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Supporting Information

Cobalt-Catalyzed Aqueous Dehydrogenation of Formic Acid

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Leibniz-Institut für Katalyse an der Universität Rostock
Albert-Einstein-Straße 29a, 18059 Rostock (Germany)

Supporting information

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1. General information

1.1 General experimental details

All reactions were performed under Argon atmosphere with exclusion of air using standard Schlenk techniques. Formic acid (FA), N,N-dimethyl-n-octylamine (DMOA) were refluxed and distilled following standard procedures and stored under Argon atmosphere. Heptane, toluene, tetrahydrofuran (THF), ether (Et_2O), dichloromethane (DCM) and ethanol (EtOH) were dried by passing through a column of anhydrous alumina using a solvent purification system equipment from *Innovative Technology* and stored under Argon atmosphere. Water was degassed overnight by bubbling Argon overnight. Pentane, HCOOK, tBuOK and $NaBEt_3H$ were purchased from Sigma-Aldrich or Alfa Aesar and used as received. Complexes (^{iPr}PNP)CoCl (**1**),[1,2] (^{Ph}PNP)$CoCl_2$ (**4**),[1] (^{iPr}PNP)$CoBr_2$[1] and (^{iPr}PNP)$Mn(CO)_2Br$ (**7**)[3] were prepared according to reported procedures.

^{1}H NMR spectra were obtained at 300 MHz (Bruker AV-300) or 400 MHz (Bruker AV-400). ^{13}C{1H} NMR spectra were obtained at 75 MHz or 101 MHz. ^{31}P{^{1}H} NMR spectra were obtained at 121 MHz or 162 MHz. NMR chemical shifts are reported in ppm downfield from tetramethylsilane and were referenced to the residual proton resonance and the natural abundance ^{13}C resonance of the solvents. ^{31}P NMR chemical shifts are reported in ppm downfield from H_3PO_4 and referenced to an external 85% solution of phosphoric acid. Abbreviations used in the reported NMR experiments: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Solution magnetic moments were determined by the method of Evans at 25 ºC using a ferrocene standard.

Diffraction data were collected on a Bruker Kappa APEX II Duo diffractometer. The structures were solved by direct methods (SHELXS-97: Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.) and refined by full-matrix least-squares procedures on F^2 (SHELXL-2014: Sheldrick, G. M. *Acta Cryst.* **2015**, *C71*, 3.). XP (Bruker AXS) was used for graphical representations.

1.2 Calculation of TON

The measured gas volumes were corrected by a blank value (volume increase measured in a reaction performed under same conditions but without catalyst).
The turnover number (TON) was calculated by equation **S1:**

$$TON = \frac{\frac{V_{obs} - V_{blank}}{(V_{m,H_2,25°C} + V_{m,CO_2,25°C})}}{n_{cat}} \qquad (\boldsymbol{S1})$$

where V_{obs} and V_{blank} are the gas volume measured in the catalytic reaction and blank reaction, respectively.

The calculation of $V_{m,H_2,25°C}$ was carried out using Van der Waals equation (equation **S2**):

$$V_{m,H_2,25°C} = \frac{RT}{p} + b - \frac{a}{RT} = 24.48\ \frac{L}{mol} \qquad (\boldsymbol{S2})$$

Where:

R: 8.3145 $m^3 \cdot Pa \cdot mol^{-1} \cdot K^{-1}$;
T: 298.15 K;
P: 101325 Pa;
a: $24.7 \cdot 10^{-3} \cdot Pa \cdot m^6 \cdot mol^{-2}$;
b: $26.6 \cdot 10^{-6}$ $m^3 \cdot mol^{-1}$

The calculation of $V_{m,CO_2,25°C}$ was carried out using Van der Waals equation (equation **S3**):

$$V_{m,CO_2,25°C} = \frac{RT}{p} + b - \frac{a}{RT} = 24.36 \frac{L}{mol} \qquad (\boldsymbol{S3})$$

Where:

R: 8.3145 $m^3 \cdot Pa \cdot mol^{-1} \cdot K^{-1}$;
T: 298.15 K;
P: 101325 Pa;
a: $36.5 \cdot 10^{-2} \cdot Pa \cdot m^6 \cdot mol^{-2}$;
b: $42.7 \cdot 10^{-6}$ $m^3 \cdot mol^{-1}$

1.3 GC calibrations

The gas constitution was determined by gas-phase GC. A GC sample was taken from the reaction system and was analyzed by one of the two available systems:

GC a): HP Plot Q / FID – hydrocarbons, Carboxen / TCD - permanent gases, He carrier gas.

GC b): Carboxen / TCD / Methanizer / FID - permanent gases, He carrier gas.

