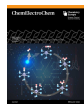


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Supporting Information



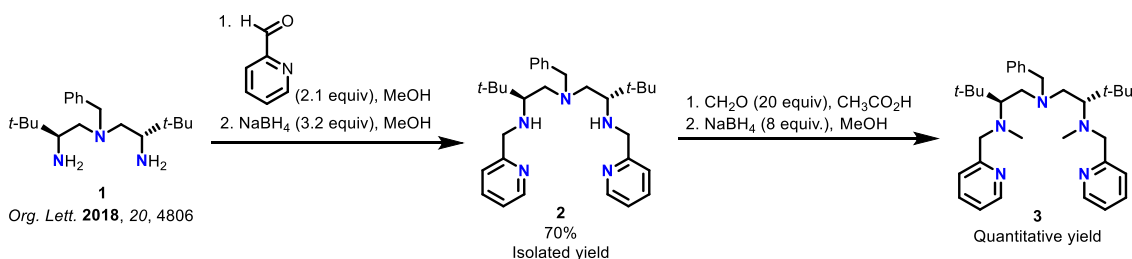
The Dual Effect of Coordinating –NH Groups and Light in the Electrochemical CO₂ Reduction with Pyridylamino Co Complexes

Sergio Fernández, Santiago Cañellas, Federico Franco, Josep M. Luis, Miquel À. Pericàs,* and Julio Lloret-Fillol*

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1. Synthesis and characterization and of ligands

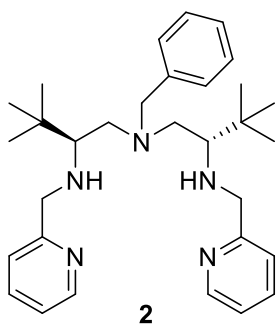


Compound **1** was synthesized according to the literature precedence.¹

(S)-N¹-benzyl-N¹-((S)-3,3-dimethyl-2-((pyridin-2-ylmethyl)amino)butyl)-3,3-dimethyl-N²-(pyridin-2-ylmethyl)butane-1,2-diamine (2, L^H). Triamine **1** (800 mg, 2.6 mmol) and 2-pyridinecarboxaldehyde (589 mg, 5.5 mmol, 2.1 equiv.) were dissolved in MeOH (8 mL) and stirred at room temperature for 30 minutes. Then, the reaction was cooled down to 0 °C and sodium borohydride (314 mg, 8.32 mmol, 3.2 equiv.) was added portionwise. The reaction was stirred at 0 °C for 4 hours. Then, water (20 mL) was added, and the product was extracted with DCM (20 mL x 3). The combined organic layers were concentrated in vacuo and submitted to silica gel column chromatography to afford compound **2** (887.7 mg, 1.82 mmol, 70% yield) as a white solid.

(S)-N¹-benzyl-N¹-((S)-3,3-dimethyl-2-(methyl(pyridin-2-ylmethyl)amino)butyl)-N²,3,3-trimethyl-N²-(pyridin-2-ylmethyl)butane-1,2-diamine (3, L^{Me}). Compound **2** (400 mg, 0.83 mmol), formaldehyde (1.24 mL, 37 wt % in H₂O, 16.6 mmol, 20 equiv.) and acetic acid (0.48 mL, 16.6 mmol, 20 equiv.) were stirred at room temperature for 30 minutes. Then, methanol (8 mL) was added and the reaction was cooled down to 0 °C, followed by the addition of sodium borohydride (251.2 mg, 6.64 mmol, 8 equiv.) and stirred at this temperature for 4 hours. Water (20 mL) was added, and the product was extracted with DCM (20 mL x 3). The combined organic layers were concentrated in vacuo and submitted to silica gel column chromatography to afford compound **3** (428 mg, 0.83 mmol, quantitative yield) as a white solid.

¹ Cañellas, S.; Alonso, P.; Pericàs, M. A. *Org. Lett.* 2018, 20, 4806-4810

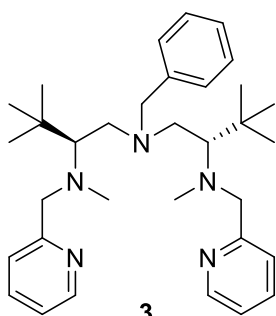


2

(S)-N¹-benzyl-N¹-((S)-3,3-dimethyl-2-((pyridin-2-ylmethyl)amino)butyl)-3,3-dimethyl-N²-(pyridin-2-

ylmethyl)butane-1,2-diamine (2, L^H). White solid. IR (film): $\nu = 612, 700, 751, 917, 992, 1027, 1047, 1073, 1125, 1213, 1330, 1357, 1389, 1433, 1475, 1570, 1590, 2865, 2904, 2952, 3009, 3062, 3307 \text{ cm}^{-1}$. ¹H NMR (400 MHz, CDCl₃): $\delta = 0.99$ (s, 18H), 2.28 (br s, 2H), 2.38 (dd, $J = 2.0, 12.3$ Hz, 2H), 2.48 (dd, $J = 2.0,$

10.5 Hz, 2H), 2.55 (dd, $J = 10.5, 12.3$ Hz, 2H), 3.15 (d, $J = 13.4$ Hz, 1H), 3.90 (d, $J = 14.5$ Hz, 2H), 4.04 (s, 1H), 4.08 (d, $J = 14.5$ Hz, 2H), 6.96 (m, 2H), 7.20 (m, 5H), 7.41 (m, 4H), 8.34 (m, 2H). ¹³C NMR (100.4 MHz, CDCl₃): $\delta = 27.3$ (6C), 36.3 (2C), 57.0 (2C), 57.7 (2C), 59.7, 65.0 (2C), 121.3 (2C), 121.9 (2C), 127.1, 128.4 (2C), 129.4 (2C), 136.0 (2C), 139.1, 148.9 (2C), 161.0 (2C). HRMS (ESI⁺): calcd for C₃₁H₄₆N₅ [M+H]⁺: 488.3748, found: 488.3733.



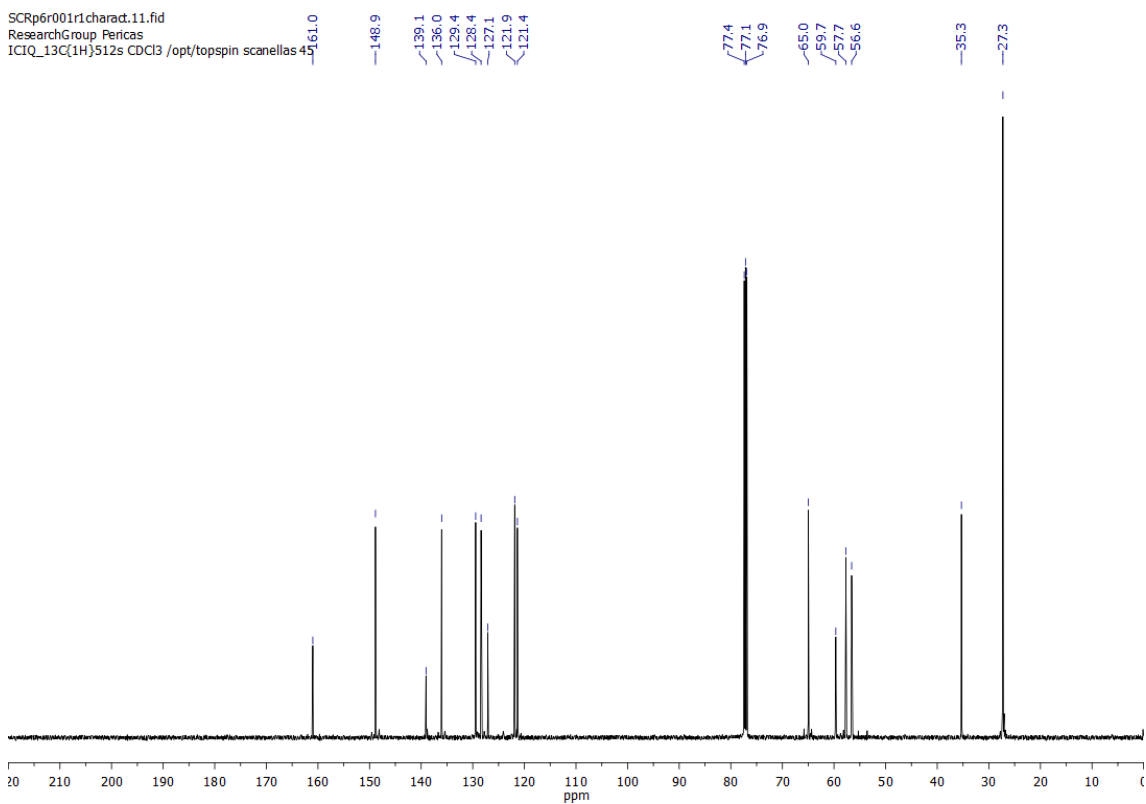
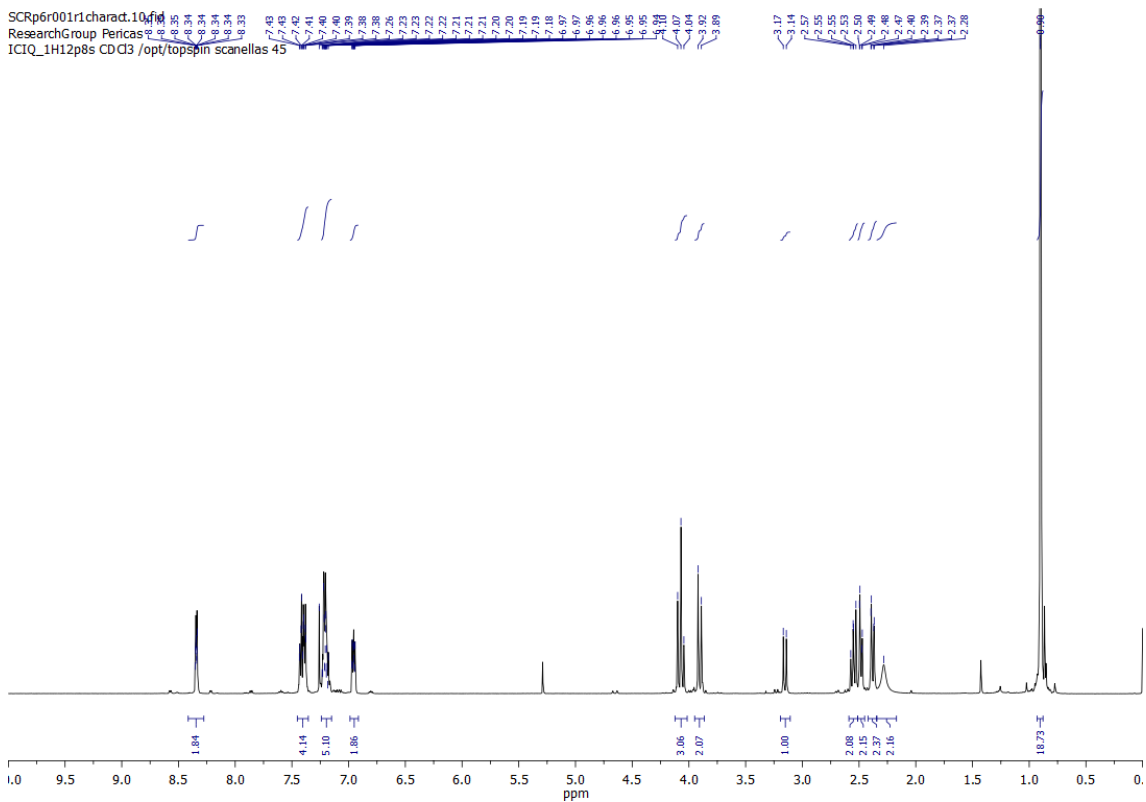
3

(S)-N¹-benzyl-N¹-((S)-3,3-dimethyl-2-(methyl(pyridin-2-ylmethyl)amino)butyl)-N²,3,3-trimethyl-N²-(pyridin-2-

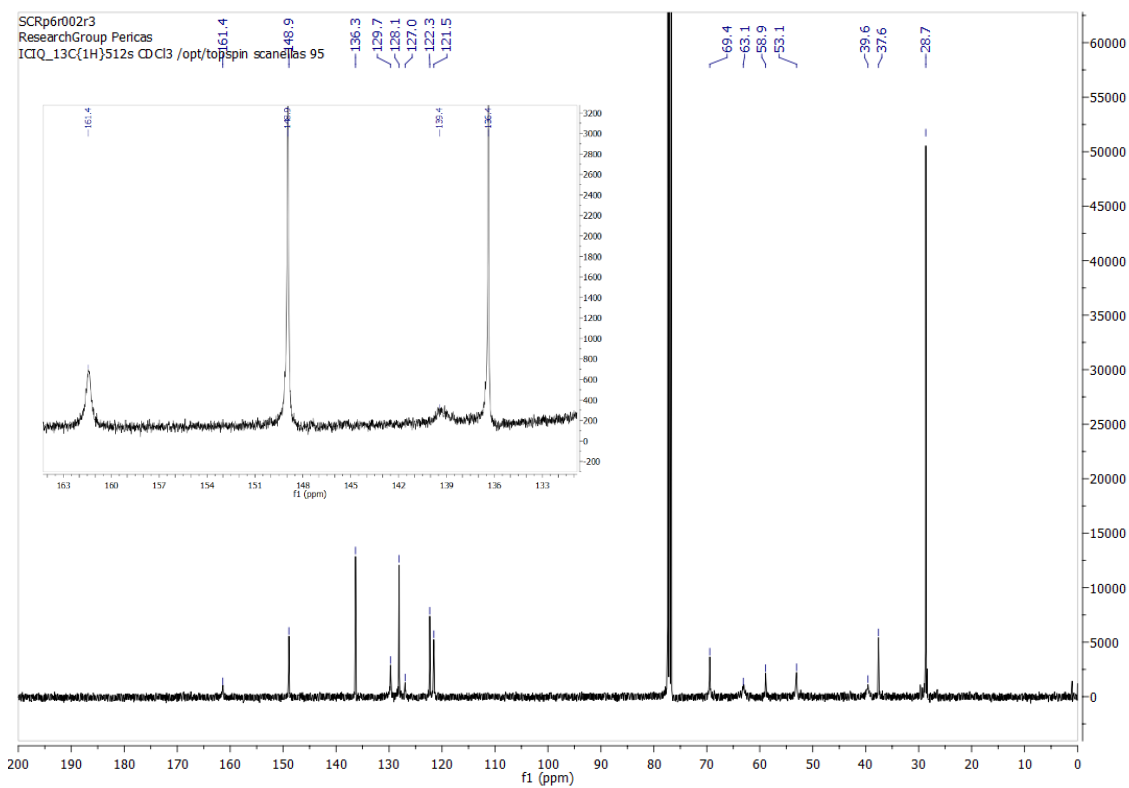
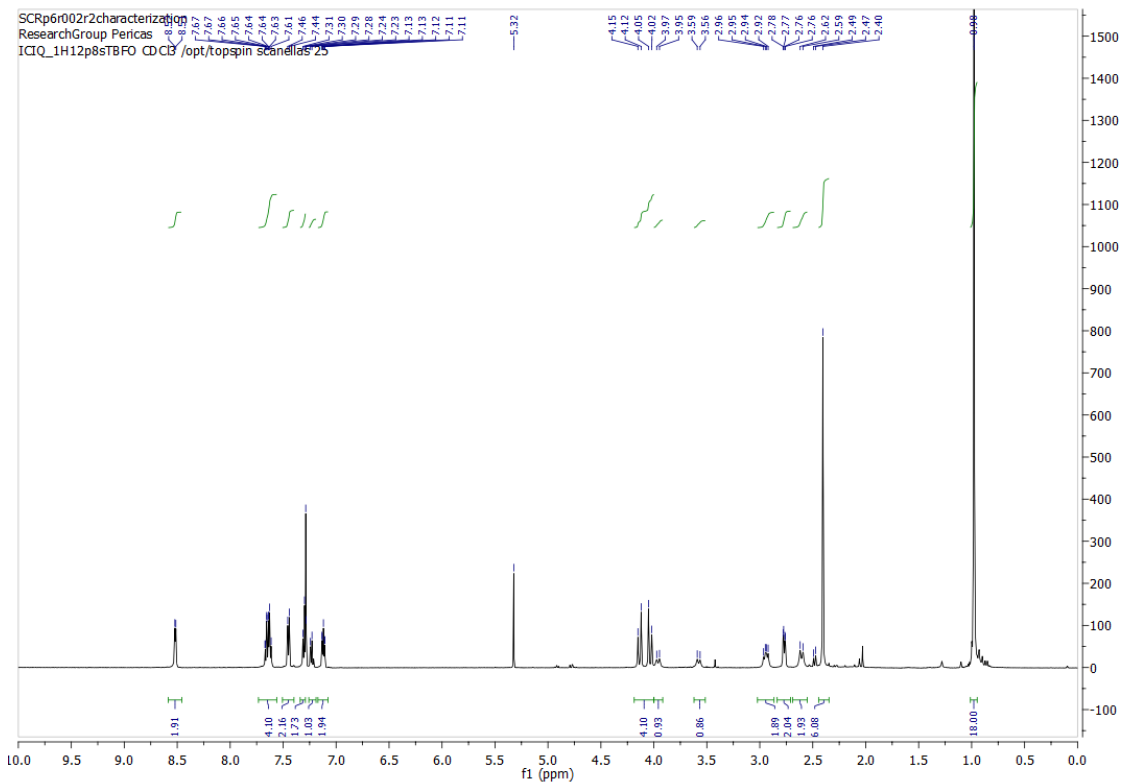
ylmethyl)butane-1,2-diamine (3, L^{Me}). White solid. ¹H NMR (400 MHz, CDCl₃): $\delta = 0.99$ (s, 18H), 2.40 (s, 6H), 2.61 (d, $J = 13.2$ Hz, 2H), 2.77 (dd, $J = 2.6, 8.2$ Hz, 2H), 2.91 (dd, $J = 8.2, 13.2$ Hz, 2H), 3.58 (d, $J = 13.2$ Hz, 1H), 3.96 (d, $J = 13.2$ Hz, 1H), 4.04 (d, $J = 15.3$ Hz, 2H), 4.14 (d, $J = 15.3$ Hz, 2H), 7.12 (m, 2H),

7.23 (m, 1H), 7.30 (m, 2H), 7.43 (m, 2H), 7.65 (ddd, $J = 4.6, 10.2, 14.2$ Hz, 4H), 8.52 (d, $J = 4.6$ Hz, 2H). ¹³C NMR (100.4 MHz, CDCl₃): $\delta = 28.7$ (6C), 37.6 (2C), 39.6 (2C), 53.1 (2C), 58.9 (2C), 63.1, 69.4 (2C), 121.5 (2C), 122.3 (2C), 127.0, 128.1 (2C), 129.7 (2C), 136.3 (2C), 139.4, 148.9 (2C), 161.4 (2C). HRMS (ESI⁺): calcd for C₃₃H₅₀N₅ [M+H]⁺: 516.4061, found: 516.4069.

