2.589872000 | 0.124376000 |
| 1 | 1.985594000 | -2.563209000 | 1.024482000 |
| 6 | 3.162640000 | -0.768648000 | 1.240111000 |
| 1 | 3.602493000 | -1.146995000 | 2.171237000 |
| 1 | 3.963188000 | -0.243240000 | 0.715879000 |
| 6 | 2.394120000 | 1.599114000 | 1.263913000 |
| 1 | 3.292291000 | 1.910926000 | 1.820181000 |
| 1 | 1.553942000 | 2.195966000 | 1.631133000 |
| 6 | 2.605340000 | 1.880130000 | -0.228905000 |
| 1 | 2.658553000 | 2.965681000 | -0.373459000 |
| 1 | 3.565279000 | 1.478656000 | -0.558045000 |
| 6 | 1.290454000 | -2.716784000 | -1.434054000 |
| 1 | 2.060528000 | -3.453221000 | -1.708889000 |
| 1 | 0.758161000 | -2.405921000 | -2.334657000 |
| 1 | 0.578068000 | -3.181291000 | -0.748134000 |
| 6 | 1.549180000 | 0.014565000 | 2.907471000 |
| 1 | 2.291888000 | 0.331078000 | 3.656339000 |
| 1 | 1.300633000 | -1.036729000 | 3.074021000 |
| 1 | 0.638057000 | 0.608326000 | 3.029999000 |
| 7 | -0.623289000 | -1.570840000 | 1.036836000 |
| 6 | -1.250304000 | -2.364981000 | 1.601236000 |
| 6 | -2.047507000 | -3.365185000 | 2.289231000 |
| 1 | -2.207635000 | -4.223259000 | 1.627933000 |
| 1 | -1.528683000 | -3.696043000 | 3.194859000 |
| 1 | -3.017109000 | -2.935970000 | 2.561300000 |
| 1 | -0.493326000 | -0.565170000 | -1.231306000 |
| 8 | -1.263193000 | -0.785762000 | -2.201594000 |
| 1 | -1.673991000 | -1.662583000 | -1.947903000 |
| 1 | -2.000149000 | -0.111781000 | -2.061967000 |
| 1 | -3.111116000 | 1.612599000 | -1.283236000 |
| 8 | -3.384329000 | 0.790647000 | -1.724883000 |
| 1 | -3.675016000 | 0.188765000 | -0.991897000 |
| 1 | -1.799554000 | -3.621415000 | -0.893629000 |
| 8 | -2.456260000 | -3.054904000 | -1.336129000 |
| 1 | -2.867855000 | -3.616344000 | -2.015913000 |
| 1 | -4.939409000 | -1.406314000 | 0.018816000 |
| 8 | -4.003315000 | -1.166836000 | 0.124119000 |
| 1 | -3.507291000 | -1.894713000 | -0.313384000 |



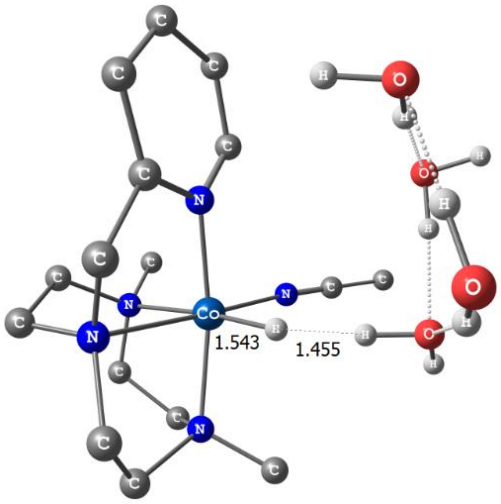
**$1^{H}$-$Co^{III}$-H_$4H_2O$ (singlet, 1 AC, G = -2588.77039738)**

| | | | |
|---|---|---|---|
| 27 | 0.624121000 | -0.123269000 | -0.050620000 |
| 7 | 1.087635000 | 1.379355000 | -1.198158000 |
| 7 | -0.880173000 | 1.002136000 | 0.490256000 |
| 7 | 1.968558000 | 0.668239000 | 1.356645000 |
| 7 | 2.190418000 | -1.093054000 | -0.816012000 |
| 6 | -0.206298000 | 2.029659000 | -1.561242000 |
| 1 | -0.696134000 | 1.402893000 | -2.312619000 |
| 1 | -0.045491000 | 3.024546000 | -1.985886000 |
| 6 | -1.069756000 | 2.058900000 | -0.337040000 |
| 6 | -2.006210000 | 3.048340000 | -0.057292000 |
| 1 | -2.118333000 | 3.886659000 | -0.736879000 |
| 6 | -2.778119000 | 2.939267000 | 1.101492000 |
| 1 | -3.513155000 | 3.700355000 | 1.344378000 |
| 6 | -2.591546000 | 1.837805000 | 1.938447000 |
| 1 | -3.173657000 | 1.707561000 | 2.844246000 |
| 6 | -1.632224000 | 0.889451000 | 1.599564000 |
| 1 | -1.450995000 | 0.023840000 | 2.222820000 |
| 6 | 1.762599000 | 0.776671000 | -2.389579000 |
| 1 | 2.226236000 | 1.555939000 | -3.005057000 |
| 1 | 0.990223000 | 0.274614000 | -2.974012000 |
| 6 | 2.790158000 | -0.233041000 | -1.907539000 |
| 1 | 3.111514000 | -0.864422000 | -2.739892000 |
| 1 | 3.684030000 | 0.255723000 | -1.521315000 |
| 6 | 3.136844000 | -1.260306000 | 0.332821000 |
| 1 | 4.102162000 | -1.637913000 | -0.026715000 |
| 1 | 2.699870000 | -2.009803000 | 0.996777000 |
| 6 | 3.309973000 | 0.058270000 | 1.068208000 |
| 1 | 3.854977000 | -0.110438000 | 2.002471000 |
| 1 | 3.905076000 | 0.759625000 | 0.482305000 |
| 6 | 1.938280000 | 2.123046000 | 1.048818000 |
| 1 | 2.775451000 | 2.644676000 | 1.531619000 |
| 1 | 1.011472000 | 2.522652000 | 1.464407000 |
| 6 | 1.995492000 | 2.344734000 | -0.459440000 |
| 1 | 1.706374000 | 3.370775000 | -0.700717000 |
| 1 | 3.010110000 | 2.203964000 | -0.830632000 |
| 6 | 1.857404000 | -2.426982000 | -1.384948000 |
| 1 | 2.775212000 | -2.925821000 | -1.718891000 |
| 1 | 1.185181000 | -2.292241000 | -2.233380000 |
| 1 | 1.371398000 | -3.041175000 | -0.626321000 |
| 6 | 1.608188000 | 0.434969000 | 2.772760000 |
| 1 | 2.313434000 | 0.952311000 | 3.436517000 |
| 1 | 1.636727000 | -0.636308000 | 2.980902000 |
| 1 | 0.601656000 | 0.809390000 | 2.963344000 |
| 7 | 0.074761000 | -1.588899000 | 1.014307000 |
| 6 | -0.325023000 | -2.476547000 | 1.633398000 |
| 6 | -0.838985000 | -3.594855000 | 2.398039000 |
| 1 | -1.355347000 | -4.286341000 | 1.724585000 |
| 1 | -0.011770000 | -4.113701000 | 2.892859000 |
| 1 | -1.542453000 | -3.226659000 | 3.151592000 |
| 1 | -0.226986000 | -0.640681000 | -1.113583000 |
| 8 | -2.479908000 | -0.667088000 | -3.018866000 |
| 1 | -2.201757000 | -1.489447000 | -2.563423000 |
| 1 | -3.075055000 | -0.238571000 | -2.360806000 |
| 1 | -3.819740000 | 1.107962000 | -0.656977000 |
| 8 | -4.203977000 | 0.283884000 | -0.999177000 |
| 1 | -3.919036000 | -0.413342000 | -0.356496000 |
| 1 | -0.914027000 | -2.871595000 | -1.191391000 |
| 8 | -1.852827000 | -2.950398000 | -1.430874000 |
| 1 | -1.985945000 | -3.887501000 | -1.654704000 |
| 1 | -4.201200000 | -2.389228000 | 0.675747000 |
| 8 | -3.402635000 | -1.838834000 | 0.613038000 |
| 1 | -2.839567000 | -2.291262000 | -0.059208000 |