The gas integration was calibrated using certified gas mixtures from commercial suppliers (Linde and Air Liquide) with the following gas vol%:

GC a):

H_2: 0.25%, 0.5%, 1%, 10%, 25%, 50%, 100%

CO: 10 ppm, 100 ppm, 250 ppm, 1000 ppm, 1%, 10%

CO_2: 1%, 5%, 10%, 25%, 50%, 100%

CH_4: 1%, 5%, 10%

GC b):

H_2: 0.25%, 0.5%, 1%, 10%, 25%, 50%, 100%

CO: 1 ppm, 10 ppm, 75 ppm, 100 ppm, 250 ppm, 1000 ppm, 1%, 10%

CO_2: 1%, 5%, 10%, 25%, 50%, 100%

CH_4: 1%, 5%, 10%

The systems allow for the determination of H_2, Ar, CH_4, CO and CO_2 within the ranges:

H_2 ≥ 0.25 vol% - 100 vol%

CO ≥ 10 ppm [GC a)], CO down to 1 ppm [GC b)]

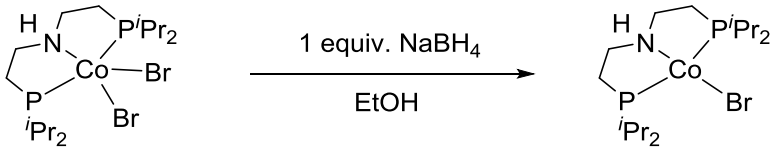
CO_2 ≥ 100 ppm - 100 vol% [GC a)], down to 1 ppm [GC b)]

CH_4 ≥ 1 ppm [GC b)]

GC analysis provides volume percentage of the different components of the collected gas: H_2, CO_2, CO, and CH_4.

2. Preparation and Characterization of Cobalt complexes

2.1 Preparation of Co(I) complex 2



(^{iPr}PNP)CoBr$_2$ (182.1 mg, 0.347 mmol) and NaBH$_4$ (13.2 mg, 0.347 mmol) were placed in a 20 mL Schlenk tube and 10 mL of EtOH was added. The purple suspension turned to brown immediately and formed a green solution within few minutes, the system stirred at room temperature for 2h during which time the solution turned to dark blue. The solvent was removed under vacuum and the solid residue was extracted with toluene (5 mL × 3). The toluene solution was concentrated to 4 mL, and 10 mL of heptane was added under vigorous stirring to yield the blue product. The solvent was removed via syringe and the product was washed with heptane (5 mL × 3), and dried under vacuum. Yield: 100.1 mg, 65%.

Crystals suitable for X-ray analysis were grown from a concentrated solution of toluene cooled to -32 ºC

^{1}H NMR (300 MHz, Benzene-d_6) δ 63.48 (br), 28.29 (br), 20.86 (br), 19.30 (br), 10.93 (br), -0.42 (br), -1.06 (br), -15.97 (br).

Anal. Calc: C, 43.26; H, 8.40; N, 3.15. Observed: C, 43.22; H, 8.58; N, 3.03; μ_{eff} = 3.09 μ_B