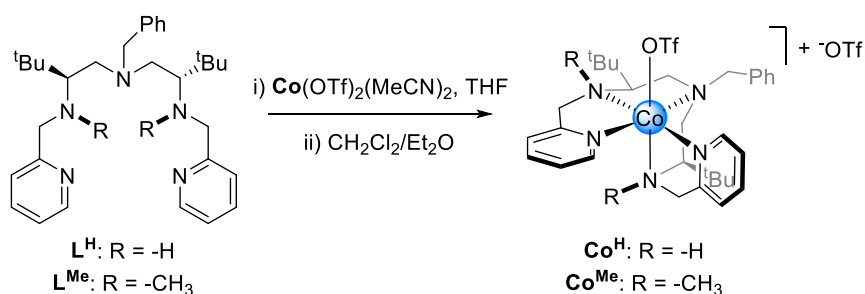
1.1. (S)-N¹-benzyl-N¹-((S)-3,3-dimethyl-2-((pyridin-2-ylmethyl)amino)butyl)-3,3-dimethyl-N²-(pyridin-2-ylmethyl)butane-1,2-diamine (2, L^H).



1.2. (S)-N¹-benzyl-N¹-((S)-3,3-dimethyl-2-(methyl(pyridin-2-ylmethyl)amino)butyl)-N²,3,3-trimethyl-N²-(pyridin-2-ylmethyl)butane-1,2-diamine (3, L^{Me}).



2. Synthesis and characterization of Co complexes

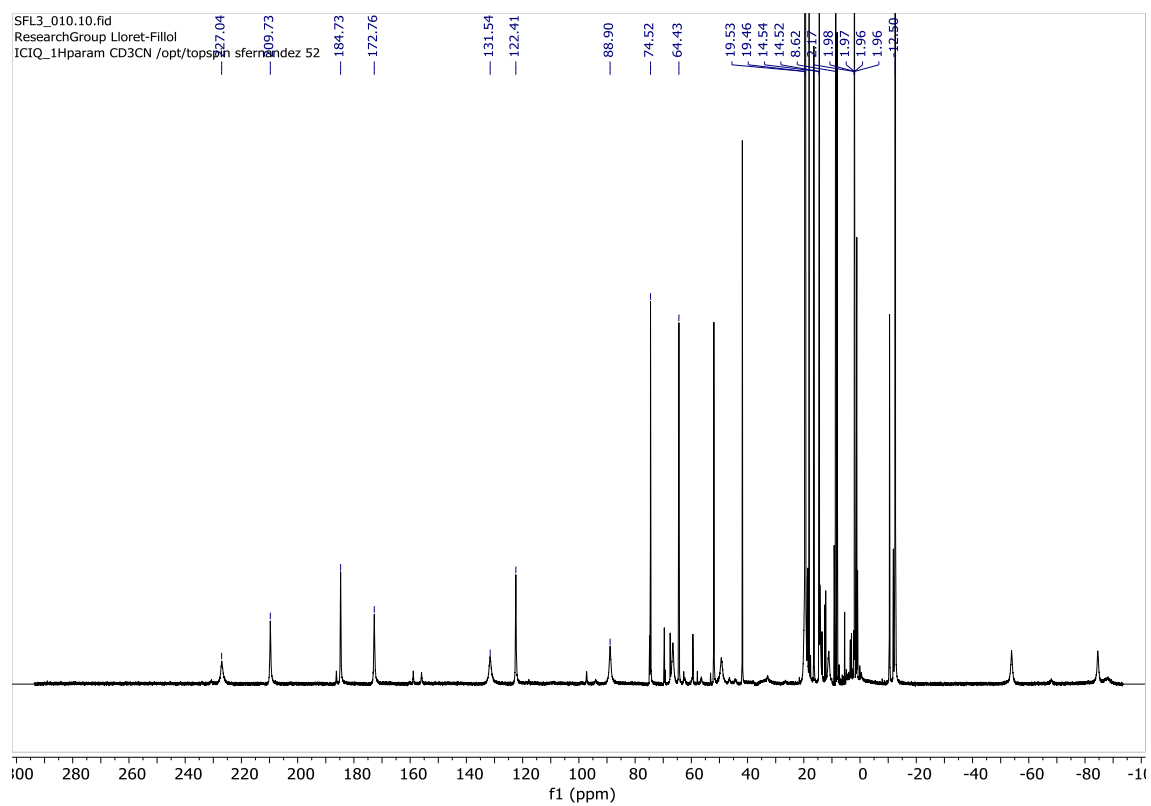
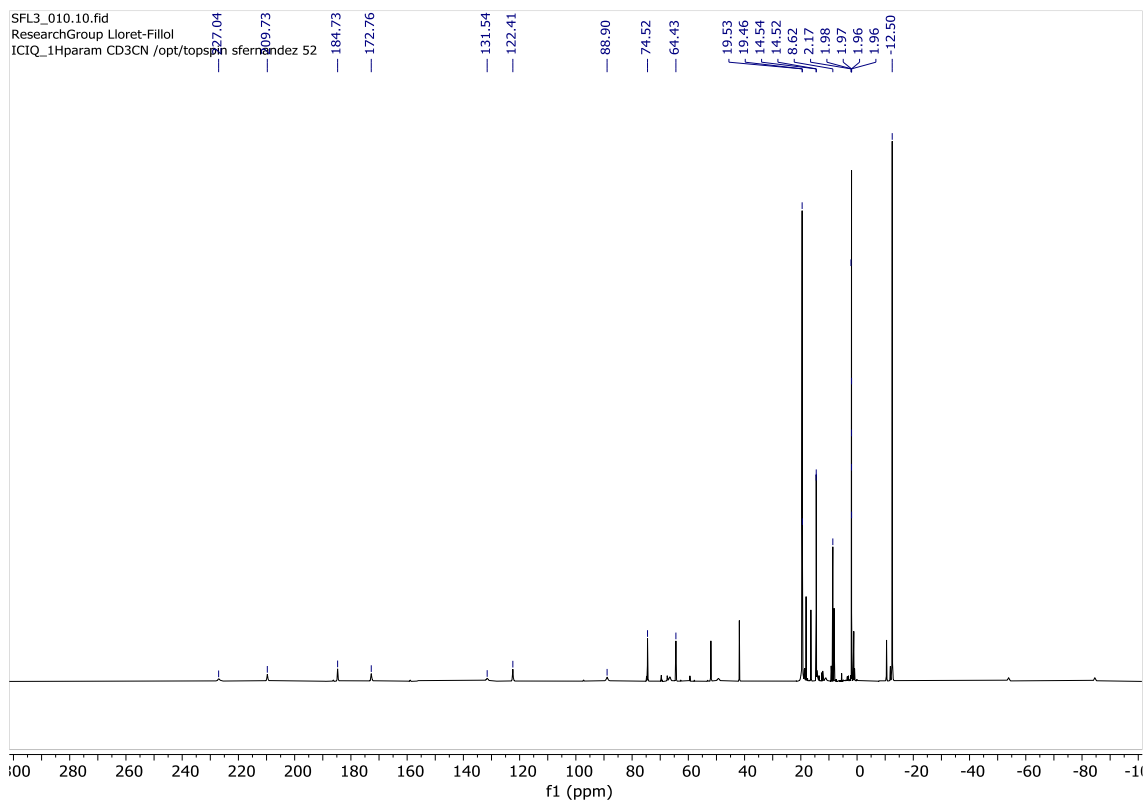


Synthesis of $[Co^H(L^H)(OTf)](OTf)$ (Co^H). In a glovebox, a solution of $Co(OTf)_2(MeCN)_2$ (90 mg, 0.205 mmol) in anhydrous THF (1 ml) was added dropwise to a vigorously stirred solution of L^H (100 mg, 0.205 mmol) in THF (1 ml). Few minutes later, a pale red-pink precipitate appeared. After stirring for an additional 5 hours the solution was filtered off and the resulting solid dried under vacuum. This solid was dissolved in DCM, filtered over Celite[®] and crystallized by slow diffusion of diethyl ether into this solution producing red crystals (61 mg, 35 % yield) suitable for X-ray diffraction (Figure S3). **HRMS** (ESI+): calculated for $C_{32}H_{45}CoF_3N_5O_3S$ $[M-(OTf)]^+$: 695.253. Found: 695.2531. Anal. Calculated for $C_{33}H_{45}CoF_6N_5O_6S_2$: C, 46.92; H, 5.37; N, 8.29 %. Found: C, 45.99; H, 5.32; N, 8.22 %.

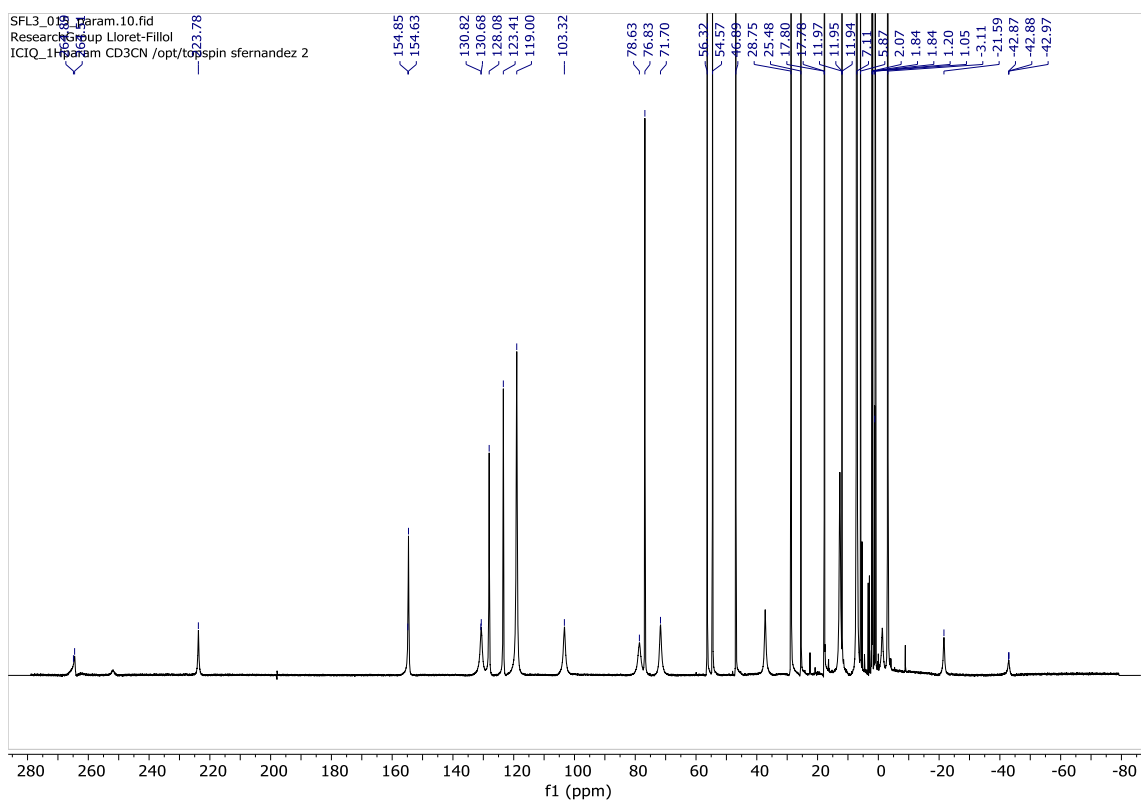
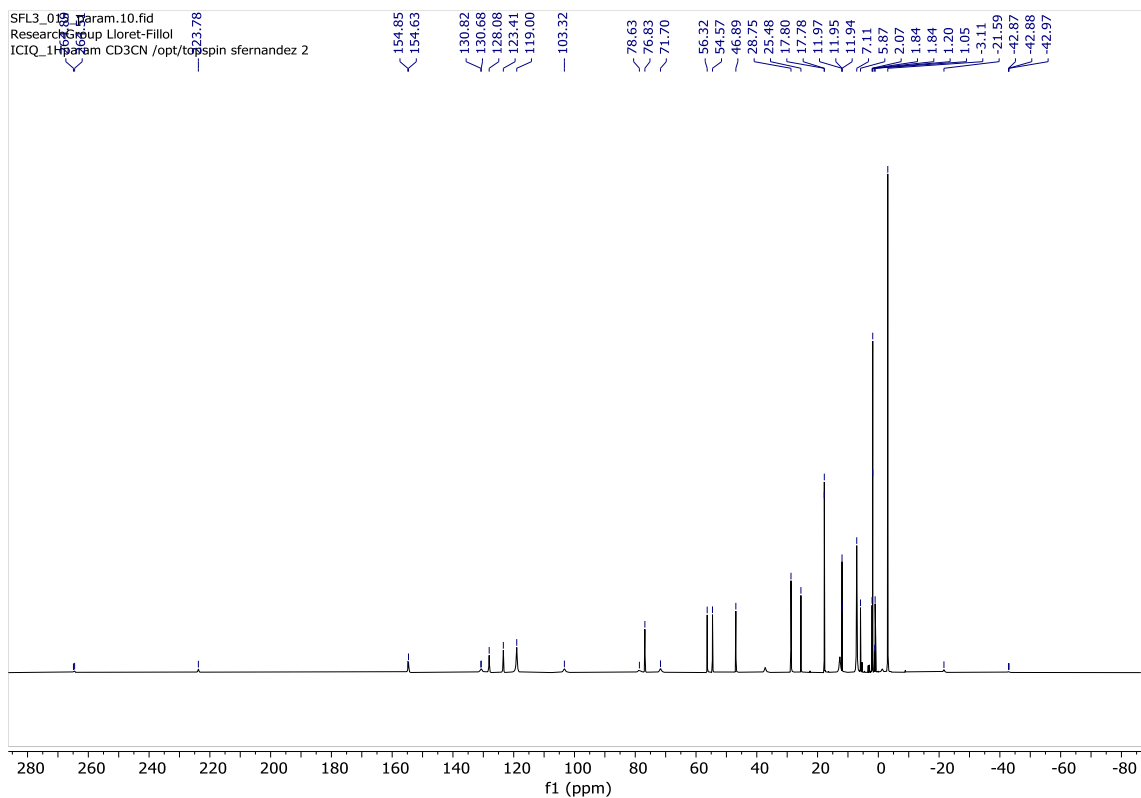
Synthesis of $[Co^{Me}(L^{Me})(OTf)](OTf)$ (Co^{Me}). In a glovebox, a solution of $Co(OTf)_2(MeCN)_2$ (128 mg, 0.291 mmol) in anhydrous THF (1 ml) was added dropwise to a vigorously stirred solution of L^{Me} (150 mg, 0.291 mmol) in THF (1 ml). After stirring for two days the reaction mixture (red-purple) was precipitated with diethyl ether, filtrated, dissolved in 2 ml DCM and filtered over Celite[®]. The slow diffusion of diethyl ether into the solution produced 163.4 mg of purple crystals (164 mg, 64 % yield) suitable for X-ray diffraction (Figure S4). **HRMS** (ESI+): calculated for $C_{34}H_{49}CoF_3N_5O_3S$ $[M-(OTf)]^+$: 723.284, found: 723.2844. Anal. Calculated for $C_{35}H_{49}CoF_6N_5O_6S_2$: C, 48.16; H, 5.66; N, 8.02 %. Found: C, 47.48; H, 5.54; N, 7.89 %.