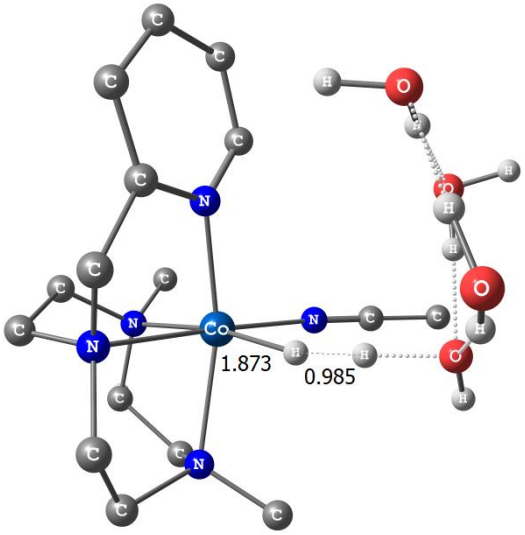
**$1^{H}$-$Co^{II}$-H_$4H_2O$ (doublet, 1 AC, G = -2588.89839432)**

| | | | |
|---|---|---|---|
| 27 | 0.597598000 | 0.217924000 | 0.002354000 |
| 7 | 1.293760000 | -1.499905000 | 1.205328000 |
| 7 | -0.798035000 | -1.095614000 | -0.550377000 |
| 7 | 2.048021000 | -0.486356000 | -1.344462000 |
| 7 | 2.147602000 | 1.238676000 | 0.882862000 |
| 6 | 0.036990000 | -2.215519000 | 1.448631000 |
| 1 | -0.508379000 | -1.682684000 | 2.235776000 |
| 1 | 0.199552000 | -3.246625000 | 1.794672000 |
| 6 | -0.841023000 | -2.214399000 | 0.212809000 |
| 6 | -1.680740000 | -3.281772000 | -0.104575000 |
| 1 | -1.677409000 | -4.168771000 | 0.521866000 |
| 6 | -2.507675000 | -3.192591000 | -1.226912000 |
| 1 | -3.166068000 | -4.014656000 | -1.492095000 |
| 6 | -2.471735000 | -2.029298000 | -1.997811000 |
| 1 | -3.099280000 | -1.908451000 | -2.874839000 |
| 6 | -1.602594000 | -1.008118000 | -1.624000000 |
| 1 | -1.535092000 | -0.085744000 | -2.189832000 |
| 6 | 1.860243000 | -0.793358000 | 2.366809000 |
| 1 | 2.428218000 | -1.464150000 | 3.031212000 |
| 1 | 1.022602000 | -0.382880000 | 2.935007000 |
| 6 | 2.779063000 | 0.352692000 | 1.923325000 |
| 1 | 3.049497000 | 0.949357000 | 2.801512000 |
| 1 | 3.713997000 | -0.046249000 | 1.526975000 |
| 6 | 3.073599000 | 1.500901000 | -0.254065000 |
| 1 | 4.022877000 | 1.930395000 | 0.100164000 |
| 1 | 2.583364000 | 2.238621000 | -0.894934000 |
| 6 | 3.335344000 | 0.223312000 | -1.038896000 |
| 1 | 3.864233000 | 0.462626000 | -1.968154000 |
| 1 | 3.987090000 | -0.447228000 | -0.477168000 |
| 6 | 2.162213000 | -1.950739000 | -1.092689000 |
| 1 | 3.031393000 | -2.365918000 | -1.623565000 |
| 1 | 1.267423000 | -2.414741000 | -1.512831000 |
| 6 | 2.268963000 | -2.272702000 | 0.404452000 |
| 1 | 2.119011000 | -3.351922000 | 0.542207000 |
| 1 | 3.274542000 | -2.051256000 | 0.767947000 |
| 6 | 1.736388000 | 2.523299000 | 1.492270000 |
| 1 | 2.613500000 | 3.095731000 | 1.828597000 |
| 1 | 1.086762000 | 2.323278000 | 2.345528000 |
| 1 | 1.181366000 | 3.110456000 | 0.757397000 |
| 6 | 1.676225000 | -0.254644000 | -2.756737000 |
| 1 | 2.411262000 | -0.710437000 | -3.435853000 |
| 1 | 1.629992000 | 0.819549000 | -2.943408000 |
| 1 | 0.693570000 | -0.687254000 | -2.952798000 |
| 7 | -0.072914000 | 1.858600000 | -1.257637000 |
| 6 | -0.665535000 | 2.781425000 | -1.635561000 |
| 6 | -1.426110000 | 3.939256000 | -2.076156000 |
| 1 | -1.918006000 | 4.400703000 | -1.212898000 |
| 1 | -0.759831000 | 4.670148000 | -2.545444000 |
| 1 | -2.187889000 | 3.629012000 | -2.798345000 |
| 1 | -0.356993000 | 0.663671000 | 1.129103000 |
| 8 | -2.955563000 | 0.576063000 | 3.246202000 |
| 1 | -2.570445000 | 1.362543000 | 2.814418000 |
| 1 | -3.371483000 | 0.086633000 | 2.497771000 |
| 1 | -3.509958000 | -1.380443000 | 0.745218000 |
| 8 | -4.120330000 | -0.670353000 | 1.004265000 |
| 1 | -3.916154000 | 0.074635000 | 0.384555000 |
| 1 | -1.165992000 | 1.869692000 | 1.218134000 |
| 8 | -1.862199000 | 2.563782000 | 1.411472000 |
| 1 | -1.447395000 | 3.407963000 | 1.163797000 |
| 1 | -4.451144000 | 2.083100000 | -0.417022000 |
| 8 | -3.612448000 | 1.601008000 | -0.511945000 |
| 1 | -3.000298000 | 2.029084000 | 0.138434000 |



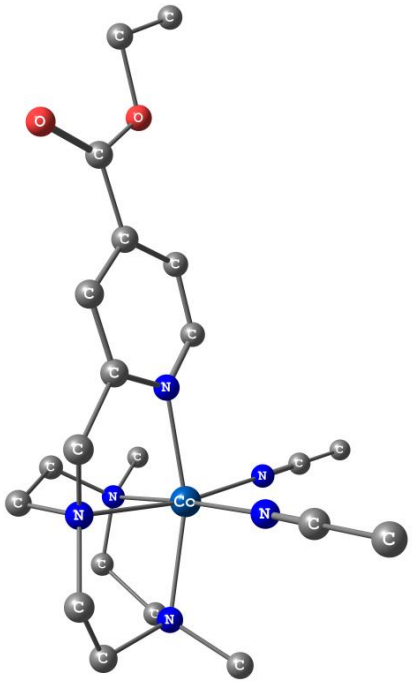
**$1^{H}$-TS2 (quartet, 1 AC, G = -2588.89270822, Imaginary frequency: -699.54 a.u.)**

| | | | |
|---|---|---|---|
| 27 | 0.602231000 | 0.210110000 | -0.074078000 |
| 7 | 1.152149000 | -1.402065000 | 1.274382000 |
| 7 | -0.912704000 | -1.203629000 | -0.519131000 |
| 7 | 2.194253000 | -0.653352000 | -1.272955000 |
| 7 | 2.292793000 | 1.224069000 | 0.897642000 |
| 6 | -0.120355000 | -2.081963000 | 1.592668000 |
| 1 | -0.671919000 | -1.446945000 | 2.294483000 |
| 1 | 0.043156000 | -3.052957000 | 2.076714000 |
| 6 | -0.970624000 | -2.233087000 | 0.351996000 |
| 6 | -1.801873000 | -3.330002000 | 0.129699000 |
| 1 | -1.819113000 | -4.146538000 | 0.845038000 |
| 6 | -2.595259000 | -3.355510000 | -1.019734000 |
| 1 | -3.249024000 | -4.200653000 | -1.214725000 |
| 6 | -2.533322000 | -2.284084000 | -1.913775000 |
| 1 | -3.132756000 | -2.263730000 | -2.818012000 |
| 6 | -1.674007000 | -1.227350000 | -1.624685000 |
| 1 | -1.582275000 | -0.370226000 | -2.284350000 |
| 6 | 1.721477000 | -0.676466000 | 2.438512000 |
| 1 | 2.159603000 | -1.372486000 | 3.168392000 |
| 1 | 0.892663000 | -0.151732000 | 2.919759000 |
| 6 | 2.778415000 | 0.347448000 | 2.008494000 |
| 1 | 3.043321000 | 0.958159000 | 2.879028000 |
| 1 | 3.697467000 | -0.152580000 | 1.699502000 |
| 6 | 3.268841000 | 1.337441000 | -0.215661000 |
| 1 | 4.232682000 | 1.730517000 | 0.142046000 |
| 1 | 2.855015000 | 2.057864000 | -0.927990000 |
| 6 | 3.489907000 | -0.004597000 | -0.912507000 |
| 1 | 4.094246000 | 0.154456000 | -1.813161000 |
| 1 | 4.061789000 | -0.679275000 | -0.273862000 |
| 6 | 2.160259000 | -2.094121000 | -0.921597000 |
| 1 | 3.025719000 | -2.624113000 | -1.346161000 |
| 1 | 1.260037000 | -2.512008000 | -1.378036000 |
| 6 | 2.128469000 | -2.306660000 | 0.597048000 |
| 1 | 1.878162000 | -3.353734000 | 0.802616000 |
| 1 | 3.118041000 | -2.136001000 | 1.023657000 |
| 6 | 1.920251000 | 2.557659000 | 1.406201000 |
| 1 | 2.799821000 | 3.096346000 | 1.788936000 |
| 1 | 1.190203000 | 2.443318000 | 2.210396000 |
| 1 | 1.462208000 | 3.140494000 | 0.603440000 |
| 6 | 1.891255000 | -0.456847000 | -2.704767000 |
| 1 | 2.607846000 | -0.996952000 | -3.340649000 |
| 1 | 1.937517000 | 0.609285000 | -2.937416000 |
| 1 | 0.880441000 | -0.816121000 | -2.915044000 |
| 7 | 0.062580000 | 1.839868000 | -1.291855000 |
| 6 | -0.449151000 | 2.801711000 | -1.682173000 |
| 6 | -1.104698000 | 4.013274000 | -2.135926000 |
| 1 | -1.782022000 | 3.778486000 | -2.962979000 |
| 1 | -1.680040000 | 4.436889000 | -1.305408000 |
| 1 | -0.356986000 | 4.738847000 | -2.471260000 |
| 1 | -0.560468000 | 0.903219000 | 1.220734000 |
| 8 | -3.447208000 | 1.116038000 | 2.993427000 |
| 1 | -2.916841000 | 1.788420000 | 2.507826000 |
| 1 | -3.755463000 | 0.514127000 | 2.277293000 |
| 1 | -3.721011000 | -1.158447000 | 0.626323000 |
| 8 | -4.303864000 | -0.392049000 | 0.755380000 |
| 1 | -3.957597000 | 0.295525000 | 0.128755000 |
| 1 | -1.144525000 | 1.696425000 | 1.208137000 |
| 8 | -1.968556000 | 2.687664000 | 1.240983000 |
| 1 | -1.406954000 | 3.454609000 | 1.033823000 |
| 1 | -4.192762000 | 2.248027000 | -0.876097000 |
| 8 | -3.393353000 | 1.700867000 | -0.801187000 |
| 1 | -2.847554000 | 2.141038000 | -0.079798000 |