¹H-NMR analysis of the two Co complexes revealed a paramagnetic behaviour when solubilized in CD₃CN solution which is in agreement with a Co^{II} (d⁷) metallic centre.

2.1. $^1\text{H-NMR}$ of Co^{H} (400 MHz, CD_3CN):



2.2. $^1\text{H-NMR}$ of Co^{Me} (400 MHz, CD_3CN):



2.3. HR-ESI-MS of Co^{H} complex

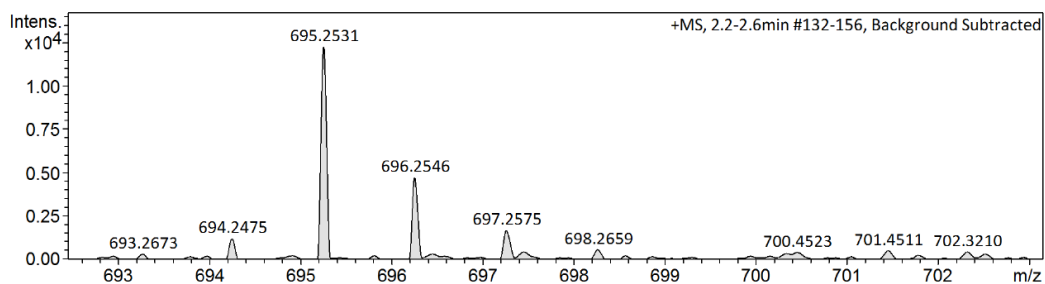


Figure S1. HR-ESI(+)-MS spectrum of Co^{H} obtained in acetonitrile solution. The peak at m/z 693.2531 corresponds to the $[\text{M}-(\text{OTf})]^+$ ion of Co^{H} .

2.4. HR-ESI-MS of Co^{Me} complex

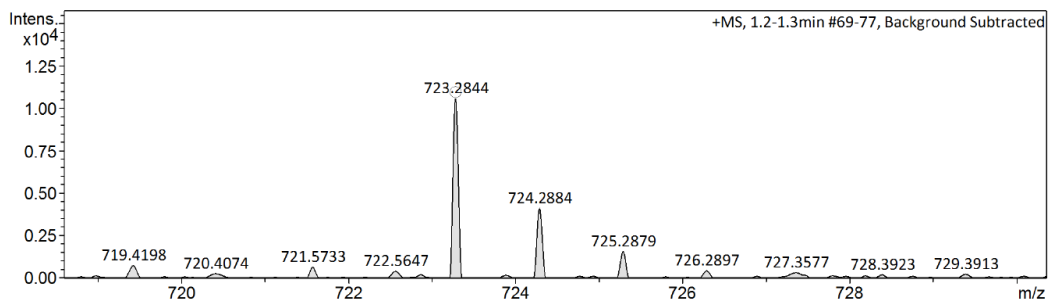


Figure S2. HR-ESI(+)-MS spectrum of Co^{Me} obtained in acetonitrile solution. The peak at m/z 723.2844 correspond to the $[\text{M}-(\text{OTf})]^+$ ion of Co^{Me} , respectively.

2.5. X-ray structure of Co^H

Full sphere single crystal data collection of mo_SFL30102_0m where performed at 100 K on a Bruker Kappa Apex II DUO diffractometer equipped with a Cryostream 700 plus low temperature device, a microsource anode with Mo K α ($\lambda = 0.71073$ Å).

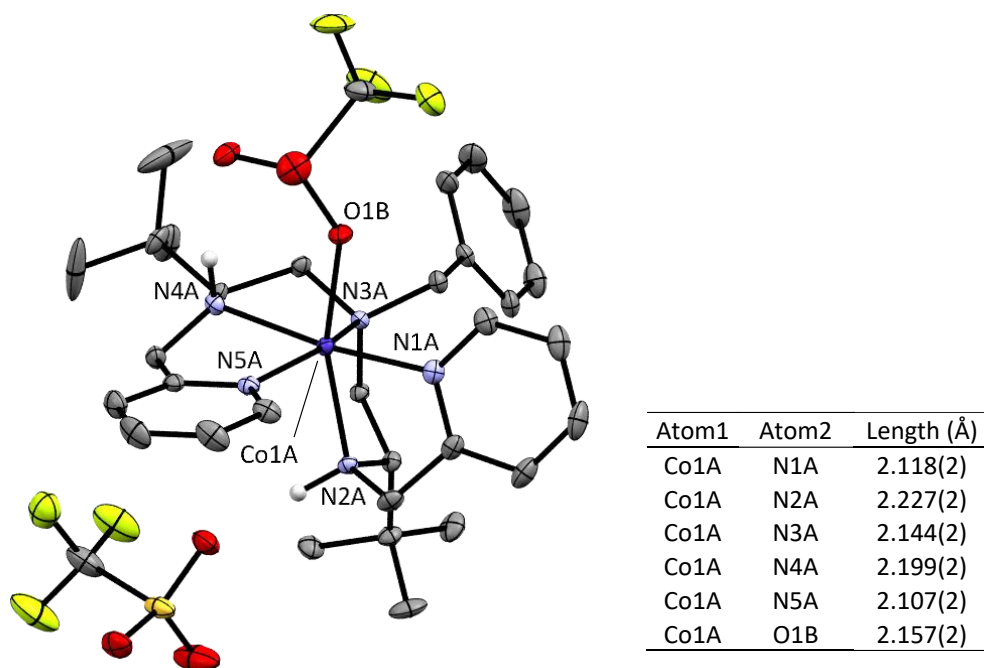


Figure S3. ORTEP plot of Co^H with elipsoids at the 50% probability and selected bond lengths. Unrelevant hydrogen atoms have been omitted for clarity. Table with relevant bond distances.

Table S1. Crystal data for Co^H.

Identification code	mo_SFL30102_0m	
Empirical formula	C33 H45 Co F6 N5 O6 S2	
Formula weight	844.79	
Temperature	100(2)K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 10.9511(8)Å	$\alpha = 90^\circ$.
	b = 15.5915(10)Å	$\beta = 90^\circ$.
	c = 22.7665(13)Å	$\gamma = 90^\circ$.
Volume	3887.2(4) Å ³	
Z	4	

Density (calculated)	1.443 Mg/m ³
Absorption coefficient	0.626 mm ⁻¹
F(000)	1756
Crystal size	0.500 x 0.250 x 0.250 mm ³
Theta range for data collection	1.789 to 30.503°.
Index ranges	-15<=h<=15,-22<=k<=12,-32<=l<=24
Reflections collected	38071
Independent reflections	11522[R(int) = 0.0514]
Completeness to theta =30.503°	97.3%
Absorption correction	Multi-scan
Max. and min. transmission	0.74 and 0.54
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11522/ 0/ 488
Goodness-of-fit on F ²	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.0815
R indices (all data)	R1 = 0.0530, wR2 = 0.0872
Flack parameter	x =-0.001(6)
Largest diff. peak and hole	0.639 and -0.782 e.Å ⁻³

2.6. X-ray structure of Co^{Me}

Full sphere single crystal data collection of mo_SFL3015_0m where performed at 100 K on a Bruker Kappa Apex II DUO diffractometer equipped with a Cryostream 700 plus low temperature device, a microsource anode with Mo K α (λ = 0.71073 Å).

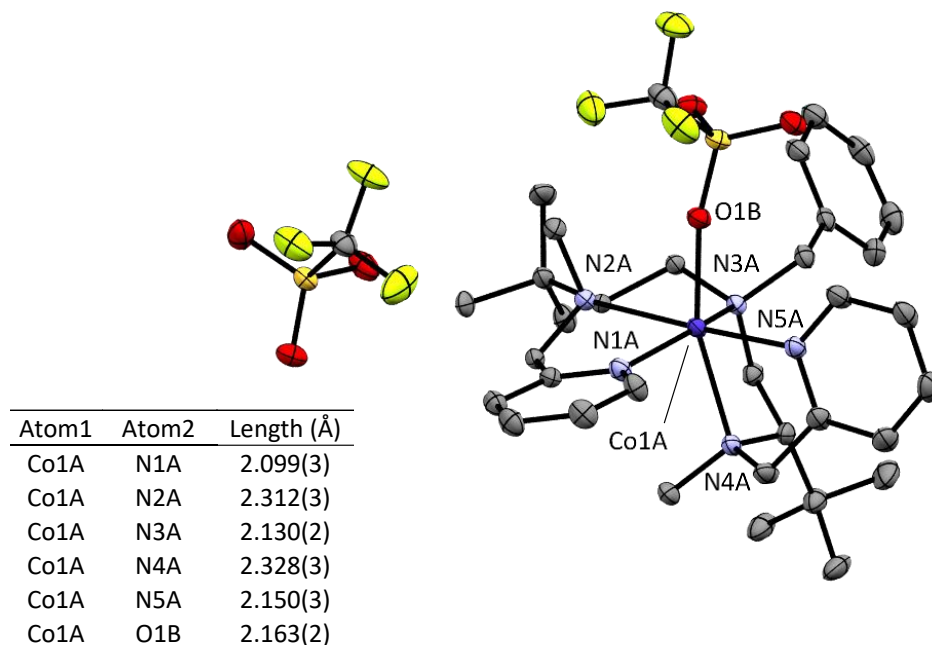


Figure S4. ORTEP plot of Co^{Me} with elipsoids at the 50% probability and selected bond lengths. Unrelevant hydrogen atoms have been omitted for clarity. Table with relevant bond distances.

Table S2. Crystal data for Co^{Me}.

Identification code	mo_SFL3015_0m	
Empirical formula	C ₃₅ H ₄₉ Co F ₆ N ₅ O ₆ S ₂	
Formula weight	872.84	
Temperature	100(2)K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.744(3)Å	α = 90°.
	b = 12.100(3)Å	β = 90°.
	c = 34.327(9)Å	γ = 90°.
Volume	4047.1(18) Å ³	
Z	4	

Density (calculated)	1.433 Mg/m ³
Absorption coefficient	0.604 mm ⁻¹
F(000)	1820
Crystal size	0.300 x 0.250 x 0.050 mm ³
Theta range for data collection	1.784 to 32.547°.
Index ranges	-14<=h<=12,-12<=k<=17,-50<=l<=47
Reflections collected	37516
Independent reflections	13652[R(int) = 0.0356]
Completeness to theta =32.547°	94.4%
Absorption correction	Multi-scan
Max. and min. transmission	0.74 and 0.61
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	13652/ 0/ 504
Goodness-of-fit on F ²	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.0780
R indices (all data)	R1 = 0.0647, wR2 = 0.0874
Flack parameter	x =0.014(5)
Largest diff. peak and hole	0.533 and -0.567 e.Å ⁻³

2.7. Relative stability of Co^H isomers

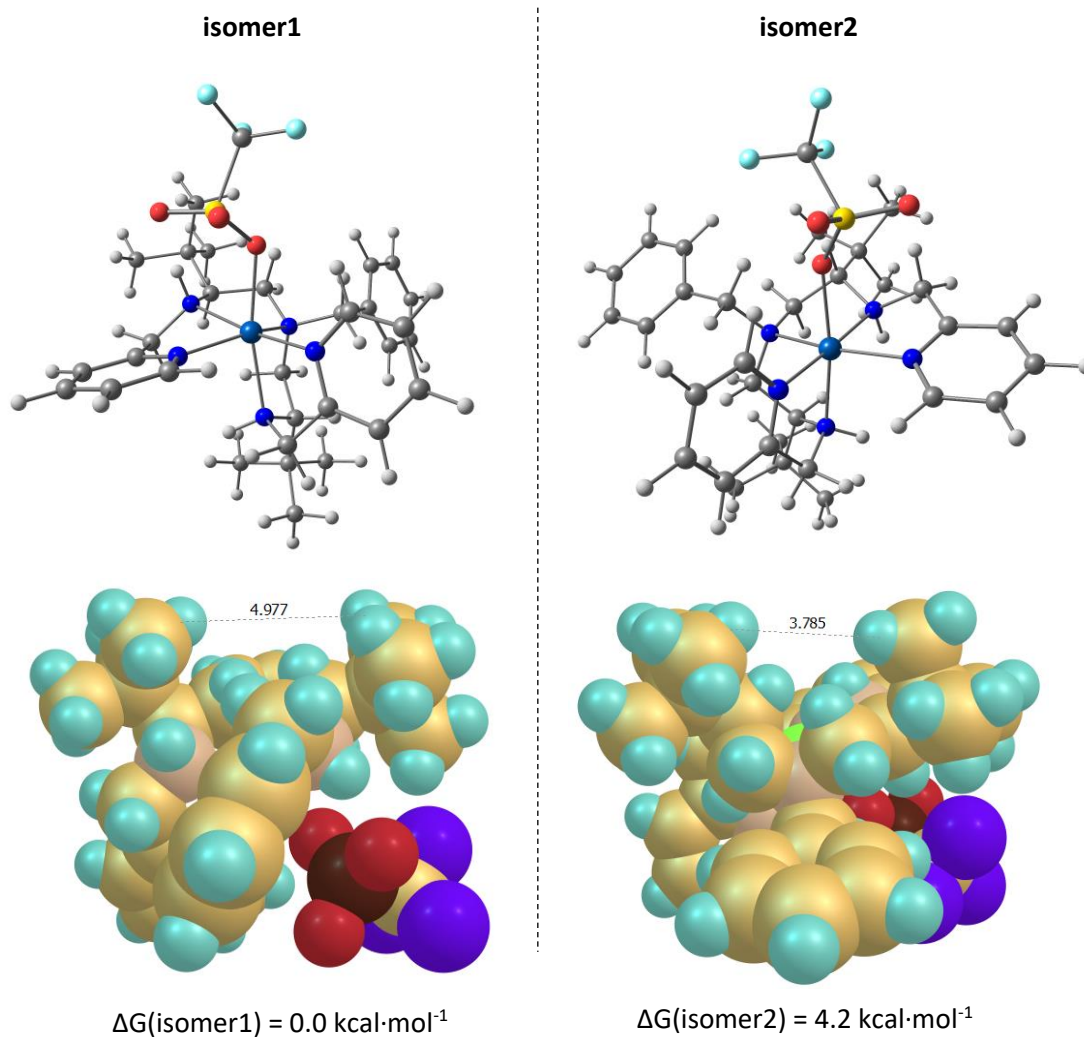


Figure S5. DFT structures of isomers 1 and 2 of [Co^H]⁺ optimized at the B3LYP/6-31+G* level of theory with relative Gibbs free energies in kcal·mol⁻¹.

3. Cyclic voltammetry (CV)

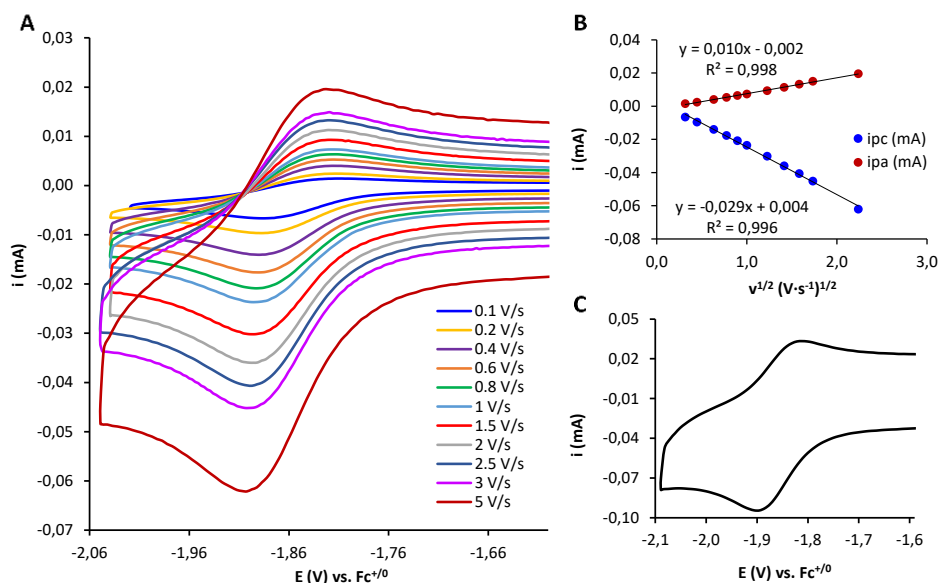


Figure S6. CVs of Co^{H} (0.4 mM) in anhydrous MeCN/TBAPF₆ 0.1 M solution under Ar atmosphere. A) At increasing scan rates (0.1 – 5 V·s⁻¹) in anhydrous MeCN/TBAPF₆ 0.1 M solution under Ar atmosphere. B) Plot of the cathodic and anodic currents *versus* the inverse of the scan rate. C) CV at 10 V·s⁻¹.