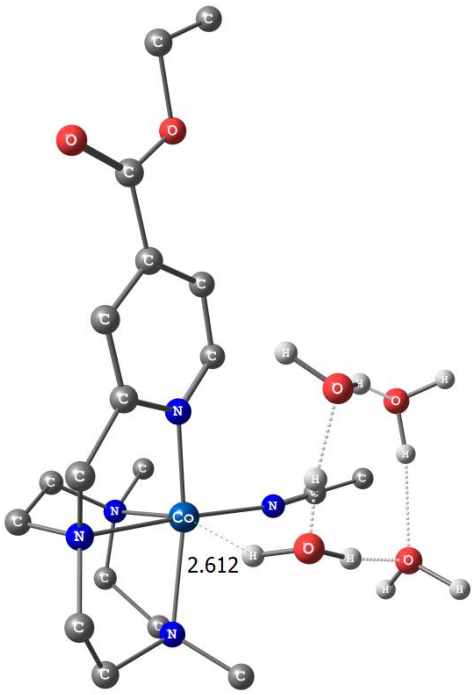
**$1^{CO2Et}$-$Co^{II}$ (quartet, 2 AC, G = -2682.36746940)**

| | | | |
|---|---|---|---|
| 27 | 1.517203000 | 0.199118000 | 0.160642000 |
| 7 | 1.206853000 | -1.813779000 | -0.595569000 |
| 7 | -0.646242000 | 0.068018000 | 0.113971000 |
| 7 | 1.690220000 | 0.658083000 | -2.007570000 |
| 7 | 3.593394000 | -0.323358000 | -0.105579000 |
| 6 | -0.045114000 | -2.288387000 | 0.029036000 |
| 1 | 0.164442000 | -2.535050000 | 1.074703000 |
| 1 | -0.422072000 | -3.197167000 | -0.455816000 |
| 6 | -1.097022000 | -1.198552000 | 0.005230000 |
| 6 | -2.457725000 | -1.480666000 | -0.090574000 |
| 1 | -2.795673000 | -2.506650000 | -0.188257000 |
| 6 | -3.373001000 | -0.424857000 | -0.064156000 |
| 6 | -2.896560000 | 0.886273000 | 0.046667000 |
| 1 | -3.568325000 | 1.735771000 | 0.062712000 |
| 6 | -1.522241000 | 1.083834000 | 0.125977000 |
| 1 | -1.101711000 | 2.080840000 | 0.207682000 |
| 6 | 2.412964000 | -2.536872000 | -0.115547000 |
| 1 | 2.462024000 | -3.552899000 | -0.531463000 |
| 1 | 2.328944000 | -2.619689000 | 0.970559000 |
| 6 | 3.690952000 | -1.771045000 | -0.475850000 |
| 1 | 4.537905000 | -2.234184000 | 0.042249000 |
| 1 | 3.899857000 | -1.853850000 | -1.543052000 |
| 6 | 4.044312000 | 0.585700000 | -1.191135000 |
| 1 | 5.077890000 | 0.356297000 | -1.489096000 |
| 1 | 4.026782000 | 1.599133000 | -0.778156000 |
| 6 | 3.124001000 | 0.512470000 | -2.405440000 |
| 1 | 3.402095000 | 1.303308000 | -3.110899000 |
| 1 | 3.258104000 | -0.430998000 | -2.937126000 |
| 6 | 0.827561000 | -0.374694000 | -2.636452000 |
| 1 | 0.964990000 | -0.383893000 | -3.727798000 |
| 1 | -0.207935000 | -0.090585000 | -2.437735000 |
| 6 | 1.103813000 | -1.780106000 | -2.088925000 |
| 1 | 0.302375000 | -2.448942000 | -2.421073000 |
| 1 | 2.029641000 | -2.175616000 | -2.508147000 |
| 6 | 4.353229000 | -0.049519000 | 1.133886000 |
| 1 | 5.434147000 | -0.148664000 | 0.961034000 |
| 1 | 4.048068000 | -0.754366000 | 1.909331000 |
| 1 | 4.134356000 | 0.965154000 | 1.478241000 |
| 6 | 1.193088000 | 2.006013000 | -2.348951000 |
| 1 | 1.155189000 | 2.148230000 | -3.438987000 |
| 1 | 1.856872000 | 2.756478000 | -1.915163000 |
| 1 | 0.191929000 | 2.143855000 | -1.933810000 |
| 7 | 1.545124000 | 2.212597000 | 0.706453000 |
| 6 | 1.559310000 | 3.330379000 | 1.003063000 |
| 6 | 1.579853000 | 4.734751000 | 1.364112000 |
| 1 | 1.459194000 | 5.344442000 | 0.462786000 |
| 1 | 0.763223000 | 4.947730000 | 2.061183000 |
| 1 | 2.536414000 | 4.974457000 | 1.840004000 |
| 7 | 1.396920000 | -0.458692000 | 2.205435000 |
| 6 | 1.330733000 | -0.898966000 | 3.273496000 |
| 6 | 1.248625000 | -1.457213000 | 4.610374000 |
| 1 | 0.203478000 | -1.675212000 | 4.852575000 |
| 1 | 1.833356000 | -2.381680000 | 4.656498000 |
| 1 | 1.647565000 | -0.738432000 | 5.333362000 |
| 6 | -4.835363000 | -0.736226000 | -0.166933000 |
| 8 | -5.271180000 | -1.867809000 | -0.346979000 |
| 8 | -5.601383000 | 0.346880000 | -0.037921000 |
| 6 | -7.051079000 | 0.166105000 | -0.121292000 |
| 1 | -7.283183000 | -0.236103000 | -1.111659000 |
| 1 | -7.344348000 | -0.563059000 | 0.638962000 |
| 6 | -7.680012000 | 1.522369000 | 0.111609000 |
| 1 | -7.360578000 | 2.240639000 | -0.651305000 |
| 1 | -8.770286000 | 1.424833000 | 0.060079000 |
| 1 | -7.414545000 | 1.912287000 | 1.100295000 |



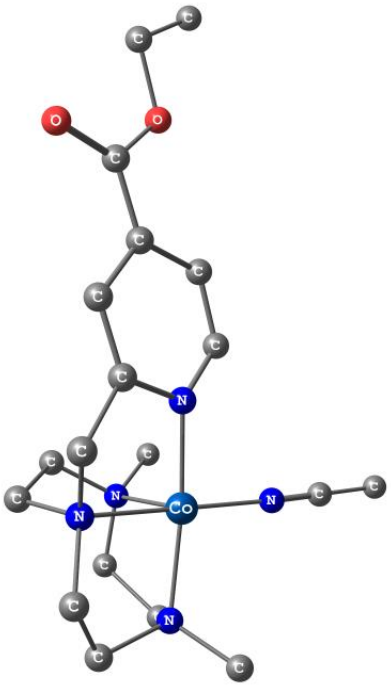
**$1^{CO2Et}$-$Co^{II}$_$H_3O^+$_$3H_2O$ (quartet, 1 AC, G = -2855.8695400)**