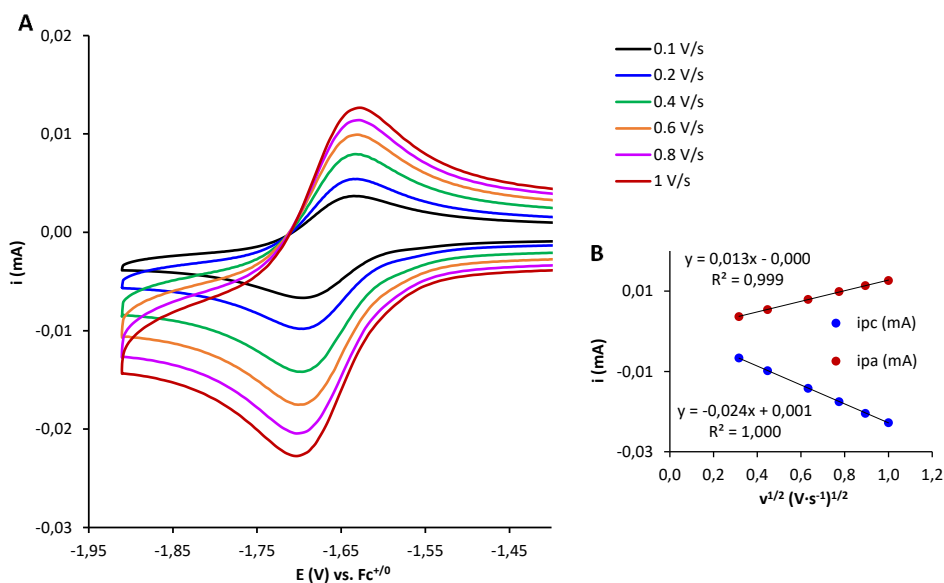


Figure S7. A) CVs of Co^{Me} (0.4 mM) in anhydrous MeCN/TBAPF₆ 0.1 M solution under Ar atmosphere at increasing scan rates (0.1 – 1 V·s⁻¹) in anhydrous MeCN/TBAPF₆ 0.1 M solution under Ar atmosphere. B) Plot of the cathodic and anodic currents *versus* the inverse of the scan rate.

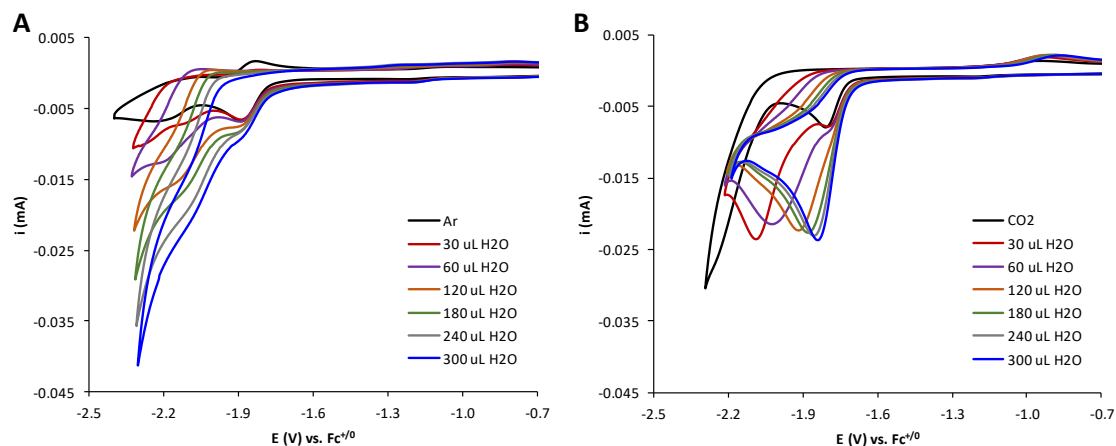


Figure S8. CVs of Co^{Me} (0.4 mM) in anhydrous MeCN/TBAPF₆ 0.1 M solution (3 mL) and upon the addition of increasing amounts of H₂O (from 30 μL (1%) to 300 μL (10%)). A) Under Ar. B) Under CO₂.

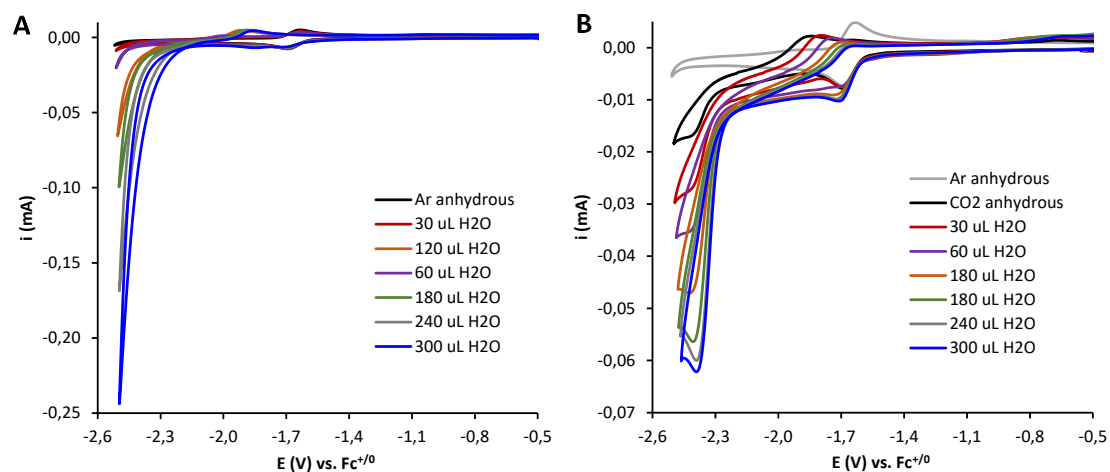


Figure S9. CVs of Co^{Me} (0.4 mM) in anhydrous MeCN/TBAPF₆ 0.1 M solution (3 mL) and upon the addition of increasing amounts of H₂O (from 30 μL (1%) to 300 μL (10%)). A) Under Ar. B) Under CO₂.

4. Spectroelectrochemistry (FTIR-SEC)

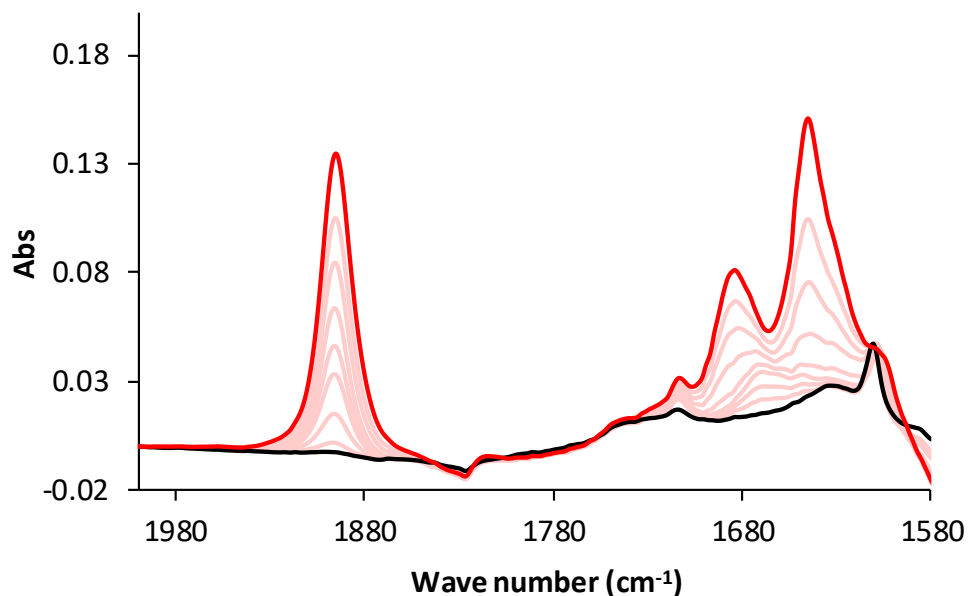


Figure S10. Thin layer *in situ* FTIR-SEC under CO₂ of Co^H. Top) Formation of [Co^I-CO]⁺. Bottom) Further reduction at the catalytic reduction wave. [Co] = 6 mM in TBAPF₆/MeCN 0.2 M.

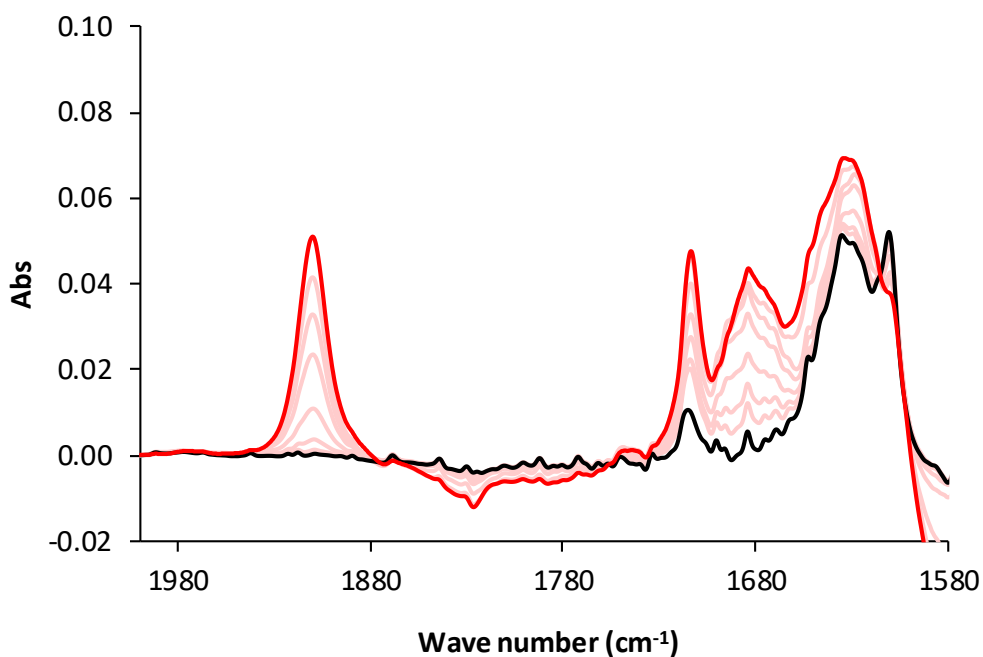


Figure S11. Thin layer *in situ* FTIR-SEC under CO₂ of Co^{Me}. Top) Formation of [Co^I-CO]⁺. Bottom) Further reduction at the catalytic reduction wave. [Co] = 6 mM in TBAPF₆/MeCN 0.2 M.

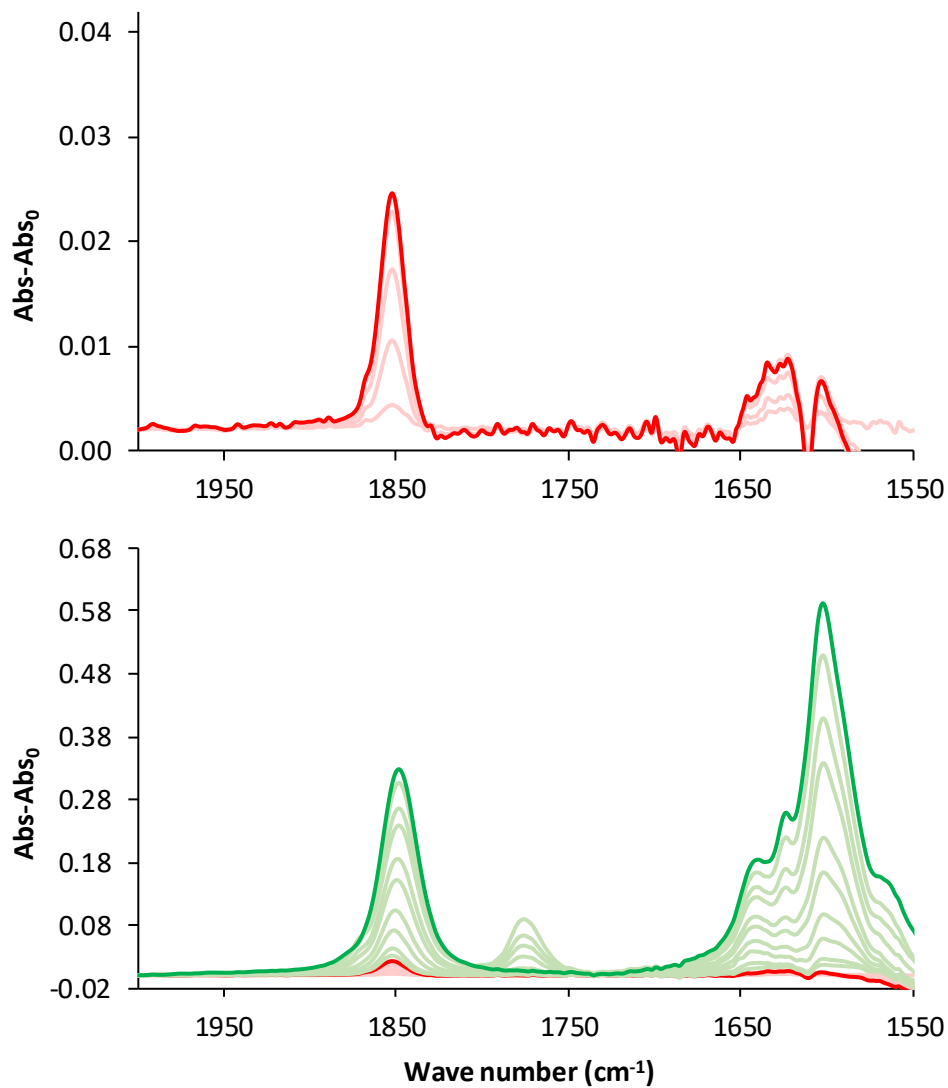


Figure S12. Thin layer *in situ* FTIR-SEC under ¹³CO₂ of **Co^H**. Top) Formation of [Co^I-CO]⁺. Bottom) Further reduction at the catalytic reduction wave. [Co] = 6 mM in TBAPF₆/MeCN 0.2 M.

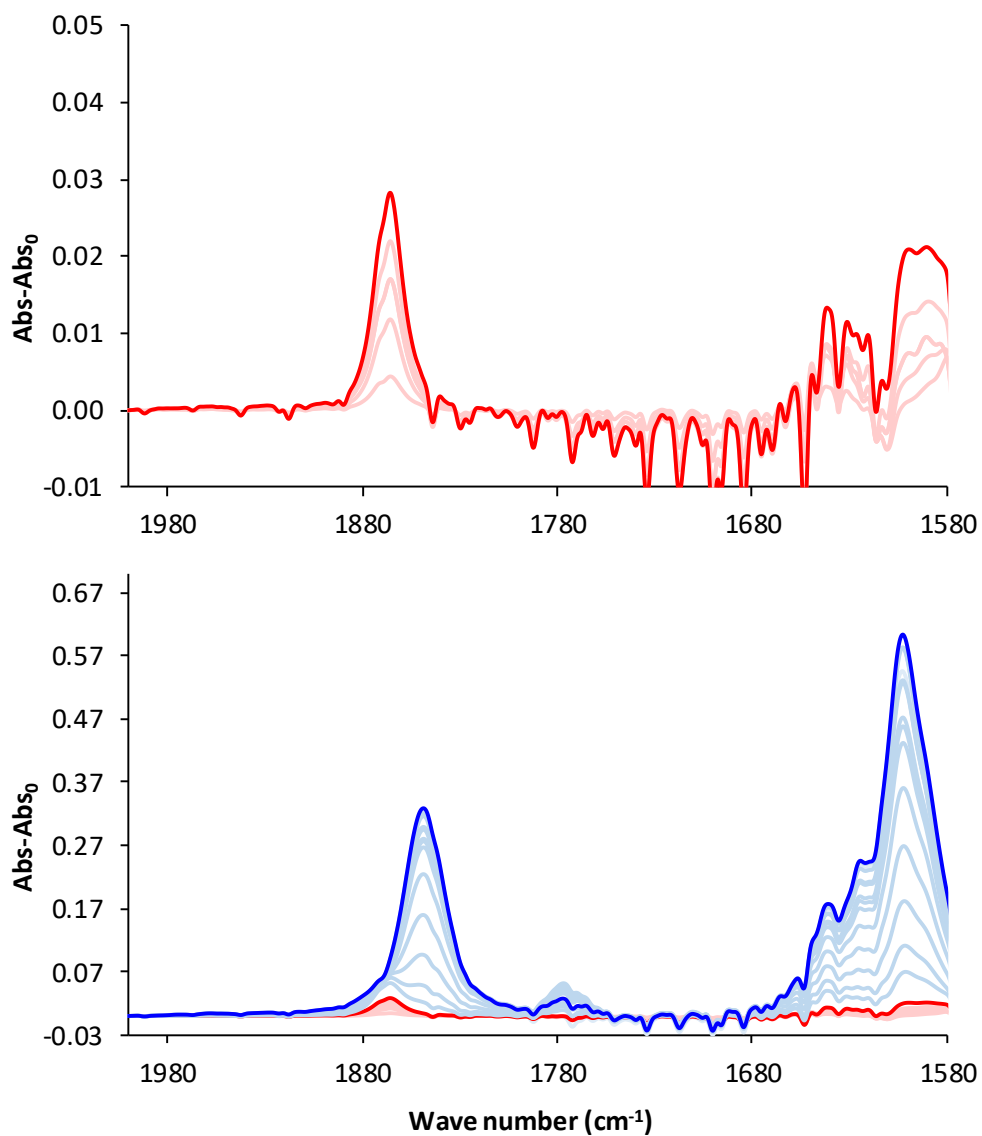


Figure S13. Thin layer *in situ* FTIR-SEC under ¹³CO₂ of **Co^{Me}**. Top) Formation of [Co^I-CO]⁺. Bottom) Further reduction at the catalytic reduction wave. [Co] = 6 mM in TBAPF₆/MeCN 0.2 M.