| | | | |
|---|---|---|---|
| 27 | -1.508529000 | -0.177455000 | 0.184498000 |
| 7 | -1.245152000 | -1.967713000 | -1.024023000 |
| 7 | 0.581388000 | -0.213647000 | 0.026708000 |
| 7 | -1.903729000 | -1.552931000 | 1.726179000 |
| 7 | -3.581116000 | -0.480856000 | -0.341657000 |
| 6 | 0.052587000 | -1.820333000 | -1.715653000 |
| 1 | -0.100597000 | -1.187601000 | -2.596729000 |
| 1 | 0.440110000 | -2.782841000 | -2.069212000 |
| 6 | 1.066458000 | -1.124653000 | -0.841665000 |
| 6 | 2.433210000 | -1.352551000 | -0.967062000 |
| 1 | 2.797620000 | -2.093095000 | -1.670257000 |
| 6 | 3.319448000 | -0.615622000 | -0.177850000 |
| 6 | 2.808242000 | 0.323543000 | 0.725654000 |
| 1 | 3.457750000 | 0.913221000 | 1.360900000 |
| 6 | 1.429133000 | 0.488243000 | 0.797507000 |
| 1 | 0.979886000 | 1.200216000 | 1.480856000 |
| 6 | -2.388047000 | -1.950976000 | -1.976589000 |
| 1 | -2.465547000 | -2.902126000 | -2.521145000 |
| 1 | -2.192870000 | -1.164355000 | -2.708980000 |
| 6 | -3.704533000 | -1.657247000 | -1.258436000 |
| 1 | -4.481635000 | -1.468088000 | -2.006852000 |
| 1 | -4.031135000 | -2.527329000 | -0.687975000 |
| 6 | -4.159264000 | -0.749895000 | 1.004811000 |
| 1 | -5.214679000 | -1.046775000 | 0.925109000 |
| 1 | -4.112703000 | 0.188925000 | 1.564198000 |
| 6 | -3.373710000 | -1.833068000 | 1.749678000 |
| 1 | -3.727526000 | -1.881572000 | 2.784861000 |
| 1 | -3.555046000 | -2.816280000 | 1.314129000 |
| 6 | -1.080903000 | -2.737525000 | 1.364200000 |
| 1 | -1.312849000 | -3.590080000 | 2.017588000 |
| 1 | -0.037869000 | -2.458323000 | 1.535476000 |
| 6 | -1.281699000 | -3.144379000 | -0.098544000 |
| 1 | -0.504584000 | -3.865194000 | -0.374900000 |
| 1 | -2.238906000 | -3.653525000 | -0.222693000 |
| 6 | -4.175877000 | 0.725755000 | -0.953201000 |
| 1 | -5.253113000 | 0.593282000 | -1.127144000 |
| 1 | -3.679626000 | 0.923786000 | -1.906801000 |
| 1 | -4.025760000 | 1.579808000 | -0.289883000 |
| 6 | -1.451828000 | -0.978651000 | 3.013943000 |
| 1 | -1.506001000 | -1.727383000 | 3.816032000 |
| 1 | -2.087632000 | -0.128528000 | 3.270489000 |
| 1 | -0.420622000 | -0.628726000 | 2.913050000 |
| 7 | -1.766208000 | 1.652063000 | 1.099410000 |
| 6 | -1.775323000 | 2.637645000 | 1.704636000 |
| 6 | -1.789597000 | 3.879296000 | 2.450812000 |
| 1 | -1.970618000 | 4.711957000 | 1.763543000 |
| 1 | -2.582969000 | 3.845633000 | 3.204583000 |
| 1 | -0.821467000 | 4.017864000 | 2.942805000 |
| 1 | -1.269509000 | 0.848703000 | -2.205221000 |
| 8 | -1.000283000 | 1.664923000 | -2.672539000 |
| 1 | -1.452677000 | 2.442984000 | -2.181878000 |
| 1 | 0.050513000 | 1.804664000 | -2.512208000 |
| 1 | 1.945645000 | 1.454761000 | -1.977895000 |
| 8 | 1.405739000 | 2.215389000 | -2.255884000 |
| 1 | 1.276004000 | 2.774871000 | -1.439850000 |
| 1 | -2.752161000 | 3.444027000 | -0.851082000 |
| 8 | -1.965468000 | 3.697055000 | -1.366875000 |
| 1 | -2.264052000 | 4.404981000 | -1.965817000 |
| 1 | 1.025368000 | 4.680391000 | -0.305467000 |
| 8 | 0.630925000 | 3.799822000 | -0.186394000 |
| 1 | -0.293208000 | 3.891410000 | -0.507235000 |
| 6 | 4.788029000 | -0.875265000 | -0.327971000 |
| 8 | 5.243059000 | -1.703584000 | -1.108378000 |
| 8 | 5.535447000 | -0.115642000 | 0.471712000 |
| 6 | 6.986339000 | -0.305349000 | 0.403725000 |
| 1 | 7.198151000 | -1.353065000 | 0.634971000 |
| 1 | 7.303784000 | -0.094791000 | -0.621466000 |
| 6 | 7.610708000 | 0.640277000 | 1.404943000 |
| 1 | 7.375176000 | 1.682650000 | 1.164421000 |
| 1 | 7.264402000 | 0.422132000 | 2.420999000 |
| 1 | 8.699376000 | 0.517105000 | 1.378156000 |



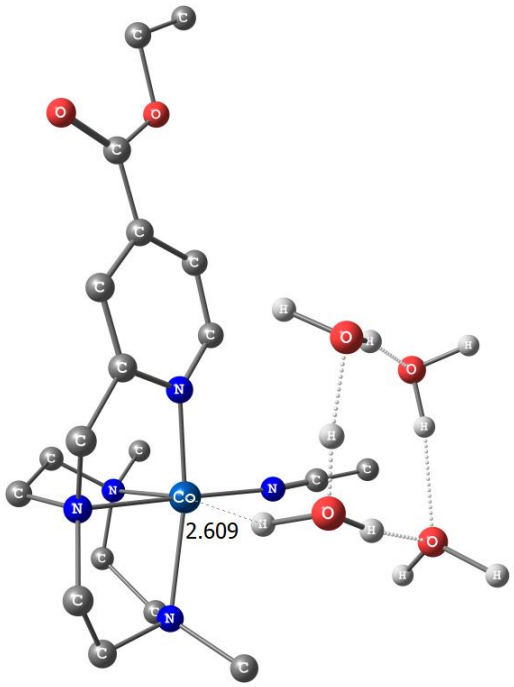
**$1^{CO2Et}$-$Co^{I}$ (triplet, 1 AC, G = -2549.70615354)**

| | | | |
|---|---|---|---|
| 27 | -0.335572000 | 0.227927000 | -0.451784000 |
| 7 | 0.456261000 | -1.840469000 | -0.444013000 |
| 7 | 1.714335000 | 0.612409000 | -0.524958000 |
| 7 | -0.512485000 | -0.180246000 | 1.710437000 |
| 7 | -2.259313000 | -0.900430000 | -0.501124000 |
| 6 | 1.739748000 | -1.722501000 | -1.156267000 |
| 1 | 1.517904000 | -1.607392000 | -2.223758000 |
| 1 | 2.366104000 | -2.619444000 | -1.040081000 |
| 6 | 2.485934000 | -0.488502000 | -0.695943000 |
| 6 | 3.860352000 | -0.471307000 | -0.469330000 |
| 1 | 4.438694000 | -1.380921000 | -0.604647000 |
| 6 | 4.470706000 | 0.718143000 | -0.058594000 |
| 1 | 5.540223000 | 0.753499000 | 0.128355000 |
| 6 | 3.675761000 | 1.854564000 | 0.115127000 |
| 1 | 4.101323000 | 2.800323000 | 0.436935000 |
| 6 | 2.307862000 | 1.754817000 | -0.128704000 |
| 1 | 1.645937000 | 2.607422000 | -0.004149000 |
| 6 | -0.562859000 | -2.608687000 | -1.185807000 |
| 1 | -0.357190000 | -3.692015000 | -1.173301000 |
| 1 | -0.520642000 | -2.270226000 | -2.225855000 |
| 6 | -1.974038000 | -2.353448000 | -0.638324000 |
| 1 | -2.698640000 | -2.825680000 | -1.314703000 |
| 1 | -2.102558000 | -2.845121000 | 0.328293000 |
| 6 | -2.826771000 | -0.532107000 | 0.812949000 |
| 1 | -3.768747000 | -1.071718000 | 1.014575000 |
| 1 | -3.058477000 | 0.536751000 | 0.767442000 |
| 6 | -1.848817000 | -0.787001000 | 1.963783000 |
| 1 | -2.282607000 | -0.383591000 | 2.888326000 |
| 1 | -1.732065000 | -1.860205000 | 2.129700000 |
| 6 | 0.598920000 | -1.119146000 | 1.967888000 |
| 1 | 0.548698000 | -1.533780000 | 2.989271000 |
| 1 | 1.525082000 | -0.543292000 | 1.894131000 |
| 6 | 0.630725000 | -2.282970000 | 0.964517000 |
| 1 | 1.583972000 | -2.815371000 | 1.083031000 |
| 1 | -0.152307000 | -3.004501000 | 1.205074000 |
| 6 | -3.111087000 | -0.423757000 | -1.598672000 |
| 1 | -4.113687000 | -0.884043000 | -1.575493000 |
| 1 | -2.635368000 | -0.665436000 | -2.554292000 |
| 1 | -3.218466000 | 0.662594000 | -1.533464000 |
| 6 | -0.340642000 | 1.059679000 | 2.478663000 |
| 1 | -0.321176000 | 0.873249000 | 3.566017000 |
| 1 | -1.165368000 | 1.740551000 | 2.251768000 |
| 1 | 0.593788000 | 1.545120000 | 2.182909000 |
| 7 | -1.076508000 | 2.006547000 | -0.559000000 |
| 6 | -1.569763000 | 3.063975000 | -0.564668000 |
| 6 | -2.185105000 | 4.383188000 | -0.559583000 |
| 1 | -2.235157000 | 4.768806000 | 0.464897000 |
| 1 | -1.598403000 | 5.078314000 | -1.170376000 |
| 1 | -3.202009000 | 4.327733000 | -0.964045000 |



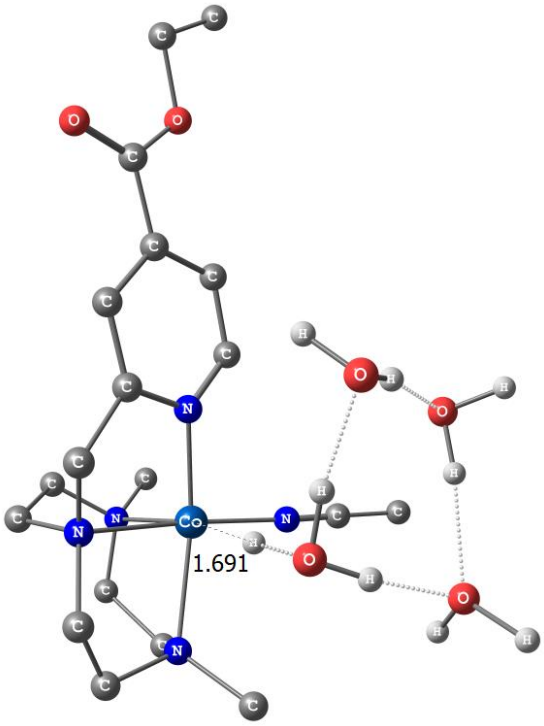
**$1^{CO2Et}$-$Co^{I}$_$H_3O^+$_$3H_2O$ (triplet, 1 AC, G = -2855.97736223)**

| | | | |
|---|---|---|---|
| 27 | -1.478947000 | -0.152309000 | 0.088438000 |
| 7 | -1.254081000 | -1.979771000 | -1.079351000 |
| 7 | 0.489099000 | -0.100058000 | -0.117084000 |
| 7 | -1.657426000 | -1.522039000 | 1.753210000 |
| 7 | -3.576476000 | -0.599262000 | -0.166696000 |
| 6 | -0.005426000 | -1.753875000 | -1.834381000 |
| 1 | -0.246779000 | -1.111497000 | -2.689204000 |
| 1 | 0.408339000 | -2.688693000 | -2.236229000 |
| 6 | 1.015227000 | -1.043015000 | -0.973648000 |
| 6 | 2.364555000 | -1.296801000 | -1.059931000 |
| 1 | 2.720729000 | -2.060805000 | -1.743941000 |
| 6 | 3.287522000 | -0.567245000 | -0.258472000 |
| 6 | 2.736796000 | 0.401279000 | 0.625253000 |
| 1 | 3.374418000 | 0.994242000 | 1.271353000 |
| 6 | 1.374936000 | 0.593877000 | 0.662763000 |
| 1 | 0.932906000 | 1.328020000 | 1.327176000 |
| 6 | -2.471757000 | -2.011493000 | -1.916436000 |
| 1 | -2.570802000 | -2.958940000 | -2.468218000 |
| 1 | -2.379849000 | -1.204311000 | -2.648930000 |
| 6 | -3.726541000 | -1.782475000 | -1.066345000 |
| 1 | -4.587826000 | -1.646097000 | -1.730775000 |
| 1 | -3.942110000 | -2.666195000 | -0.463917000 |
| 6 | -4.014848000 | -0.868442000 | 1.224813000 |
| 1 | -5.054249000 | -1.230002000 | 1.251831000 |
| 1 | -3.972953000 | 0.085359000 | 1.758708000 |
| 6 | -3.099275000 | -1.881463000 | 1.916295000 |
| 1 | -3.358266000 | -1.926037000 | 2.980331000 |
| 1 | -3.266868000 | -2.883211000 | 1.517576000 |
| 6 | -0.826896000 | -2.670961000 | 1.309211000 |
| 1 | -0.950508000 | -3.528665000 | 1.988086000 |
| 1 | 0.215168000 | -2.347980000 | 1.368565000 |
| 6 | -1.152019000 | -3.118871000 | -0.124326000 |
| 1 | -0.373090000 | -3.818216000 | -0.452261000 |
| 1 | -2.091291000 | -3.674611000 | -0.140056000 |
| 6 | -4.270863000 | 0.574499000 | -0.729446000 |
| 1 | -5.356574000 | 0.407811000 | -0.795678000 |
| 1 | -3.879342000 | 0.774348000 | -1.730902000 |
| 1 | -4.083723000 | 1.445431000 | -0.097323000 |
| 6 | -1.113315000 | -0.940832000 | 2.994445000 |
| 1 | -1.073829000 | -1.687171000 | 3.802152000 |
| 1 | -1.745442000 | -0.107086000 | 3.308839000 |
| 1 | -0.106069000 | -0.560299000 | 2.805025000 |
| 7 | -1.708077000 | 1.592750000 | 1.148206000 |
| 6 | -1.743992000 | 2.572006000 | 1.764969000 |
| 6 | -1.781210000 | 3.806004000 | 2.528183000 |
| 1 | -1.999017000 | 4.642654000 | 1.856505000 |
| 1 | -2.558164000 | 3.745267000 | 3.297094000 |
| 1 | -0.809105000 | 3.970335000 | 3.004367000 |
| 1 | -1.351278000 | 0.849510000 | -2.317553000 |
| 8 | -1.129447000 | 1.698476000 | -2.752295000 |
| 1 | -1.587506000 | 2.430437000 | -2.200141000 |
| 1 | -0.078090000 | 1.856071000 | -2.602675000 |
| 1 | 1.752315000 | 1.444739000 | -2.013720000 |
| 8 | 1.280087000 | 2.235544000 | -2.330396000 |
| 1 | 1.146331000 | 2.807384000 | -1.523110000 |
| 1 | -2.838648000 | 3.308205000 | -0.731618000 |
| 8 | -2.115512000 | 3.619431000 | -1.305705000 |
| 1 | -2.502203000 | 4.321517000 | -1.858957000 |
| 1 | 0.877727000 | 4.743594000 | -0.439229000 |
| 8 | 0.527323000 | 3.852788000 | -0.270340000 |
| 1 | -0.418135000 | 3.897585000 | -0.534468000 |
| 6 | 4.707299000 | -0.839877000 | -0.358206000 |
| 8 | 5.220604000 | -1.677378000 | -1.124290000 |
| 8 | 5.467071000 | -0.083597000 | 0.482763000 |
| 6 | 6.903001000 | -0.297929000 | 0.454728000 |
| 1 | 7.106036000 | -1.346802000 | 0.694144000 |
| 1 | 7.269198000 | -0.094071000 | -0.556692000 |
| 6 | 7.518397000 | 0.638979000 | 1.474007000 |
| 1 | 7.302828000 | 1.685037000 | 1.228601000 |
| 1 | 7.139393000 | 0.428615000 | 2.480474000 |
| 1 | 8.606062000 | 0.503232000 | 1.480200000 |



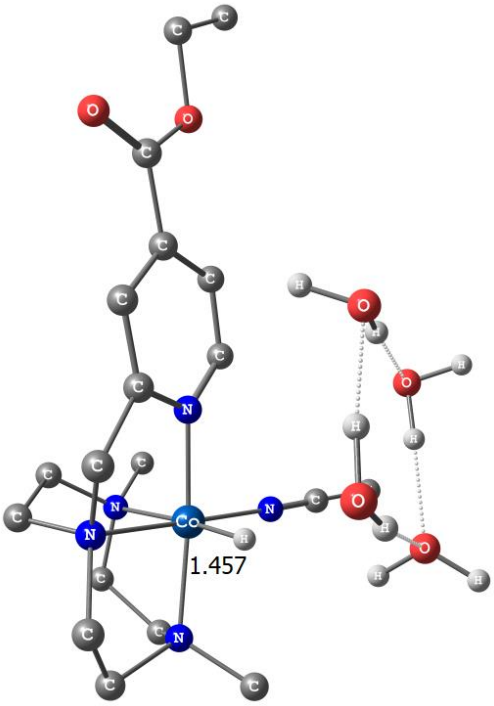
**$1^{CO2Et}$-TS1 (triplet, 1 AC, G = -2855.97490732, Imaginary frequency: -960.21)**