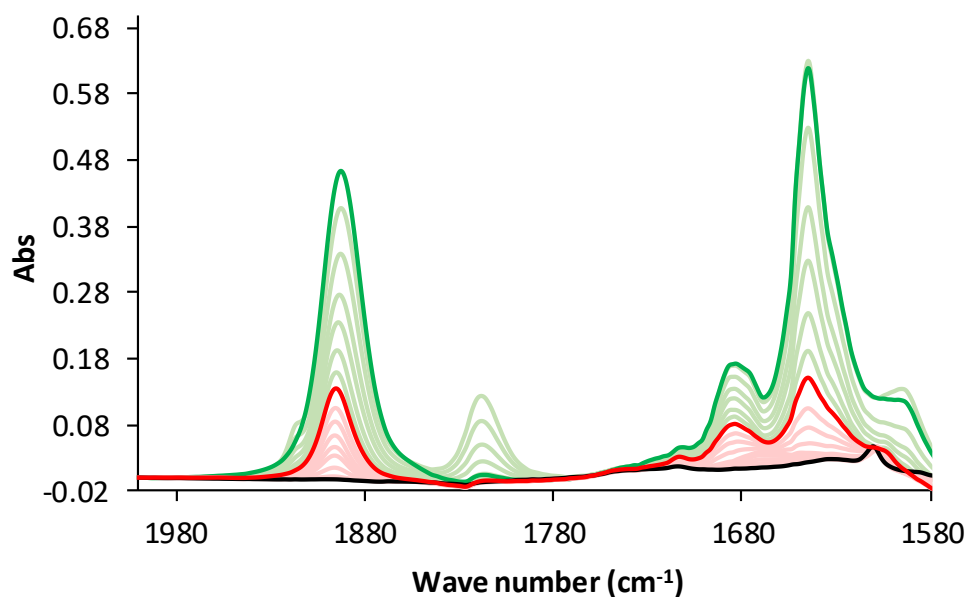


Figure S14. Thin layer *in situ* FTIR-SEC under CO₂ of **Co^H**. Formation of [Co^I-CO]⁺ (red) Further reduction at the catalytic reduction wave (green). [Co] = 6 mM in TBAPF₆/MeCN 0.2 M.

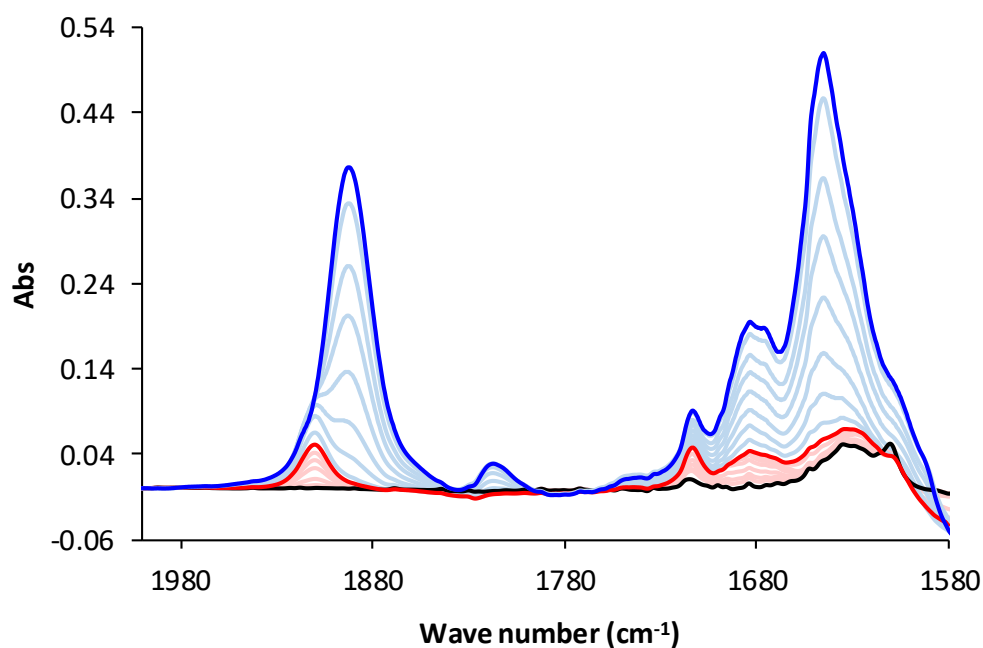


Figure S15. Thin layer *in situ* FTIR-SEC under CO₂ of **Co^{Me}**. Formation of [Co^I-CO]⁺ (red). Further reduction at the catalytic reduction wave (blue). [Co] = 6 mM in TBAPF₆/MeCN 0.2 M.

5. Controlled Potential Electrolysis (CPE)

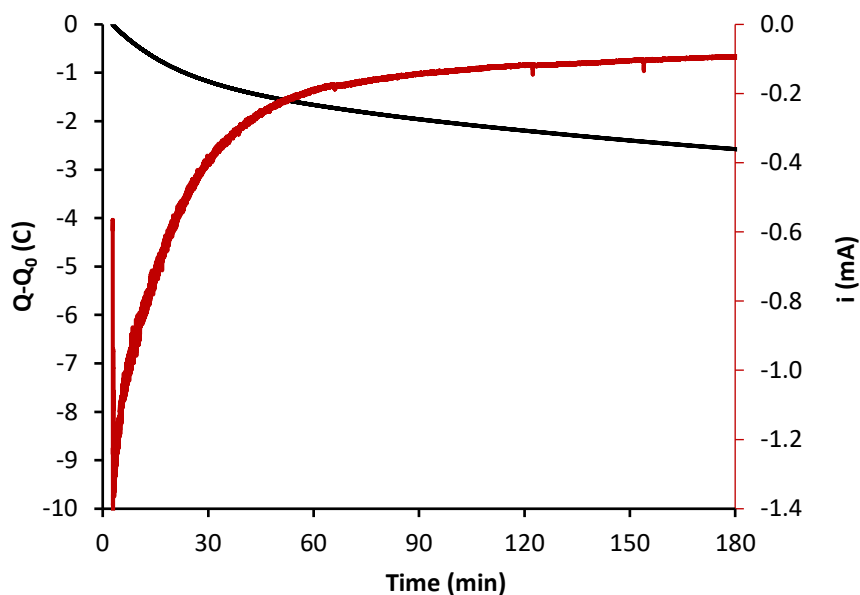


Figure S16. CPE at -2.2 V vs. $\text{Fc}^{+/0}$ in the dark of Co^{H} (1 mM) in a 0.1 M $\text{TBAPF}_6/\text{MeCN}$ solution under CO_2 saturation with 1% of added H_2O . Charge versus time plot (black trace). Current versus time plot (red trace).

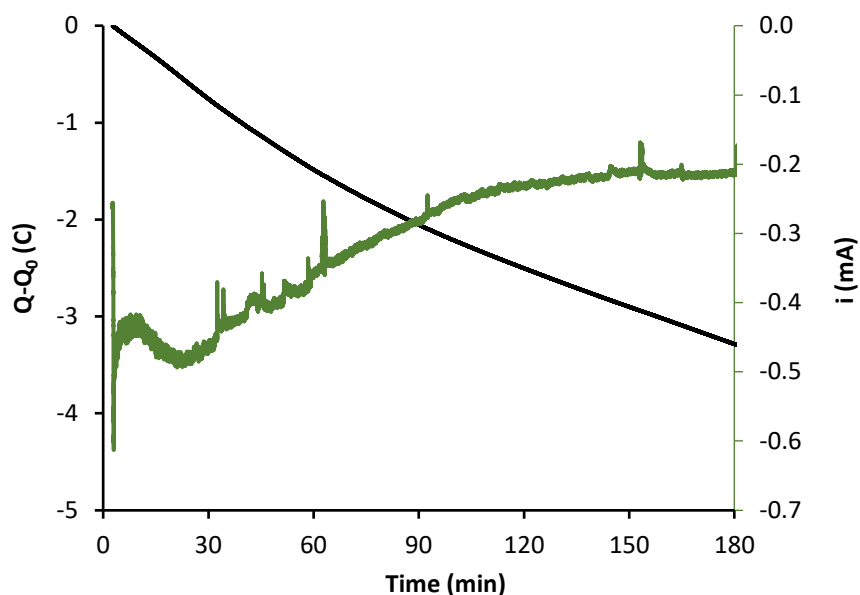


Figure S17. CPE at -2.2 V vs. $\text{Fc}^{+/0}$ in the dark of Co^{Me} (1 mM) in a 0.1 M $\text{TBAPF}_6/\text{MeCN}$ solution under CO_2 saturation with 1% of added H_2O . Charge versus time plot (black trace). Current versus time plot (red trace).

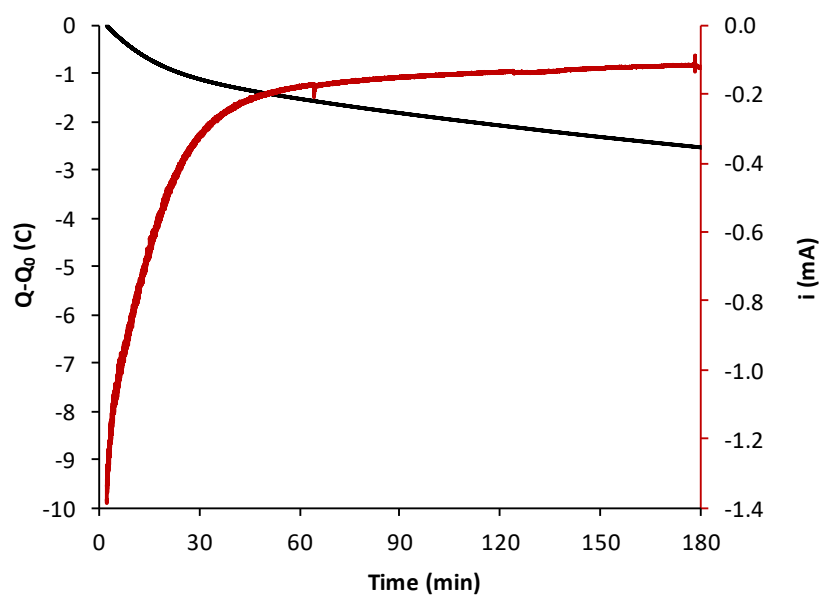


Figure S18. CPE at -1.9 V vs. $\text{Fc}^{+/0}$ in the dark of Co^{H} (1 mM) in a 0.1 M $\text{TBAPF}_6/\text{MeCN}$ solution under CO_2 saturation with 10% of added H_2O . Charge versus time plot (black trace). Current versus time plot (red trace).

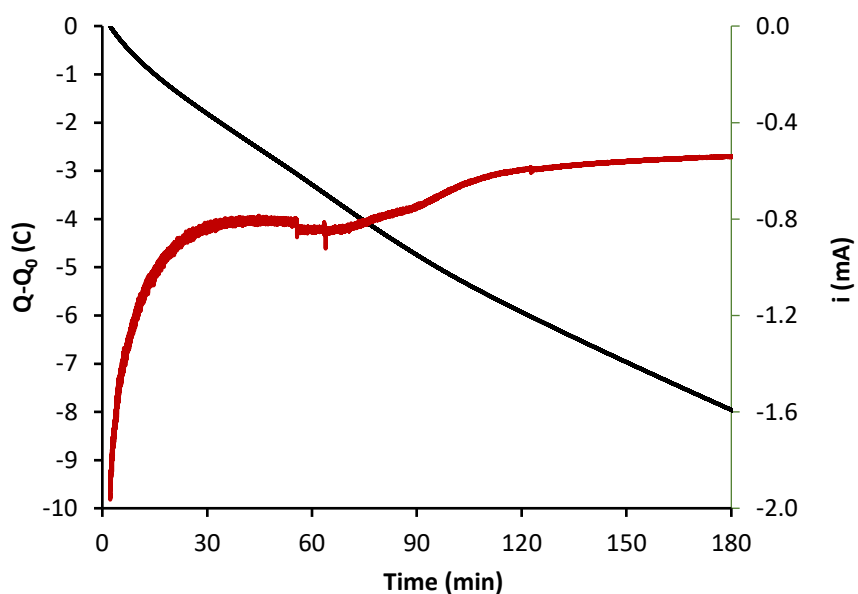


Figure S19. CPE at -1.9 V vs. $\text{Fc}^{+/0}$ in the dark of Co^{H} (1 mM) in a 0.1 M $\text{TBAPF}_6/\text{MeCN}$ solution under CO_2 saturation with 10% of added H_2O . Charge versus time plot (black trace). Current versus time plot (red trace). Temperature control at 30 °C.

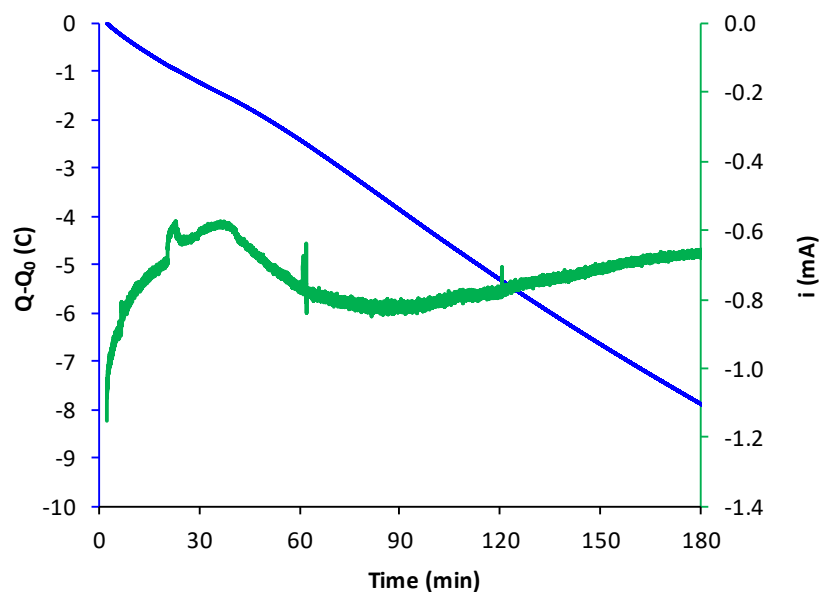


Figure S20. CPE at -1.9 V vs. $\text{Fc}^{+/0}$ irradiated at 447 nm of Co^{H} (1 mM) in a 0.1 M $\text{TBAPF}_6/\text{MeCN}$ solution under CO_2 saturation with 10% of added H_2O . Charge *versus* time plot (blue trace). Current *versus* time plot (green trace).

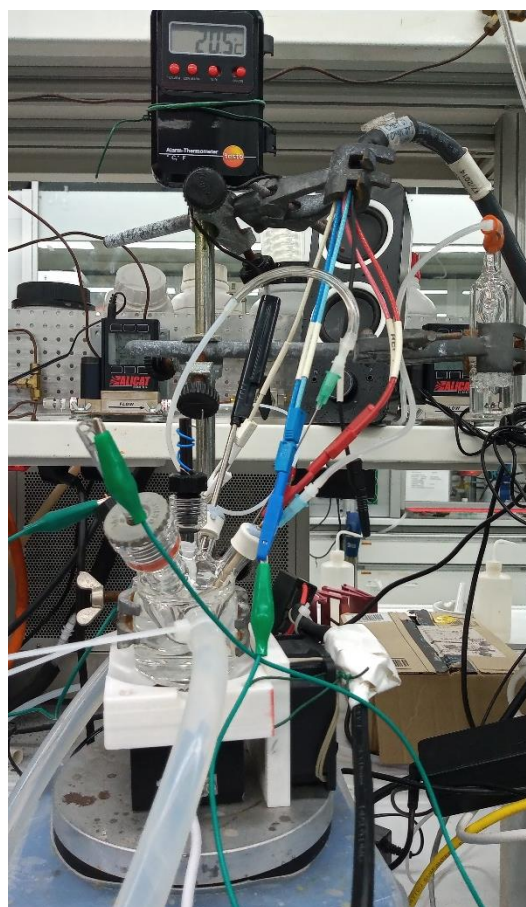


Figure S21. Picture of the employed setup for temperature-controlled electrochemical experiments under irradiation.