| | | | |
|---|---|---|---|
| 27 | -1.414557000 | -0.197573000 | 0.172481000 |
| 7 | -1.178521000 | -1.969887000 | -1.095199000 |
| 7 | 0.595653000 | -0.125076000 | -0.125098000 |
| 7 | -1.729913000 | -1.686387000 | 1.724040000 |
| 7 | -3.517197000 | -0.548162000 | -0.250600000 |
| 6 | 0.089271000 | -1.770611000 | -1.823935000 |
| 1 | -0.113404000 | -1.129489000 | -2.688859000 |
| 1 | 0.503070000 | -2.713290000 | -2.202984000 |
| 6 | 1.102796000 | -1.049928000 | -0.967912000 |
| 6 | 2.473023000 | -1.265717000 | -1.067861000 |
| 1 | 2.856200000 | -2.015126000 | -1.751859000 |
| 6 | 3.341840000 | -0.513148000 | -0.269757000 |
| 6 | 2.806380000 | 0.436428000 | 0.608522000 |
| 1 | 3.439298000 | 1.040138000 | 1.247325000 |
| 6 | 1.426672000 | 0.597837000 | 0.646258000 |
| 1 | 0.960391000 | 1.325239000 | 1.301388000 |
| 6 | -2.359316000 | -1.923532000 | -1.992900000 |
| 1 | -2.451917000 | -2.844914000 | -2.586870000 |
| 1 | -2.205925000 | -1.088371000 | -2.679666000 |
| 6 | -3.651712000 | -1.689065000 | -1.207267000 |
| 1 | -4.463929000 | -1.493295000 | -1.916299000 |
| 1 | -3.934916000 | -2.589735000 | -0.660366000 |
| 6 | -4.014191000 | -0.893850000 | 1.112093000 |
| 1 | -5.070423000 | -1.200975000 | 1.070628000 |
| 1 | -3.952592000 | 0.019862000 | 1.710845000 |
| 6 | -3.184805000 | -1.996306000 | 1.775936000 |
| 1 | -3.515412000 | -2.107468000 | 2.815773000 |
| 1 | -3.366190000 | -2.957764000 | 1.292667000 |
| 6 | -0.894727000 | -2.818394000 | 1.258127000 |
| 1 | -1.054967000 | -3.713873000 | 1.879029000 |
| 1 | 0.148267000 | -2.511729000 | 1.383028000 |
| 6 | -1.157622000 | -3.172803000 | -0.210793000 |
| 1 | -0.386289000 | -3.877320000 | -0.543935000 |
| 1 | -2.112498000 | -3.692432000 | -0.307743000 |
| 6 | -4.223858000 | 0.646736000 | -0.754470000 |
| 1 | -5.310482000 | 0.478619000 | -0.797098000 |
| 1 | -3.859570000 | 0.884534000 | -1.755565000 |
| 1 | -4.019094000 | 1.493473000 | -0.095184000 |
| 6 | -1.239713000 | -1.162323000 | 3.011051000 |
| 1 | -1.243544000 | -1.937985000 | 3.792310000 |
| 1 | -1.877425000 | -0.333292000 | 3.328259000 |
| 1 | -0.220041000 | -0.785046000 | 2.883519000 |
| 7 | -1.690725000 | 1.521598000 | 1.147021000 |
| 6 | -1.811689000 | 2.519794000 | 1.721881000 |
| 6 | -1.967673000 | 3.786297000 | 2.414448000 |
| 1 | -2.358369000 | 4.535129000 | 1.717512000 |
| 1 | -2.663805000 | 3.670978000 | 3.251457000 |
| 1 | -0.996788000 | 4.119931000 | 2.794138000 |
| 1 | -1.393870000 | 0.779561000 | -1.206917000 |
| 8 | -1.338005000 | 1.483145000 | -2.253537000 |
| 1 | -1.747230000 | 2.345674000 | -1.954036000 |
| 1 | -0.354649000 | 1.684561000 | -2.339101000 |
| 1 | 1.823682000 | 1.585784000 | -2.027737000 |
| 8 | 1.227084000 | 2.286926000 | -2.340438000 |
| 1 | 1.065118000 | 2.863397000 | -1.550020000 |
| 1 | -3.056579000 | 3.575366000 | -0.698945000 |
| 8 | -2.309992000 | 3.814303000 | -1.276789000 |
| 1 | -2.674622000 | 4.443162000 | -1.923643000 |
| 1 | 0.719591000 | 4.813384000 | -0.431855000 |
| 8 | 0.366106000 | 3.920560000 | -0.282741000 |
| 1 | -0.574695000 | 3.972219000 | -0.562611000 |
| 6 | 4.812978000 | -0.763701000 | -0.372134000 |
| 8 | 5.305916000 | -1.581676000 | -1.141792000 |
| 8 | 5.526082000 | -0.006875000 | 0.464083000 |
| 6 | 6.978192000 | -0.184101000 | 0.457092000 |
| 1 | 7.190372000 | -1.232131000 | 0.687199000 |
| 1 | 7.340696000 | 0.039987000 | -0.550207000 |
| 6 | 7.548191000 | 0.756750000 | 1.495449000 |
| 1 | 7.157453000 | 0.525412000 | 2.492380000 |
| 1 | 7.313108000 | 1.799349000 | 1.255062000 |
| 1 | 8.638172000 | 0.645124000 | 1.517567000 |



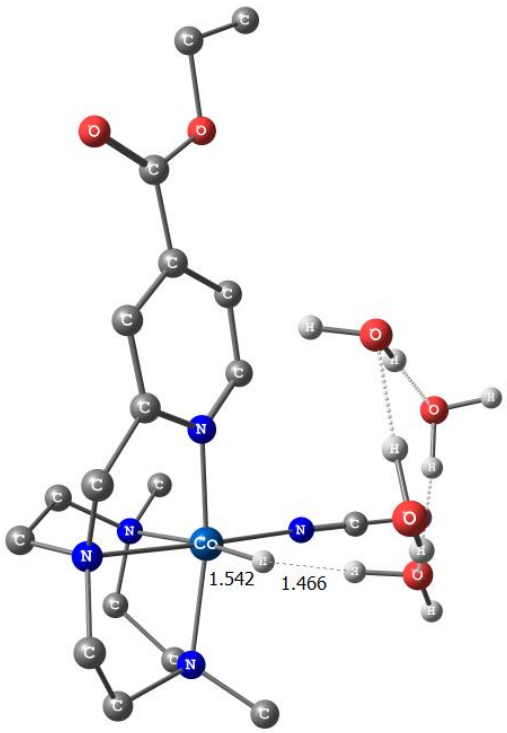
**$1^{CO2Et}$-$Co^{III}$-H_4$H_2O$ (singlet, 1 AC, G = -2856.01034731)**

| | | | |
|---|---|---|---|
| 27 | -1.591427000 | -0.157113000 | 0.046762000 |
| 7 | -1.461514000 | -1.584434000 | -1.270799000 |
| 7 | 0.360204000 | -0.210786000 | 0.018162000 |
| 7 | -1.805867000 | -1.651121000 | 1.504472000 |
| 7 | -3.569761000 | -0.247646000 | -0.168824000 |
| 6 | -0.190498000 | -1.347574000 | -2.015250000 |
| 1 | -0.360256000 | -0.526049000 | -2.717824000 |
| 1 | 0.111321000 | -2.234287000 | -2.579815000 |
| 6 | 0.851344000 | -0.913362000 | -1.030971000 |
| 6 | 2.208993000 | -1.166599000 | -1.170258000 |
| 1 | 2.567108000 | -1.745976000 | -2.013572000 |
| 6 | 3.093370000 | -0.665648000 | -0.210133000 |
| 6 | 2.582088000 | 0.079266000 | 0.856881000 |
| 1 | 3.227043000 | 0.495391000 | 1.620801000 |
| 6 | 1.209185000 | 0.281214000 | 0.936155000 |
| 1 | 0.774793000 | 0.842162000 | 1.752249000 |
| 6 | -2.660467000 | -1.428276000 | -2.153045000 |
| 1 | -2.772562000 | -2.299931000 | -2.807652000 |
| 1 | -2.494401000 | -0.540664000 | -2.764657000 |
| 6 | -3.882753000 | -1.237124000 | -1.271981000 |
| 1 | -4.721782000 | -0.869315000 | -1.867975000 |
| 1 | -4.202610000 | -2.178180000 | -0.825940000 |
| 6 | -4.079936000 | -0.724831000 | 1.156707000 |
| 1 | -5.145540000 | -0.974016000 | 1.080392000 |
| 1 | -3.971155000 | 0.106286000 | 1.856920000 |
| 6 | -3.277365000 | -1.924795000 | 1.636443000 |
| 1 | -3.525790000 | -2.138237000 | 2.680467000 |
| 1 | -3.528116000 | -2.821140000 | 1.067252000 |
| 6 | -1.075601000 | -2.796229000 | 0.896584000 |
| 1 | -1.304495000 | -3.731656000 | 1.424380000 |
| 1 | -0.008023000 | -2.598694000 | 1.013451000 |
| 6 | -1.440351000 | -2.933573000 | -0.576639000 |
| 1 | -0.724833000 | -3.588040000 | -1.080019000 |
| 1 | -2.424385000 | -3.385864000 | -0.691204000 |
| 6 | -4.201395000 | 1.058965000 | -0.503048000 |
| 1 | -5.291609000 | 0.944434000 | -0.531555000 |
| 1 | -3.842477000 | 1.389562000 | -1.478618000 |
| 1 | -3.939718000 | 1.799138000 | 0.253470000 |
| 6 | -1.234009000 | -1.329717000 | 2.831712000 |
| 1 | -1.296232000 | -2.201749000 | 3.495737000 |
| 1 | -1.789413000 | -0.500852000 | 3.274329000 |
| 1 | -0.187451000 | -1.040521000 | 2.724337000 |
| 7 | -1.662825000 | 1.291021000 | 1.266145000 |
| 6 | -1.660043000 | 2.202153000 | 1.973863000 |
| 6 | -1.646122000 | 3.358384000 | 2.846101000 |
| 1 | -1.767119000 | 4.265020000 | 2.244572000 |
| 1 | -2.464048000 | 3.285224000 | 3.569985000 |
| 1 | -0.690180000 | 3.399438000 | 3.377869000 |
| 1 | -1.507560000 | 0.813156000 | -1.036613000 |
| 8 | -0.229338000 | 2.247986000 | -3.264085000 |
| 1 | -0.773441000 | 2.721421000 | -2.600351000 |
| 1 | 0.664223000 | 2.230978000 | -2.849547000 |
| 1 | 2.510358000 | 1.492206000 | -1.718053000 |
| 8 | 2.245445000 | 2.406164000 | -1.911697000 |
| 1 | 1.826327000 | 2.731859000 | -1.075995000 |
| 1 | -2.135081000 | 2.995367000 | -0.716563000 |
| 8 | -1.518106000 | 3.625763000 | -1.125100000 |
| 1 | -1.991673000 | 4.475074000 | -1.146479000 |
| 1 | 1.245044000 | 4.417897000 | 0.284392000 |
| 8 | 0.906256000 | 3.506874000 | 0.266704000 |
| 1 | 0.020175000 | 3.580050000 | -0.161769000 |
| 6 | 4.557042000 | -0.943471000 | -0.369707000 |
| 8 | 5.010468000 | -1.632531000 | -1.276013000 |
| 8 | 5.298621000 | -0.363096000 | 0.572238000 |
| 6 | 6.746378000 | -0.575196000 | 0.509214000 |
| 1 | 6.928944000 | -1.652485000 | 0.555879000 |
| 1 | 7.098885000 | -0.194575000 | -0.453506000 |
| 6 | 7.358831000 | 0.162660000 | 1.678664000 |
| 1 | 7.150228000 | 1.236463000 | 1.621199000 |
| 1 | 6.978179000 | -0.223006000 | 2.630722000 |
| 1 | 8.445276000 | 0.020160000 | 1.658523000 |



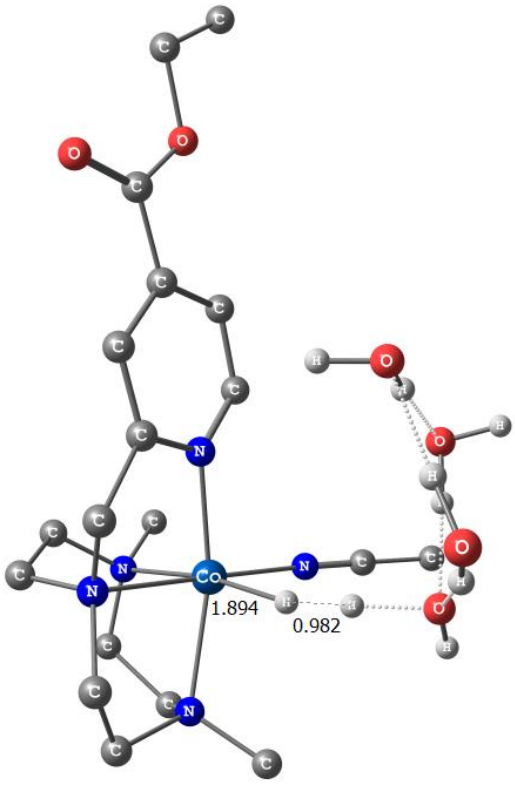
**$1^{CO2Et}$-$Co^{II}$-H_$4H_2O$ (doublet, 1 AC, G = -2856.13899550)**

| | | | |
|---|---|---|---|
| 27 | 1.664566000 | -0.046859000 | 0.007358000 |
| 7 | 1.360488000 | -1.744194000 | 1.332284000 |
| 7 | -0.470342000 | -0.205410000 | 0.025859000 |
| 7 | 1.870938000 | -1.728886000 | -1.504025000 |
| 7 | 3.756988000 | -0.556859000 | 0.340648000 |
| 6 | 0.099440000 | -1.431553000 | 2.033626000 |
| 1 | 0.300283000 | -0.612822000 | 2.733284000 |
| 1 | -0.274843000 | -2.288863000 | 2.607271000 |
| 6 | -0.939867000 | -0.951059000 | 1.048068000 |
| 6 | -2.296550000 | -1.228734000 | 1.184407000 |
| 1 | -2.646624000 | -1.841168000 | 2.008062000 |
| 6 | -3.192492000 | -0.719719000 | 0.238420000 |
| 6 | -2.698283000 | 0.057686000 | -0.814905000 |
| 1 | -3.353602000 | 0.472848000 | -1.570961000 |
| 6 | -1.327347000 | 0.286651000 | -0.880736000 |
| 1 | -0.893951000 | 0.877323000 | -1.680666000 |
| 6 | 2.546008000 | -1.683392000 | 2.221838000 |
| 1 | 2.585278000 | -2.548056000 | 2.899969000 |
| 1 | 2.444292000 | -0.777128000 | 2.823290000 |
| 6 | 3.838741000 | -1.606413000 | 1.403769000 |
| 1 | 4.673837000 | -1.390953000 | 2.079615000 |
| 1 | 4.059669000 | -2.570386000 | 0.943728000 |
| 6 | 4.215896000 | -1.036788000 | -0.987880000 |
| 1 | 5.250692000 | -1.408086000 | -0.934932000 |
| 1 | 4.204881000 | -0.169632000 | -1.655818000 |
| 6 | 3.306469000 | -2.127428000 | -1.552503000 |
| 1 | 3.608638000 | -2.335489000 | -2.585996000 |
| 1 | 3.442689000 | -3.061516000 | -1.003886000 |
| 6 | 1.010850000 | -2.791849000 | -0.939002000 |
| 1 | 1.155877000 | -3.745308000 | -1.471220000 |
| 1 | -0.025118000 | -2.484108000 | -1.097255000 |
| 6 | 1.271655000 | -3.018260000 | 0.555907000 |
| 1 | 0.472907000 | -3.649121000 | 0.962377000 |
| 1 | 2.200845000 | -3.572358000 | 0.694528000 |
| 6 | 4.509511000 | 0.650056000 | 0.736935000 |
| 1 | 5.590872000 | 0.450269000 | 0.766910000 |
| 1 | 4.173460000 | 0.976874000 | 1.722976000 |
| 1 | 4.310737000 | 1.454870000 | 0.023662000 |
| 6 | 1.394093000 | -1.338977000 | -2.841563000 |
| 1 | 1.389765000 | -2.195906000 | -3.533610000 |
| 1 | 2.045084000 | -0.560637000 | -3.246231000 |
| 1 | 0.380355000 | -0.937196000 | -2.768221000 |
| 7 | 1.855469000 | 1.436144000 | -1.447173000 |
| 6 | 1.855540000 | 2.388628000 | -2.104036000 |
| 6 | 1.855495000 | 3.600973000 | -2.898621000 |
| 1 | 1.981566000 | 4.465326000 | -2.238111000 |
| 1 | 2.675963000 | 3.569741000 | -3.622817000 |
| 1 | 0.903533000 | 3.687874000 | -3.431762000 |
| 1 | 1.637333000 | 1.143226000 | 1.325038000 |
| 8 | -0.207093000 | 3.807238000 | 3.195781000 |
| 1 | 0.502698000 | 3.835094000 | 2.522208000 |
| 1 | -0.960164000 | 3.388573000 | 2.717884000 |
| 1 | -2.192273000 | 1.723103000 | 1.625384000 |
| 8 | -2.254193000 | 2.691914000 | 1.588195000 |
| 1 | -1.752135000 | 2.945884000 | 0.773246000 |
| 1 | 1.657928000 | 2.529271000 | 1.079310000 |
| 8 | 1.603505000 | 3.544405000 | 0.991858000 |
| 1 | 2.382050000 | 3.794899000 | 0.465088000 |
| 1 | -0.986063000 | 4.598506000 | -0.520363000 |
| 8 | -0.718970000 | 3.663944000 | -0.514341000 |
| 1 | 0.144702000 | 3.655441000 | -0.026696000 |
| 6 | -4.647016000 | -1.039202000 | 0.385656000 |
| 8 | -5.094388000 | -1.730259000 | 1.294776000 |
| 8 | -5.398063000 | -0.496675000 | -0.574181000 |
| 6 | -6.838174000 | -0.751156000 | -0.522240000 |
| 1 | -6.990448000 | -1.833217000 | -0.571053000 |
| 1 | -7.210773000 | -0.381860000 | 0.437371000 |
| 6 | -7.463603000 | -0.031012000 | -1.696117000 |
| 1 | -7.067286000 | -0.406858000 | -2.645758000 |
| 1 | -8.546070000 | -0.202020000 | -1.682094000 |
| 1 | -7.283227000 | 1.047926000 | -1.638411000 |



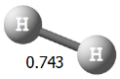
### $1^{CO2Et}$-TS2 (quartet, 1 AC, G = -2856.13034575, imaginary frequency: -656.12)