6. Density Functional Theory (DFT) calculations

6.1. Computational details

Geometry optimizations and frequency calculations at the ground state structure have been performed at the B3LYP/6-31+G* level of theory with the *Gaussian09* software package.² Solvent effects and dispersion interactions are considered through the SMD model³ for acetonitrile and Grimme-D₃ correction⁴, respectively. The free energy (G) was calculated following equation S1

$$G = E_{\text{elec}} + \Delta G_{\text{corr}} + \Delta G^{0/*} \quad (\text{S1})$$

in which E_{elec} is the single point energy at the B3LYP/6-31+G* ground state geometry and ΔG_{corr} is the Gibbs energy correction obtained from the frequency calculation. $\Delta G^{0/*}$ is the free energy change associated with the conversion from the standard-state gas-phase pressure of 1 atm to the desired concentration in mol·L⁻¹ according to equation S2

$$\Delta G^{0/*} = RT \ln(24.4 \cdot c) \quad (\text{S2})$$

where 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⁻¹.⁵ In our calculations we have considered that the concentration of CO₂ and CO in acetonitrile under saturation conditions is of 0.28 M and 0.028 M, respectively.

6.2. Thermodynamic data of optimized structures

All geometries were optimized at the B3LYP-D₃/6-31+G* level of theory. The charge and spin multiplicity of the corresponding structure are indicated at the beginning of each set of xyz coordinates as [**name**, **q**, **s**] e.g. **Co^H (Co-CO, 1, 3)** where Co-CO is the name of the [Co^I-CO]⁺ intermediate of **Co^H**; 1 is the charge (q) and 3 is the spin multiplicity (s). The associated electronic energy value (E_{elec}) and the different thermodynamic corrections to Gibbs energy (ΔG_{corr}) and Enthalpy (ΔH_{corr}) as well as the corresponding G and H obtained after a vibrational analysis at the same level of theory are shown in Table S3.

² Gaussian 09, Revision E.01, Frisch et. al. Gaussian, Inc., Wallingford CT, **2009**.

³ A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 6378–6396.

⁴ S. Grimme, J. Antony, S. Ehrlich, H. J. Krieg, *Chem. Phys.* **2010**, *132*, 154104.

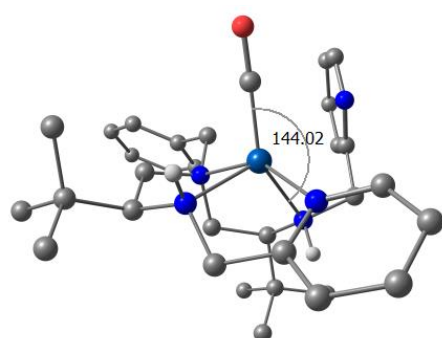
⁵ C. P. Kelly, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2007**, *111*, 408–422.

Table S3. DFT data of relevant intermediates calculated at the B3LYP/6-31+G* (SMD, acetonitrile).

Co ^H	Charge	Spin multiplicity	E	G _{corr}	H _{corr}	G	H
Co	1	3	-2864.9584	0.6530	0.7593	-2864.3055	-2864.1991
Co-CO ₂	1	1	-3053.5765	0.6753	0.7806	-3052.9012	-3052.7959
Co-CO ₂	1	3	-3053.5707	0.6675	0.7785	-3052.9032	-3052.7922
Co-CO 6coord	1	3	-2978.3173	0.6604	0.7714	-2977.6569	-2977.5459
Co-CO 5coord	1	3	-2978.3119	0.6594	0.7718	-2977.6525	-2977.5401

Co ^{Me}	Charge	Spin multiplicity	E	G _{corr}	H _{corr}	G	H
Co	1	3	-2943.5719	0.7123	0.8194	-2942.8596	-2942.7524
Co-CO ₂	1	1	-3132.1718	0.7333	0.8405	-3131.4385	-3131.3313
Co-CO ₂	1	3	-3132.172	0.7258	0.8385	-3131.4462	-3131.3335
Co-CO 6coord	1	3	-3056.9258	0.7197	0.8316	-3056.2061	-3056.0941
Co-CO 5coord	1	3	-3056.9184	0.7172	0.8311	-3056.2012	-3056.0873

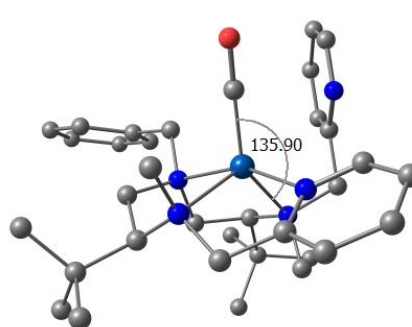
Ligands	Charge	Spin multiplicity	E	G _{corr}	H _{corr}	G	H
CO ₂	0	1	-188.5912	-0.0073	0.0140	-188.5986	-188.5773
CO	0	1	-113.3125	-0.0141	0.0083	-113.3267	-113.3042



Co^H 5-coordinate Co^I-CO

$$\Delta G = G(5\text{-coord}) - G(6\text{-coord}) = 2.7 \text{ kcal}\cdot\text{mol}^{-1}$$

$$\text{Theoretical } \nu_{\text{st}}(\text{CO}) = 1906 \text{ cm}^{-1}$$



Co^{Me} 5-coordinate Co^I-CO

$$\Delta G = G(5\text{-coord}) - G(6\text{-coord}) = 3.1 \text{ kcal}\cdot\text{mol}^{-1}$$

$$\text{Theoretical } \nu_{\text{st}}(\text{CO}) = 1916 \text{ cm}^{-1}$$

Figure 22. DFT computed 5-coordinate structures of the Co(I)-CO intermediate with a dangling pyridine ligand for both Co^H and Co^{Me}.

6.3. XYZ coordinates

Co ^H (Co, 1, 3)				7	3.151011000	-0.072051000	-0.384700000
27	1.090508000	-0.162967000	-0.718025000	6	0.375714000	-1.859625000	-3.062413000
7	0.727243000	-1.805302000	-1.750872000	1	0.534713000	-0.944258000	-3.626048000
7	0.749603000	-1.525509000	1.016053000	6	-0.167520000	-2.990957000	-3.659158000
1	1.442475000	-1.322798000	1.733373000	1	-0.433791000	-2.966614000	-4.712358000
7	-0.985939000	0.417072000	-0.188553000	6	-0.367403000	-4.141370000	-2.883612000
7	1.382114000	1.963478000	-0.197368000	1	-0.800586000	-5.039839000	-3.313918000
1	1.795863000	2.390012000	-1.027618000	6	0.007893000	-4.099684000	-1.533640000
				1	-0.124902000	-4.966528000	-0.891031000

6	0.560267000	-2.937573000	-1.004303000	1	0.553906000	-1.352795000	-3.354692000
6	1.058818000	-2.842970000	0.418278000	6	0.400576000	-3.505027000	-3.182680000
1	0.678123000	-3.689099000	0.998588000	1	0.185304000	-3.655530000	-4.236916000
1	2.153790000	-2.918465000	0.403680000	6	0.467049000	-4.583115000	-2.291455000
6	-0.621212000	-1.351703000	1.571637000	1	0.300728000	-5.601548000	-2.631094000
1	-1.262023000	-2.062441000	1.039144000	6	0.750628000	-4.314139000	-0.946738000
6	-0.759995000	-1.675672000	3.101343000	1	0.810212000	-5.116915000	-0.216366000
6	-0.197533000	-3.078716000	3.403502000	6	0.961901000	-3.000361000	-0.537265000
1	-0.358778000	-3.322597000	4.461142000	6	1.350846000	-2.637040000	0.875175000
1	0.880142000	-3.138388000	3.213834000	1	1.196005000	-3.491833000	1.540511000
1	-0.698185000	-3.848497000	2.803320000	1	2.425856000	-2.419041000	0.882371000
6	-2.252871000	-1.677406000	3.493582000	6	-0.810251000	-1.497404000	1.444433000
1	-2.362817000	-1.981197000	4.542397000	1	-1.092119000	-2.173343000	0.631485000
1	-2.821007000	-2.386835000	2.878592000	6	-1.465531000	-2.117529000	2.741725000
1	-2.716840000	-0.691166000	3.388094000	6	-0.751992000	-3.410729000	3.181799000
6	-0.007945000	-0.652534000	3.977961000	1	-1.290717000	-3.854103000	4.029383000
1	-0.041178000	-0.968320000	5.028167000	1	0.276798000	-3.234200000	3.507659000
1	-0.452430000	0.347249000	3.922465000	1	-0.738403000	-4.154172000	2.375708000
1	1.050178000	-0.568966000	3.696803000	6	-2.921683000	-2.512762000	2.394744000
6	-1.069304000	0.085490000	1.250070000	1	-3.374837000	-3.036801000	3.245819000
1	-2.077015000	0.281502000	1.635009000	1	-2.956133000	-3.188107000	1.530324000
1	-0.388625000	0.763080000	1.764933000	1	-3.551740000	-1.645580000	2.174141000
6	-1.981492000	-0.309780000	-1.025235000	6	-1.517206000	-1.145094000	3.940762000
1	-1.787089000	-1.377158000	-0.909445000	1	-2.035313000	-1.630712000	4.777996000
1	-1.751947000	-0.056343000	-2.064384000	1	-2.072860000	-0.230636000	3.704817000
6	-3.440957000	-0.019813000	-0.728163000	1	-0.523785000	-0.857424000	4.294486000
6	-4.139532000	-0.778134000	0.224469000	6	-1.396075000	-0.109256000	1.131402000
1	-3.629788000	-1.592458000	0.733254000	1	-2.482553000	-0.104025000	1.266452000
6	-5.476005000	-0.497879000	0.526641000	1	-0.993900000	0.608166000	1.846333000
1	-5.99521000	-1.095854000	1.269151000	6	-1.865552000	-0.251308000	-1.303946000
6	-6.138136000	0.547294000	-0.127673000	1	-1.725172000	-1.330386000	-1.223871000
1	-7.177817000	0.766296000	0.103704000	1	-1.412280000	0.061701000	-2.249418000
6	-5.455946000	1.304452000	-1.087473000	6	-3.349982000	0.070349000	-1.308959000
1	-5.965345000	2.112877000	-1.606939000	6	-4.262618000	-0.773816000	-0.657947000
6	-4.118703000	1.020750000	-1.383112000	1	-3.898966000	-1.672656000	-0.168691000
1	-3.593905000	1.611341000	-2.131004000	6	-5.630180000	-0.479995000	-0.638735000
6	-1.072478000	1.876807000	-0.416373000	1	-6.319495000	-1.148397000	-0.127851000
1	-2.003316000	2.279507000	0.002270000	6	-6.109032000	0.666605000	-1.281381000
1	-1.111530000	2.010752000	-1.500779000	1	-7.171556000	0.897524000	-1.270443000
6	0.122494000	2.671548000	0.153990000	6	-5.212296000	1.507945000	-1.950963000
1	0.058439000	2.666458000	1.246669000	1	-5.576875000	2.393815000	-2.465975000
6	0.082523000	4.179978000	-0.275586000	6	-3.846542000	1.208742000	-1.965463000
6	-1.200755000	4.836127000	0.276486000	1	-3.160306000	1.863262000	-2.497661000
1	-1.179128000	5.916635000	0.086258000	6	-1.137742000	1.856622000	-0.287058000
1	-1.287409000	4.687024000	1.360878000	1	-2.081902000	2.198804000	0.150337000
1	-2.106239000	4.438910000	-0.194941000	1	-1.164040000	2.131377000	-1.342316000
6	0.114166000	4.356811000	-1.807722000	6	0.049431000	2.569535000	0.388480000
1	0.189094000	5.423122000	-2.055176000	1	0.162187000	2.169891000	1.400919000
1	-0.792084000	3.973185000	-2.288740000	6	-0.256147000	4.105977000	0.582791000
1	0.977709000	3.856845000	-2.265340000	6	-1.267228000	4.234615000	1.747097000
6	1.295525000	4.917707000	0.325692000	1	-1.485326000	5.293109000	1.937517000
1	1.217339000	5.993133000	0.123115000	1	-0.861568000	3.804178000	2.672045000
1	2.239966000	4.572609000	-0.110113000	1	-2.219447000	3.736910000	1.533785000
1	1.347297000	4.782157000	1.413286000	6	-0.867765000	4.777983000	-0.665881000
6	2.411309000	1.884637000	0.855196000	1	-1.048144000	5.840158000	-0.455504000
1	1.925406000	1.469676000	1.747251000	1	-1.830707000	4.334537000	-0.942570000
1	2.838253000	2.854661000	1.134693000	1	-0.206172000	4.722552000	-1.535338000
6	3.520012000	0.945879000	0.425814000	6	1.007868000	4.884259000	0.992917000
6	4.834226000	1.094280000	0.871627000	1	0.738933000	5.920707000	1.234729000
1	5.094593000	1.933520000	1.510908000	1	1.749713000	4.917526000	0.189891000
6	5.794998000	0.154680000	0.488950000	1	1.479244000	4.447872000	1.881453000
1	6.823288000	0.248850000	0.827314000	6	2.529649000	2.202064000	0.513090000
6	5.409833000	-0.902057000	-0.341402000	1	2.259665000	1.978313000	1.550780000
1	6.121280000	-1.654549000	-0.668633000	1	2.992196000	3.196524000	0.500869000
6	4.082112000	-0.971284000	-0.757376000	6	3.564418000	1.189113000	0.062535000
1	3.730817000	-1.766424000	-1.409052000	6	4.931351000	1.429224000	0.212836000
				1	5.267677000	2.378853000	0.620496000
				6	5.846562000	0.444679000	-0.165846000
				1	6.914611000	0.610890000	-0.054342000
				6	5.359014000	-0.750950000	-0.702358000
				1	6.028225000	-1.544537000	-1.021690000
				6	3.982480000	-0.908963000	-0.833730000
				1	3.554482000	-1.813303000	-1.255322000
				6	1.393637000	-0.785415000	2.455878000
				1	0.908613000	0.152200000	2.733624000
				1	1.447929000	-1.431864000	3.342912000
Co^{Me} (Co, 1, 3)							
27	1.038113000	-0.141670000	-0.549061000				
7	0.878739000	-1.947837000	-1.399097000				
7	0.680587000	-1.397516000	1.327382000				
7	-1.046860000	0.379589000	-0.224301000				
7	1.301839000	2.131024000	-0.295332000				
7	3.093714000	0.031904000	-0.452988000				
6	0.608459000	-2.217630000	-2.699193000				

1	2.413516000	-0.555572000	2.135323000
6	1.534277000	2.644066000	-1.655396000
1	2.321636000	2.048752000	-2.127758000
1	0.632284000	2.535849000	-2.259629000
1	1.847459000	3.697482000	-1.663722000

Co^H (Co-CO₂, 1, 1)

27	0.929917000	0.148356000	-0.478420000
7	1.013143000	-1.680454000	-1.387597000
7	0.782739000	-1.405073000	1.345650000
1	1.180540000	-1.047646000	2.211061000
7	-1.101501000	0.241472000	-0.117223000
7	0.987812000	1.909351000	0.437892000
1	1.431723000	2.506994000	-0.267376000
7	2.869547000	0.229676000	-0.137314000
6	0.791990000	-1.879671000	-2.704753000
1	0.496032000	-1.001172000	-3.262588000
6	0.918633000	-3.123994000	-3.312108000
1	0.728376000	-3.220092000	-4.376479000
6	1.279750000	-4.221593000	-2.530190000
1	1.382136000	-5.210692000	-2.967861000
6	1.491721000	-4.024080000	-1.167740000
1	1.754030000	-4.851253000	-0.514939000
6	1.357165000	-2.745147000	-0.624190000
6	1.610246000	-2.506678000	0.843182000
1	1.468920000	-3.447699000	1.379406000
1	2.657567000	-2.216316000	0.982630000
6	-0.671499000	-1.666773000	1.508717000
1	-0.946908000	-2.387986000	0.732816000
6	-1.115307000	-2.276474000	2.888362000
6	-0.263343000	-3.509473000	3.243620000
1	-0.651861000	-3.970451000	4.160250000
1	0.783359000	-3.244896000	3.431419000
1	-0.297345000	-4.265620000	2.449849000
6	-2.585309000	-2.735556000	2.780128000
1	-2.895353000	-3.216587000	3.716300000
1	-2.711511000	-3.465517000	1.970398000
1	-3.271252000	-1.902652000	2.595465000
6	-0.986158000	-1.252344000	4.035156000
1	-1.217236000	-1.737373000	4.991530000
1	-1.678874000	-0.411695000	3.918877000
1	0.032181000	-0.848711000	4.111677000
6	-1.355783000	-0.326117000	1.246956000
1	-2.434215000	-0.368543000	1.414483000
1	-0.946808000	0.383748000	1.962218000
6	-1.922373000	-0.447323000	-1.175955000
1	-1.647221000	-1.502076000	-1.140882000
1	-1.564757000	-0.039366000	-2.121222000
6	-3.425022000	-0.303041000	-1.059308000
6	-4.186045000	-1.264769000	-0.376937000
1	-3.684334000	-2.117217000	0.073943000
6	-5.575032000	-1.138797000	-0.272487000
1	-6.148183000	-1.894307000	0.259822000
6	-6.224355000	-0.045207000	-0.856111000
1	-7.304393000	0.054444000	-0.778821000
6	-5.477521000	0.914860000	-1.549255000
1	-5.975754000	1.762160000	-2.014437000
6	-4.089446000	0.783345000	-1.650926000
1	-3.514684000	1.527902000	-2.196562000
6	-1.397932000	1.708766000	-0.071017000
1	-2.403620000	1.871889000	0.327474000
1	-1.375658000	2.058236000	-1.102079000
6	-0.362553000	2.471458000	0.778060000
1	-0.525263000	2.261395000	1.873914000
6	-0.469958000	4.022218000	0.610823000
6	-1.843837000	4.474350000	1.149898000
1	-1.906537000	5.569262000	1.131659000
1	-1.991852000	4.144974000	2.186692000
1	-2.672907000	4.087609000	0.547249000
6	-0.327430000	4.472940000	-0.857279000
1	-0.299820000	5.568604000	-0.900319000
1	-1.168625000	4.141982000	-1.475817000
1	0.594846000	4.101487000	-1.319513000
6	0.627535000	4.712099000	1.445404000
1	0.461357000	5.795978000	1.449730000