| | | | |
|---|---|---|---|
| 27 | 1.590895000 | -0.147319000 | -0.129939000 |
| 7 | 1.307487000 | -1.675111000 | 1.387605000 |
| 7 | -0.525546000 | -0.198297000 | -0.027084000 |
| 7 | 1.896719000 | -1.899729000 | -1.396294000 |
| 7 | 3.705037000 | -0.471688000 | 0.315257000 |
| 6 | 0.027228000 | -1.333407000 | 2.041519000 |
| 1 | 0.207910000 | -0.479360000 | 2.703545000 |
| 1 | -0.355407000 | -2.158483000 | 2.654521000 |
| 6 | -1.001514000 | -0.900185000 | 1.022134000 |
| 6 | -2.362264000 | -1.154370000 | 1.167827000 |
| 1 | -2.721386000 | -1.728507000 | 2.014842000 |
| 6 | -3.251237000 | -0.663950000 | 0.205642000 |
| 6 | -2.748735000 | 0.067231000 | -0.876333000 |
| 1 | -3.399749000 | 0.465768000 | -1.644783000 |
| 6 | -1.374644000 | 0.271244000 | -0.952882000 |
| 1 | -0.930342000 | 0.823535000 | -1.774148000 |
| 6 | 2.479388000 | -1.457701000 | 2.275675000 |
| 1 | 2.547273000 | -2.238814000 | 3.046378000 |
| 1 | 2.324946000 | -0.497542000 | 2.773518000 |
| 6 | 3.789257000 | -1.405118000 | 1.482805000 |
| 1 | 4.590412000 | -1.085085000 | 2.158264000 |
| 1 | 4.067479000 | -2.400105000 | 1.133296000 |
| 6 | 4.209651000 | -1.076702000 | -0.944188000 |
| 1 | 5.253542000 | -1.406306000 | -0.831969000 |
| 1 | 4.183781000 | -0.289387000 | -1.703684000 |
| 6 | 3.346849000 | -2.253758000 | -1.397644000 |
| 1 | 3.659759000 | -2.558446000 | -2.403134000 |
| 1 | 3.503689000 | -3.119960000 | -0.753178000 |
| 6 | 1.052676000 | -2.942944000 | -0.763927000 |
| 1 | 1.239338000 | -3.927672000 | -1.217331000 |
| 1 | 0.012882000 | -2.676301000 | -0.967650000 |
| 6 | 1.284768000 | -3.024395000 | 0.749126000 |
| 1 | 0.495649000 | -3.639625000 | 1.195801000 |
| 1 | 2.228093000 | -3.529054000 | 0.963000000 |
| 6 | 4.407058000 | 0.793963000 | 0.603519000 |
| 1 | 5.487214000 | 0.628638000 | 0.729453000 |
| 1 | 4.000392000 | 1.229476000 | 1.518581000 |
| 1 | 4.243659000 | 1.496440000 | -0.217669000 |
| 6 | 1.423917000 | -1.608643000 | -2.764680000 |
| 1 | 1.431074000 | -2.513480000 | -3.389850000 |
| 1 | 2.073902000 | -0.855795000 | -3.215713000 |
| 1 | 0.406474000 | -1.210110000 | -2.720973000 |
| 7 | 1.876773000 | 1.329569000 | -1.565118000 |
| 6 | 1.983369000 | 2.331266000 | -2.133745000 |
| 6 | 2.116520000 | 3.603599000 | -2.815635000 |
| 1 | 1.189867000 | 3.831107000 | -3.351957000 |
| 1 | 2.305917000 | 4.386429000 | -2.073048000 |
| 1 | 2.948804000 | 3.562603000 | -3.525430000 |
| 1 | 1.511742000 | 1.220253000 | 1.177958000 |
| 8 | 0.021417000 | 3.615557000 | 3.205984000 |
| 1 | 0.706550000 | 3.659671000 | 2.500860000 |
| 1 | -0.773527000 | 3.285688000 | 2.728051000 |
| 1 | -2.156168000 | 1.776566000 | 1.581155000 |
| 8 | -2.136850000 | 2.747737000 | 1.574184000 |
| 1 | -1.614151000 | 2.983929000 | 0.764466000 |
| 1 | 1.601743000 | 2.191436000 | 1.059825000 |
| 8 | 1.665181000 | 3.481266000 | 0.964399000 |
| 1 | 2.480578000 | 3.629897000 | 0.455052000 |
| 1 | -0.802432000 | 4.557278000 | -0.561706000 |
| 8 | -0.558644000 | 3.617368000 | -0.523230000 |
| 1 | 0.311833000 | 3.600463000 | -0.017940000 |
| 6 | -4.711885000 | -0.951360000 | 0.367881000 |
| 8 | -5.163988000 | -1.637230000 | 1.278203000 |
| 8 | -5.460164000 | -0.384676000 | -0.579389000 |
| 6 | -6.905007000 | -0.609173000 | -0.515580000 |
| 1 | -7.079279000 | -1.687932000 | -0.562863000 |
| 1 | -7.261789000 | -0.232164000 | 0.447028000 |
| 6 | -7.524847000 | 0.123722000 | -1.684542000 |
| 1 | -7.141536000 | -0.258142000 | -2.637097000 |
| 1 | -8.610089000 | -0.027815000 | -1.663778000 |
| 1 | -7.325012000 | 1.199228000 | -1.626944000 |



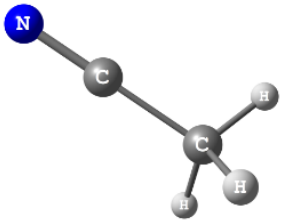

### $H_2$ (singlet, G = -1.178796004)

| | | | |
|---|---|---|---|
| 1 | -0.491715000 | 0.000982000 | -7.962985000 |
| 1 | -0.505985000 | -0.531402000 | -7.445272000 |



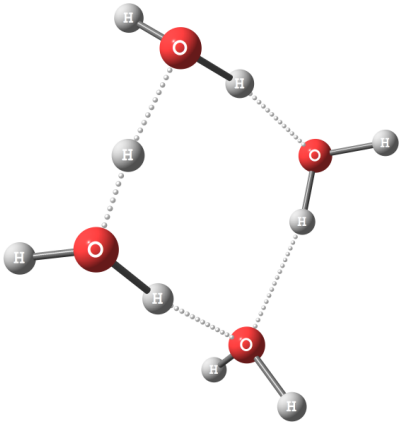
**Acetonitrile (singlet, G = -132.790418679)**

| | | | |
|---|---|---|---|
| 7 | 1.419014000 | -0.152560000 | 2.190818000 |
| 6 | 1.414018000 | -0.524571000 | 3.294355000 |
| 6 | 1.408779000 | -0.988987000 | 4.674229000 |
| 1 | 2.375606000 | -0.775133000 | 5.141245000 |
| 1 | 0.618838000 | -0.478674000 | 5.234712000 |
| 1 | 1.227350000 | -2.068275000 | 4.701515000 |



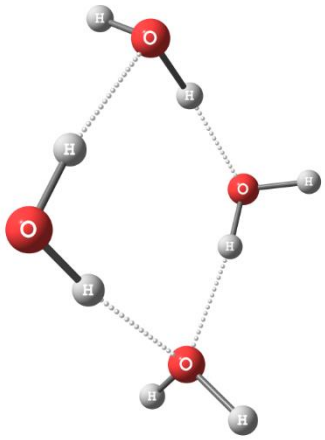
**H3O_3H2O (singlet, G = -306.288178479)**

| | | | |
|---|---|---|---|
| 1 | -0.067739000 | -2.310285000 | 0.694904000 |
| 8 | -0.049134000 | -1.757277000 | -0.111952000 |
| 1 | -0.837252000 | -1.109686000 | -0.049336000 |
| 1 | 0.841367000 | -1.138768000 | -0.075291000 |
| 1 | 2.406503000 | -0.310069000 | 0.732302000 |
| 8 | 1.899668000 | -0.210518000 | -0.093565000 |
| 1 | 1.401426000 | 0.652774000 | -0.003778000 |
| 1 | -2.454273000 | 0.031547000 | 0.812330000 |
| 8 | -1.903063000 | 0.081816000 | 0.011005000 |
| 1 | -2.526243000 | 0.043867000 | -0.736343000 |
| 1 | 0.293998000 | 2.454362000 | -0.704111000 |
| 8 | 0.243477000 | 1.921917000 | 0.108043000 |
| 1 | -0.585360000 | 1.398766000 | 0.021070000 |



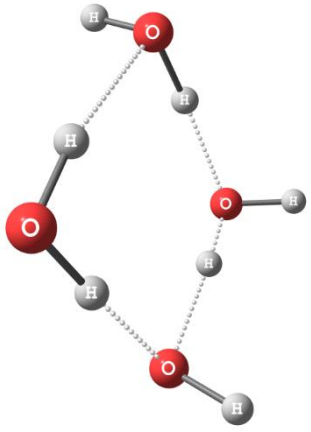
**H2O_3H2O (singlet, G = -305.864937777)**

| | | | |
|---|---|---|---|
| 8 | 0.060240000 | 1.980177000 | -0.022368000 |
| 1 | -0.711861000 | 1.375286000 | -0.000277000 |
| 1 | 0.833753000 | 1.372468000 | 0.025752000 |
| 1 | 2.587809000 | 0.051644000 | -0.711849000 |
| 8 | 2.107632000 | 0.020414000 | 0.132515000 |
| 1 | 1.437297000 | -0.700006000 | 0.018177000 |
| 1 | -2.603500000 | 0.004723000 | -0.754489000 |
| 8 | -2.016262000 | 0.028512000 | 0.020568000 |
| 1 | -2.608634000 | -0.025979000 | 0.790008000 |
| 1 | 0.052825000 | -2.379795000 | 0.675689000 |
| 8 | 0.063861000 | -1.837229000 | -0.130787000 |
| 1 | -0.711460000 | -1.233328000 | -0.042433000 |



**HO_3H2O (singlet, G = -305.395351198)**

| | | | |
|---|---|---|---|
| 8 | -3.024788000 | 1.025000000 | 2.882992000 |
| 1 | -2.594614000 | 1.706782000 | 2.268892000 |
| 1 | -3.614229000 | 0.518521000 | 2.284764000 |
| 1 | -4.145545000 | -1.104161000 | 0.681395000 |
| 8 | -4.580405000 | -0.241977000 | 0.789987000 |
| 1 | -4.079570000 | 0.372747000 | 0.187714000 |
| 8 | -1.910058000 | 2.763257000 | 1.193579000 |
| 1 | -2.389923000 | 3.597164000 | 1.327038000 |
| 1 | -3.774433000 | 2.157882000 | -1.113125000 |
| 8 | -3.138701000 | 1.534370000 | -0.724275000 |
| 1 | -2.658897000 | 2.066234000 | 0.027767000 |



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