1	1.627057000	4.540745000	1.029193000
1	0.619545000	4.365151000	2.486290000
6	1.975290000	1.732781000	1.534327000
1	1.512682000	1.128185000	2.319304000
1	2.287109000	2.681045000	1.976837000
6	3.160330000	1.015937000	0.927933000
6	4.465655000	1.152248000	1.392995000
1	4.668058000	1.795063000	2.244240000
6	5.492019000	0.464912000	0.742243000
1	6.517615000	0.555558000	1.088561000
6	5.184567000	-0.324017000	-0.368314000
1	5.954107000	-0.861823000	-0.912679000
6	3.858432000	-0.412090000	-0.780406000
1	3.561659000	-1.006941000	-1.636554000
6	1.026778000	1.231030000	-2.169223000
8	0.113030000	1.032456000	-2.996600000
8	1.984329000	2.035172000	-2.213561000

Co^{Me} (Co-CO₂, 1, 1)

27	0.939394000	0.155486000	-0.557198000
7	1.042308000	-1.776617000	-1.108144000
7	0.752869000	-1.193308000	1.591477000
7	-1.102563000	0.188153000	-0.231804000
7	0.977550000	2.151635000	0.026882000
7	2.874003000	0.318387000	-0.321677000
6	0.754173000	-2.207211000	-2.355851000
1	0.368130000	-1.470852000	-3.045187000
6	0.921497000	-3.524970000	-2.763783000
1	0.668993000	-3.803098000	-3.781954000
6	1.407697000	-4.455948000	-1.846582000
1	1.554627000	-5.494707000	-2.128700000
6	1.676958000	-4.027756000	-0.548921000
1	2.023464000	-4.721268000	0.210989000
6	1.481924000	-2.689410000	-0.206330000
6	1.738088000	-2.207566000	1.194773000
1	1.778761000	-3.067579000	1.871700000
1	2.725271000	-1.733966000	1.237271000
6	-0.676873000	-1.627688000	1.492896000
1	-0.707031000	-2.314400000	0.645451000
6	-1.348880000	-2.435298000	2.672225000
6	-0.440147000	-3.588774000	3.139322000
1	-0.975951000	-4.200740000	3.876193000
1	0.477771000	-3.235892000	3.617317000
1	-0.165183000	-4.241800000	2.301778000
6	-2.642355000	-3.080258000	2.117091000
1	-3.066881000	-3.759366000	2.866964000
1	-2.442781000	-3.665841000	1.210538000
1	-3.409962000	-2.337326000	1.880850000
6	-1.746439000	-1.571600000	3.888704000
1	-2.292003000	-2.194924000	4.608937000
1	-2.411214000	-0.746972000	3.606417000
1	-0.884727000	-1.150501000	4.412365000
6	-1.477916000	-0.386249000	1.112141000
1	-2.550050000	-0.586872000	1.107170000
1	-1.319207000	0.376643000	1.869410000
6	-1.896923000	-0.509317000	-1.313956000
1	-1.673975000	-1.572310000	-1.216588000
1	-1.481285000	-0.153269000	-2.252803000
6	-3.400038000	-0.305953000	-1.312360000
6	-4.254449000	-1.287909000	-0.787931000
1	-3.827261000	-2.195149000	-0.370479000
6	-5.643362000	-1.121448000	-0.805969000
1	-6.285831000	-1.895934000	-0.393507000
6	-6.201962000	0.035722000	-1.357925000
1	-7.280856000	0.170014000	-1.373209000
6	-5.362831000	1.013692000	-1.905522000
1	-5.788637000	1.908584000	-2.353330000
6	-3.976111000	0.839827000	-1.887616000
1	-3.337002000	1.598106000	-2.332142000
6	-1.391445000	1.656215000	-0.212502000
1	-2.410888000	1.825067000	0.139386000
1	-1.319835000	2.004037000	-1.241394000
6	-0.375149000	2.386968000	0.669219000
1	-0.282444000	1.854323000	1.615275000
6	-0.850433000	3.829448000	1.078201000

6	-2.006860000	3.630026000	2.092518000	6	-2.006848000	-0.298103000	-1.052667000
1	-2.346386000	4.606861000	2.456768000	1	-1.771707000	-1.362510000	-1.006413000
1	-1.677048000	3.045649000	2.960762000	1	-1.711230000	0.059241000	-2.040661000
1	-2.873410000	3.125550000	1.653387000	6	-3.491138000	-0.093152000	-0.828432000
6	-1.386786000	4.677114000	-0.094442000	6	-4.225604000	-1.004112000	-0.053389000
1	-1.800896000	5.614526000	0.298122000	1	-3.718815000	-1.863803000	0.378849000
1	-2.192495000	4.165629000	-0.633288000	6	-5.593049000	-0.816125000	0.171497000
1	-0.610179000	4.941952000	-0.816551000	1	-6.145583000	-1.532080000	0.775499000
6	0.249453000	4.613121000	1.822116000	6	-6.247654000	0.289830000	-0.382286000
1	-0.177609000	5.539672000	2.225607000	1	-7.311124000	0.437962000	-0.210522000
1	1.081710000	4.899879000	1.173975000	6	-5.527965000	1.200313000	-1.165211000
1	0.649015000	4.037160000	2.665191000	1	-6.031265000	2.057469000	-1.606318000
6	2.104847000	2.182013000	1.004881000	6	-4.160707000	1.007294000	-1.386245000
1	1.746806000	1.788360000	1.955580000	1	-3.607167000	1.714223000	-1.999821000
1	2.458715000	3.200213000	1.182293000	6	-1.233919000	1.869132000	-0.174374000
6	3.234355000	1.332346000	0.942853000	1	-2.197738000	2.184945000	0.238329000
6	4.567619000	1.564612000	0.830292000	1	-1.220164000	2.106673000	-1.237465000
1	4.817615000	2.399237000	1.478079000	6	-0.096490000	2.620549000	0.550097000
6	5.552305000	0.722630000	0.316184000	1	-0.260147000	2.550714000	1.629706000
1	6.597352000	0.879635000	0.568154000	6	-0.082353000	4.149576000	0.215080000
6	5.174078000	-0.311474000	-0.544497000	6	-1.427966000	4.767784000	0.649450000
1	5.906784000	-0.980568000	-0.984243000	1	-1.389661000	5.858684000	0.540308000
6	3.828173000	-0.471469000	-0.849456000	1	-1.647809000	4.542133000	1.701246000
1	3.486593000	-1.235770000	-1.533083000	1	-2.264248000	4.406425000	0.041136000
6	1.058279000	0.672186000	-2.488787000	6	0.135035000	4.429823000	-1.286228000
8	2.164100000	0.462371000	-3.011738000	1	0.202259000	5.512693000	-1.448193000
8	-0.002951000	1.112264000	-2.971760000	1	-0.689185000	4.055388000	-1.902001000
6	1.159663000	-0.559750000	2.849696000	1	1.064237000	3.987780000	-1.665793000
1	0.474679000	0.250141000	3.108391000	6	1.045330000	4.836103000	1.012051000
1	1.200210000	-1.265933000	3.689067000	1	0.997991000	5.921991000	0.864458000
1	2.162335000	-0.142776000	2.723696000	1	2.038947000	4.508359000	0.684485000
6	1.299983000	3.102539000	-1.073982000	1	0.953671000	4.636204000	2.087042000
1	2.204385000	2.760749000	-1.578114000	6	2.069062000	1.696555000	1.441808000
1	0.486749000	3.129284000	-1.792492000	1	1.478529000	1.168129000	2.198366000
1	1.478247000	4.103117000	-0.675034000	1	2.431677000	2.624851000	1.894211000

Co^H (Co-CO₂, 1, 3)

27	0.949657000	-0.055794000	-0.632564000
7	0.772432000	-1.913283000	-1.598274000
7	0.623759000	-1.491798000	1.153266000
1	1.218215000	-1.173538000	1.916210000
7	-1.097789000	0.393106000	-0.079656000
7	1.197326000	1.928484000	0.270647000
1	1.734537000	2.469683000	-0.406242000
7	2.961674000	-0.091404000	0.078918000
6	0.527820000	-2.085109000	-2.913163000
1	0.489421000	-1.183182000	-3.510753000
6	0.312247000	-3.335486000	-3.482724000
1	0.118836000	-3.415962000	-4.547779000
6	0.339896000	-4.460316000	-2.656285000
1	0.164825000	-5.452998000	-3.061887000
6	0.586932000	-4.286175000	-1.295468000
1	0.606966000	-5.132911000	-0.615618000
6	0.808046000	-3.000615000	-0.796672000
6	1.145221000	-2.776694000	0.656901000
1	0.804532000	-3.638792000	1.232503000
1	2.236117000	-2.739990000	0.752565000
6	-0.799451000	-1.471790000	1.591756000
1	-1.327097000	-2.187904000	0.953153000
6	-1.065930000	-1.888733000	3.084782000
6	-0.380254000	-3.226627000	3.420900000
1	-0.640671000	-3.523510000	4.444529000
1	0.711869000	-3.152589000	3.372057000
1	-0.708305000	-4.029805000	2.749900000
6	-2.584578000	-2.081066000	3.287173000
1	-2.782597000	-2.422039000	4.311176000
1	-2.980462000	-2.838929000	2.599126000
1	-3.150364000	-1.156038000	3.134526000
6	-0.550321000	-0.825823000	4.078704000
1	-0.634235000	-1.207232000	5.103633000
1	-1.124765000	0.105344000	4.028909000
1	0.506359000	-0.582130000	3.906588000
6	-1.311181000	-0.053011000	1.317878000
1	-2.365703000	0.052889000	1.589182000
1	-0.749123000	0.629577000	1.951043000

Co^{Me} (Co-CO₂, 1, 3)

27	0.970586000	-0.105003000	-0.600411000
7	0.936147000	-2.167682000	-1.144800000
7	0.635708000	-1.308646000	1.508631000
7	-1.093418000	0.303720000	-0.188508000
7	1.142934000	2.279697000	-0.044628000
7	2.986853000	0.172768000	-0.083608000
6	0.669499000	-2.617578000	-2.386057000
1	0.507283000	-1.864118000	-3.147124000
6	0.593457000	-3.971272000	-2.698403000
1	0.372619000	-4.278342000	-3.715729000
6	0.800811000	-4.903208000	-1.679929000
1	0.746313000	-5.969147000	-1.883228000
6	1.067101000	-4.441865000	-0.390830000
1	1.218754000	-5.132400000	0.433053000
6	1.129274000	-3.067804000	-0.155729000
6	1.440951000	-2.507839000	1.206787000
1	1.352296000	-3.294768000	1.960031000
1	2.490009000	-2.191776000	1.212860000
6	-0.847862000	-1.530554000	1.531164000
1	-1.026900000	-2.236953000	0.716485000
6	-1.548782000	-2.176326000	2.792321000
6	-0.777672000	-3.403314000	3.317971000
1	-1.362701000	-3.886096000	4.111184000
1	0.191870000	-3.138230000	3.748705000
1	-0.616988000	-4.146499000	2.527839000
6	-2.937953000	-2.688538000	2.338964000

1	-3.417604000	-3.230333000	3.163619000	6	0.794604000	-3.659584000	-3.160675000
1	-2.849985000	-3.380634000	1.491672000	1	0.553289000	-3.914602000	-4.188209000
1	-3.611920000	-1.877220000	2.048051000	6	1.114861000	-4.640613000	-2.218558000
6	-1.768689000	-1.191509000	3.961259000	1	1.128514000	-5.692114000	-2.492608000
1	-2.309126000	-1.704505000	4.767287000	6	1.406801000	-4.244069000	-0.913748000
1	-2.375129000	-0.328168000	3.665541000	1	1.649346000	-4.973793000	-0.146327000
1	-0.831384000	-0.819537000	4.383058000	6	1.378623000	-2.884305000	-0.588533000
6	-1.506511000	-0.197103000	1.154528000	6	1.726116000	-2.398383000	0.798175000
1	-2.595301000	-0.274594000	1.188912000	1	1.675518000	-3.241905000	1.489366000
1	-1.233016000	0.553352000	1.892526000	1	2.766697000	-2.055184000	0.793760000
6	-1.889011000	-0.368207000	-1.283571000	6	-0.522643000	-1.491524000	1.509712000
1	-1.719280000	-1.441182000	-1.178940000	1	-0.866893000	-2.265978000	0.815742000
1	-1.435409000	-0.049135000	-2.221072000	6	-0.849063000	-1.999537000	2.965575000
6	-3.379241000	-0.087813000	-1.316861000	6	0.046607000	-3.186687000	3.367109000
6	-4.290775000	-0.988529000	-0.745551000	1	-0.282050000	-3.579700000	4.337596000
1	-3.919789000	-1.893786000	-0.273768000	1	1.095571000	-2.890009000	3.475585000
6	-5.667267000	-0.741842000	-0.783142000	1	-0.014735000	-4.004942000	2.639433000
1	-6.356143000	-1.453113000	-0.333478000	6	-2.311879000	-2.492501000	3.006890000
6	-6.154386000	0.413562000	-1.402685000	1	-2.548213000	-2.877658000	4.007050000
1	-7.223607000	0.608850000	-1.434100000	1	-2.472785000	-3.306836000	2.288534000
6	-5.257355000	1.310564000	-1.995289000	1	-3.029833000	-1.697647000	2.782482000
1	-5.628172000	2.203388000	-2.493280000	6	-0.658475000	-0.884549000	4.015583000
6	-3.883163000	1.057861000	-1.955595000	1	-0.771925000	-1.300562000	5.024484000
1	-3.195604000	1.753086000	-2.430567000	1	-1.396662000	-0.082188000	3.908746000
6	-1.246202000	1.785222000	-0.260380000	1	0.342423000	-0.437379000	3.955606000
1	-2.255703000	2.060191000	0.054018000	6	-1.248829000	-0.169513000	1.224339000
1	-1.139080000	2.063322000	-1.309367000	1	-2.303752000	-0.216311000	1.514728000
6	-0.193009000	2.519553000	0.584237000	1	-0.782102000	0.584833000	1.855837000
1	-0.108997000	2.006052000	1.543211000	6	-1.964182000	-0.460699000	-1.135264000
6	-0.655429000	3.978193000	0.958120000	1	-1.612124000	-1.493875000	-1.112991000
6	-1.790428000	3.840416000	2.003322000	1	-1.729604000	-0.062712000	-2.126660000
1	-2.119778000	4.835523000	2.326787000	6	-3.462837000	-0.417801000	-0.900614000
1	-1.445395000	3.297445000	2.892624000	6	-4.093521000	-1.403420000	-0.126087000
1	-2.668286000	3.318605000	1.608107000	1	-3.499508000	-2.211282000	0.293256000
6	-1.197810000	4.787519000	-0.238580000	6	-5.470309000	-1.356384000	0.115976000
1	-1.566330000	5.758840000	0.116171000	1	-5.939956000	-2.129018000	0.720412000
1	-2.036767000	4.281886000	-0.730703000	6	-6.240444000	-0.318916000	-0.421179000
1	-0.432606000	4.986117000	-0.994101000	1	-7.311258000	-0.280101000	-0.235981000
6	0.478900000	4.771338000	1.635361000	6	-5.625596000	0.664449000	-1.205607000
1	0.086937000	5.728160000	2.003435000	1	-6.218231000	1.469081000	-1.634780000
1	1.298647000	4.999961000	0.949062000	6	-4.248385000	0.612196000	-1.442609000
1	0.889000000	4.228054000	2.494956000	1	-3.776627000	1.376887000	-2.055695000
6	2.269458000	2.282062000	0.906681000	6	-1.417694000	1.759334000	-0.239430000
1	1.901774000	1.965179000	1.885798000	1	-2.410427000	1.962747000	0.180522000
1	2.700125000	3.281683000	1.033842000	1	-1.446490000	2.017905000	-1.299770000
6	3.366909000	1.333727000	0.482387000	6	-0.375640000	2.644161000	0.487126000
6	4.714232000	1.632167000	0.700396000	1	-0.506954000	2.523981000	1.567129000
1	4.985516000	2.583835000	1.147939000	6	-0.593510000	4.169160000	0.196252000
6	5.687955000	0.706017000	0.329340000	6	-2.003090000	4.583463000	0.666644000
1	6.741049000	0.920974000	0.488946000	1	-2.119637000	5.671426000	0.584936000
6	5.286824000	-0.493207000	-0.264991000	1	-2.168417000	4.305387000	1.715916000
1	6.006940000	-1.240538000	-0.582825000	1	-2.793654000	4.122931000	0.064386000
6	3.927837000	-0.712552000	-0.459524000	6	-0.442853000	4.513457000	-1.300091000
1	3.565181000	-1.615066000	-0.938375000	1	-0.532733000	5.598016000	-1.438557000
6	1.237032000	0.493027000	-2.631333000	1	-1.213971000	4.037886000	-1.915696000
8	2.368511000	0.137575000	-2.962082000	1	0.536200000	4.218305000	-1.699093000
8	0.260069000	1.018975000	-3.166202000	6	0.442180000	4.987434000	0.993523000
6	1.201260000	-0.618472000	2.677427000	1	0.238761000	6.059962000	0.882891000
1	0.623102000	0.276872000	2.906615000	1	1.463673000	4.811243000	0.637619000
1	1.231040000	-1.254187000	3.571778000	1	0.405154000	4.745365000	2.063256000
1	2.225022000	-0.318549000	2.442689000	6	1.944028000	2.029086000	1.275696000
6	1.476222000	3.121510000	-1.208397000	1	1.463240000	1.438847000	2.064168000
1	2.357025000	2.704357000	-1.704227000	1	2.233017000	2.987810000	1.723582000
1	0.654760000	3.122061000	-1.921539000	6	3.188611000	1.305719000	0.794748000
1	1.706672000	4.153515000	-0.917106000	6	4.437267000	1.528327000	1.382497000

Co^H (Co-CO 6coord, 1, 3)

27	0.980556000	0.155673000	-0.838043000
7	1.067118000	-1.939203000	-1.496276000
7	0.904555000	-1.244317000	1.186560000
7	-1.120399000	0.307293000	-0.171472000
7	0.990939000	2.160317000	0.166250000
7	3.030285000	0.425281000	-0.215922000
6	0.782587000	-2.328221000	-2.752223000
1	0.533304000	-1.533931000	-3.449427000

6	5.545824000	0.819980000	0.917616000
1	6.524470000	0.976532000	1.363400000
6	5.378465000	-0.082455000	-0.136420000
1	6.213552000	-0.648434000	-0.537973000
6	4.103069000	-0.243168000	-0.672497000
1	3.913354000	-0.934136000	-1.489133000
6	0.917542000	0.887848000	-2.496391000
8	0.882751000	1.431429000	-3.529337000
1	1.410341000	2.758477000	-0.543156000
1	1.356900000	-0.761407000	1.959109000

Co^{Me} (Co-CO 6coord, 1, 3)

27	1.002638000	0.014411000	-0.827411000
7	0.987120000	-2.176395000	-1.127291000
7	0.667075000	-1.214583000	1.527115000
7	-1.107944000	0.336534000	-0.272334000
7	1.182140000	2.285469000	-0.121259000
7	3.050490000	0.202412000	-0.343163000
6	0.700595000	-2.730874000	-2.318985000
1	0.475575000	-2.039038000	-3.124124000
6	0.677977000	-4.106141000	-2.539190000
1	0.436330000	-4.493229000	-3.524450000
6	0.965549000	-4.954741000	-1.468489000
1	0.955532000	-6.033924000	-1.595051000
6	1.251982000	-4.388587000	-0.226332000
1	1.462302000	-5.011101000	0.638343000
6	1.255500000	-2.997735000	-0.090048000
6	1.568051000	-2.337866000	1.227632000
1	1.596454000	-3.096211000	2.018765000
1	2.578149000	-1.915800000	1.166499000
6	-0.795280000	-1.496533000	1.450948000
1	-0.900838000	-2.181369000	0.606151000
6	-1.525374000	-2.218598000	2.652269000
6	-0.704896000	-3.417501000	3.165853000
1	-1.293015000	-3.975723000	3.905967000
1	0.222806000	-3.108583000	3.655607000
1	-0.453135000	-4.108017000	2.351860000
6	-2.864484000	-2.786183000	2.124156000
1	-3.351206000	-3.379233000	2.908874000
1	-2.706207000	-3.442762000	1.258743000
1	-3.565325000	-1.999307000	1.829664000
6	-1.843469000	-1.286604000	3.840944000
1	-2.389932000	-1.850997000	4.608177000
1	-2.478876000	-0.444018000	3.545532000
1	-0.942880000	-0.884043000	4.312062000
6	-1.503005000	-0.187985000	1.066026000
1	-2.588584000	-0.312518000	1.102523000
1	-1.266824000	0.570236000	1.810336000
6	-1.918236000	-0.291999000	-1.367068000
1	-1.718549000	-1.365248000	-1.323550000
1	-1.502910000	0.077060000	-2.307601000
6	-3.417974000	-0.048025000	-1.354273000
6	-4.297077000	-1.020522000	-0.854482000
1	-3.894727000	-1.957718000	-0.480171000
6	-5.679292000	-0.804063000	-0.837599000
1	-6.342055000	-1.571469000	-0.444304000
6	-6.205580000	0.394998000	-1.329025000
1	-7.279005000	0.568193000	-1.316809000
6	-5.341794000	1.365753000	-1.850727000
1	-5.743146000	2.294124000	-2.250509000
6	-3.962126000	1.141628000	-1.867508000
1	-3.302372000	1.895299000	-2.289851000
6	-1.227447000	1.818886000	-0.296738000
1	-2.220651000	2.117341000	0.052048000
1	-1.146413000	2.131940000	-1.340028000
6	-0.136898000	2.519346000	0.538203000
1	-0.039250000	1.982461000	1.483081000
6	-0.569742000	3.976254000	0.954760000
6	-1.672049000	3.838722000	2.033465000
1	-1.979451000	4.832866000	2.381208000
1	-1.305180000	3.279445000	2.903808000
1	-2.567923000	3.331904000	1.659421000
6	-1.135557000	4.815188000	-0.210704000
1	-1.463155000	5.792282000	0.168156000
1	-2.006493000	4.338820000	-0.675589000
1	-0.394237000	5.001079000	-0.993212000
6	0.598487000	4.741221000	1.605652000
1	0.235222000	5.698070000	2.002291000
1	1.397969000	4.967057000	0.894551000
1	1.029722000	4.177664000	2.441527000
6	2.341123000	2.260609000	0.785253000
1	2.003174000	1.927232000	1.769256000
1	2.783558000	3.255219000	0.921548000
6	3.431006000	1.318301000	0.309611000
6	4.778332000	1.587380000	0.571330000

1	5.050781000	2.501182000	1.092045000
6	5.752303000	0.681406000	0.153224000
1	6.803913000	0.874777000	0.347135000
6	5.352182000	-0.469635000	-0.531602000
1	6.072648000	-1.199348000	-0.888303000
6	3.993367000	-0.663070000	-0.759701000
1	3.626291000	-1.535500000	-1.291528000
6	1.073129000	0.415449000	-2.597509000
8	1.194397000	0.648091000	-3.732896000
6	1.150286000	-0.504859000	2.711979000
1	0.521829000	0.360344000	2.928995000
1	1.187258000	-1.138797000	3.610940000
1	2.167340000	-0.151985000	2.516118000
6	1.484107000	3.113502000	-1.298858000
1	2.353431000	2.691603000	-1.811802000
1	0.644438000	3.105970000	-1.994881000
1	1.716848000	4.153151000	-1.032503000

Co^H (Co-CO 5coord, 1, 3)

27	1.040859000	-0.273854000	-0.780956000
7	-0.334627000	-2.822248000	-2.017700000
7	0.342823000	-1.669192000	0.880110000
7	-0.731649000	0.759438000	-0.088029000
7	1.978469000	1.564289000	-0.090306000
7	3.026465000	-0.944664000	-0.328952000
6	-1.201059000	-2.819869000	-3.040190000
1	-0.793988000	-2.549943000	-4.012756000
6	-2.554966000	-3.137040000	-2.901824000
1	-3.215027000	-3.110703000	-3.764069000
6	-3.023228000	-3.493927000	-1.636191000
1	-4.066632000	-3.756700000	-1.482662000
6	-2.125981000	-3.501078000	-0.566771000
1	-2.452702000	-3.769367000	0.433758000
6	-0.790775000	-3.140942000	-0.792206000
6	0.201266000	-3.055252000	0.346014000
1	-0.084077000	-3.767110000	1.124047000
1	1.190346000	-3.335291000	-0.025575000
6	-0.823156000	-1.101967000	1.621574000
1	-1.717963000	-1.565220000	1.199745000
6	-0.848689000	-1.397142000	3.164202000
6	-0.796268000	-2.915571000	3.425926000
1	-0.949174000	-3.110783000	4.494631000
1	0.174536000	-3.343960000	3.154622000
1	-1.579442000	-3.447885000	2.872484000
6	-2.172477000	-0.866664000	3.757462000
1	-2.264755000	-1.182218000	4.804195000
1	-3.037874000	-1.261662000	3.209861000
1	-2.230004000	0.226281000	3.740583000
6	0.334501000	-0.743985000	3.908206000
1	0.327728000	-1.060536000	4.958685000
1	0.282544000	0.349869000	3.897046000
1	1.303097000	-1.042983000	3.487050000
6	-0.871627000	0.413098000	1.342906000
1	-1.789571000	0.850336000	1.750918000
1	-0.037012000	0.881942000	1.860450000
6	-1.914283000	0.361412000	-0.909757000
1	-1.982818000	-0.726257000	-0.868531000
1	-1.671775000	0.629481000	-1.941549000
6	-3.242856000	0.973676000	-0.508397000
6	-4.094103000	0.305142000	0.385342000
1	-3.802533000	-0.668023000	0.772255000
6	-5.309626000	0.872570000	0.780482000
1	-5.955856000	0.338911000	1.473661000
6	-5.693717000	2.122732000	0.282505000
1	-6.638881000	2.565832000	0.587000000
6	-4.857976000	2.795821000	-0.616678000
1	-5.153237000	3.763774000	-1.014993000
6	-3.643598000	2.223042000	-1.008169000
1	-3.000389000	2.747634000	-1.711192000
6	-0.410942000	2.196202000	-0.267047000
1	-1.180977000	2.821921000	0.199872000
1	-0.436672000	2.376872000	-1.344139000
6	0.974602000	2.598389000	0.290221000
1	0.925942000	2.600846000	1.383548000

6	1.379661000	4.052633000	-0.125461000	6	-1.683003000	-0.026012000	3.986256000
6	0.326926000	5.048170000	0.405608000	1	-2.264297000	-0.208277000	4.899262000
1	0.673050000	6.076943000	0.246090000	1	-1.918265000	0.990956000	3.653052000
1	0.159236000	4.912543000	1.482056000	1	-0.625366000	-0.055551000	4.260939000
1	-0.636628000	4.943902000	-0.104691000	6	-1.274870000	0.566344000	1.126060000
6	1.499794000	4.221488000	-1.654299000	1	-2.269443000	1.010342000	1.240472000
1	1.860566000	5.231751000	-1.884024000	1	-0.611617000	1.114075000	1.792623000
1	0.538932000	4.092610000	-2.163780000	6	-1.757270000	0.338875000	-1.297445000
1	2.213820000	3.516038000	-2.098835000	1	-1.870586000	-0.743148000	-1.195466000
6	2.738917000	4.401572000	0.514252000	1	-1.274842000	0.520970000	-2.260482000
1	2.991628000	5.448909000	0.307550000	6	-3.118813000	1.007378000	-1.273944000
1	3.551253000	3.784707000	0.112897000	6	-4.210311000	0.375814000	-0.660227000
1	2.713260000	4.268561000	1.603257000	1	-4.072034000	-0.603587000	-0.210938000
6	2.884233000	1.100449000	0.978742000	6	-5.467128000	0.988297000	-0.620060000
1	2.260579000	0.783086000	1.823068000	1	-6.300090000	0.482768000	-0.136935000
1	3.564212000	1.878345000	1.343166000	6	-5.650632000	2.247362000	-1.201677000
6	3.677875000	-0.095894000	0.494812000	1	-6.626060000	2.727002000	-1.172628000
6	4.994944000	-0.329930000	0.895418000	6	-4.573054000	2.881958000	-1.831667000
1	5.494336000	0.378856000	1.549744000	1	-4.710283000	3.854567000	-2.298608000
6	5.649274000	-1.476958000	0.441390000	6	-3.319654000	2.263638000	-1.869817000
1	6.674215000	-1.678991000	0.740431000	1	-2.491510000	2.757629000	-2.371926000
6	4.970541000	-2.352129000	-0.410238000	6	-0.371262000	2.192286000	-0.458350000
1	5.442744000	-3.251349000	-0.793947000	1	-1.172062000	2.864740000	-0.135243000
6	3.660526000	-2.042769000	-0.771725000	1	-0.247354000	2.335621000	-1.533774000
1	3.087902000	-2.682474000	-1.437490000	6	0.943927000	2.549241000	0.262589000
6	1.019004000	-0.003178000	-2.552765000	1	0.870429000	2.200232000	1.295323000
8	0.981448000	0.189854000	-3.703858000	6	1.124629000	4.110799000	0.379972000
1	2.544524000	1.901651000	-0.867061000	6	0.121319000	4.611299000	1.448565000
1	1.157975000	-1.670890000	1.493390000	1	0.237559000	5.693187000	1.588608000
				1	0.301527000	4.126999000	2.417188000
				1	-0.921869000	4.427783000	1.169861000
				6	0.846532000	4.865904000	-0.936757000
				1	0.975969000	5.943464000	-0.772947000
				1	-0.179440000	4.712364000	-1.289976000
				1	1.528695000	4.571365000	-1.738925000
				6	2.531450000	4.482894000	0.886007000
				1	2.573590000	5.560965000	1.087438000
				1	3.312557000	4.259486000	0.154336000
				1	2.772310000	3.961719000	1.820061000
				6	3.148150000	1.405742000	0.628799000
				1	2.728367000	1.338245000	1.638101000
				1	3.904736000	2.197790000	0.636970000
				6	3.826574000	0.087432000	0.315033000
				6	5.201546000	-0.094612000	0.481581000
				1	5.820173000	0.737888000	0.804526000
				6	5.758606000	-1.347954000	0.222149000
				1	6.825718000	-1.511832000	0.345689000
				6	4.924452000	-2.381909000	-0.211714000
				1	5.314520000	-3.370159000	-0.435884000
				6	3.565639000	-2.118516000	-0.364875000
				1	2.868334000	-2.874633000	-0.714070000
				6	1.108257000	-0.611051000	-2.290677000
				8	1.232079000	-0.788860000	-3.435729000
				6	1.042156000	-1.093277000	2.453741000
				1	1.020332000	-0.015537000	2.623363000
				1	0.825543000	-1.606402000	3.398535000
				1	2.052337000	-1.365345000	2.142853000
				6	2.571503000	2.096592000	-1.624078000
				1	3.176269000	1.276473000	-2.020511000
				1	1.751640000	2.274657000	-2.321022000
				1	3.200663000	2.994252000	-1.567477000

Co^{Me} (Co-CO 5coord, 1, 3)

27	1.048648000	-0.328435000	-0.509592000
7	0.282033000	-3.394879000	-1.274608000
7	0.101579000	-1.450038000	1.373998000
7	-0.778352000	0.778439000	-0.254208000
7	2.039159000	1.695192000	-0.308458000
7	3.027054000	-0.915428000	-0.098414000
6	-0.276353000	-3.774014000	-2.433016000
1	0.380503000	-3.780667000	-3.300597000
6	-1.617681000	-4.142200000	-2.557873000
1	-2.018679000	-4.435505000	-3.523876000
6	-2.411541000	-4.133272000	-1.409453000
1	-3.458360000	-4.422417000	-1.453464000
6	-1.835101000	-3.748505000	-0.198206000
1	-2.422748000	-3.739546000	0.713748000
6	-0.486042000	-3.367055000	-0.169126000
6	0.193527000	-2.916134000	1.107448000
1	-0.187366000	-3.497926000	1.951718000
1	1.258720000	-3.135635000	1.009621000
6	-1.290580000	-0.912816000	1.548692000
1	-1.887042000	-1.456252000	0.815231000
6	-2.058266000	-1.087278000	2.926754000
6	-1.873501000	-2.485953000	3.550844000
1	-2.509344000	-2.565569000	4.442134000
1	-0.846375000	-2.679896000	3.870127000
1	-2.176801000	-3.281554000	2.862451000
6	-3.571126000	-0.941784000	2.632882000
1	-4.142060000	-1.076556000	3.560246000
1	-3.910141000	-1.702140000	1.918514000
1	-3.829371000	0.041150000	2.227928000