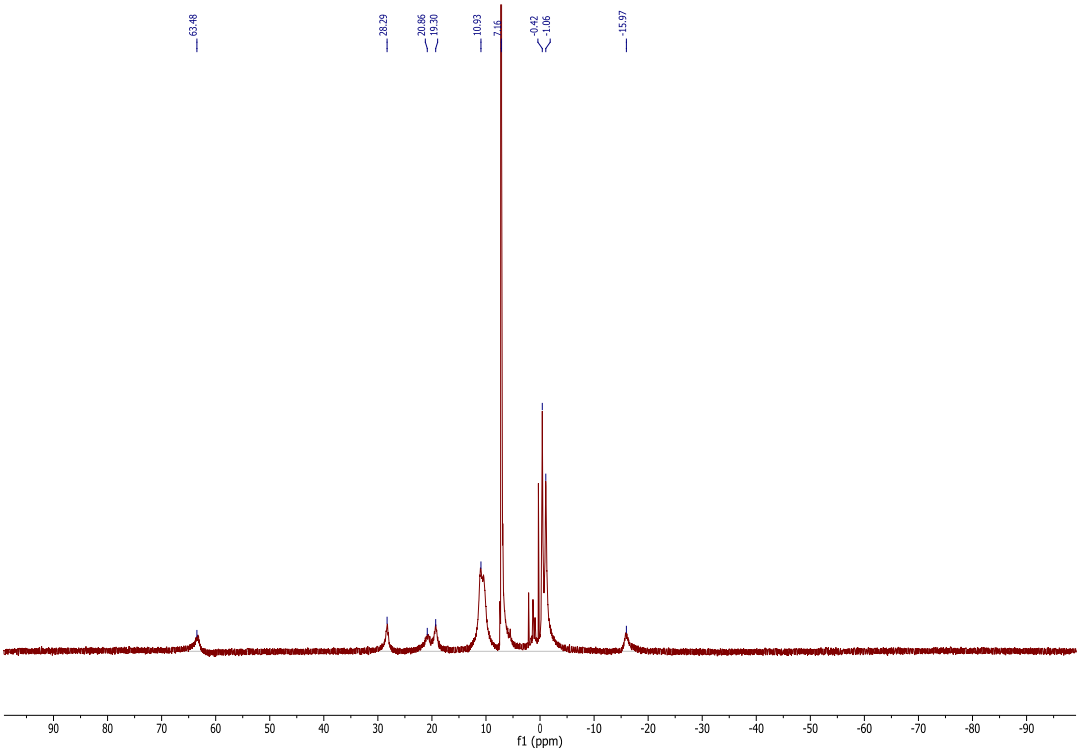


Figure S1 ^{1}H NMR (C_6D_6) spectrum of complex **2**

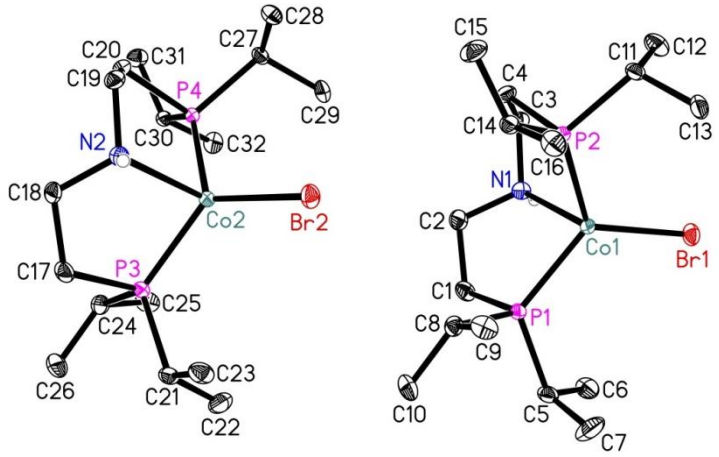
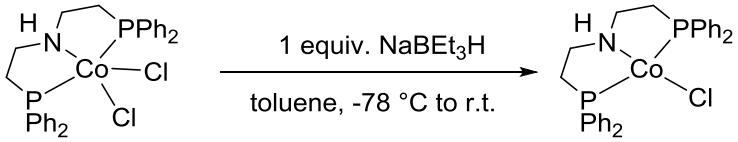


Figure S2 Molecular structure of complex **2** with thermal ellipsoids at 30% probability. All hydrogens except that attached to nitrogen were eliminated for clarity.

Table S1. Selected bond lengths and angles of complex **2**:

Bond distances [Å]				Bond Angles [°]			
Br1-Co1	2.3789(3)	Br2-Co2	2.3866(3)	N1-Co1-P2	86.39(5)	N2-Co2-P3	86.16(4)
Co1-N1	2.1479(16)	Co2-N2	2.1473(15)	N1-Co1-P1	86.44(4)	N2-Co2-P4	86.29(5)
Co1-P1	2.2408(5)	Co2-P3	2.2424(5)	P2-Co1-P1	114.747(19)	P3-Co2-P4	116.16(2)
Co1-P2	2.2395(5)	Co2-P4	2.2496(5)	N1-Co1-Br1	108.48(5)	N2-Co2-Br2	109.34(5)
				P1-Co1-Br1	123.752(16)	P3-Co2-Br2	125.178(17)
				P2-Co1-Br1	119.947(16)	P4-Co2-Br2	17.050(15)

2.2 Preparation of Co(I) complex 3



To a suspension of (^{Ph}PNP)$CoCl_2$ (571.3 mg, 1 mmol) in 25 mL toluene $NaBEt_3H$ (1 mL, 1.0 M in toluene) was added at -78 ºC. The system was allowed to warm up to r.t. gradually and stirred overnight. The resulting solution was filtered through Celite and concentrated to 5 mL. Then, pentane (15 mL) was added to the solution under stirring to give a green precipitate. The solid product was filtered, washed with pentane and dried under vacuum. Yield: 439.6 mg, 82%.

Crystals suitable for X-ray analysis were grown by layering a benzene solution with pentane.

^{1}H NMR (300 MHz, Benzene-d_6) δ 15.95 (br), 13.36 (br), 7.99 (br), 7.15 – 6.25 (m), 5.05 (br), 4.37 (br), 4.08 (br), 2.86 – 0.62 (m), -1.05 (br).

Anal. Calc: C, 62.76; H, 5.45; N, 2.61. Observed: C, 62.65; H, 5.74; N, 2.20; μ_{eff} = 2.57 μ_B

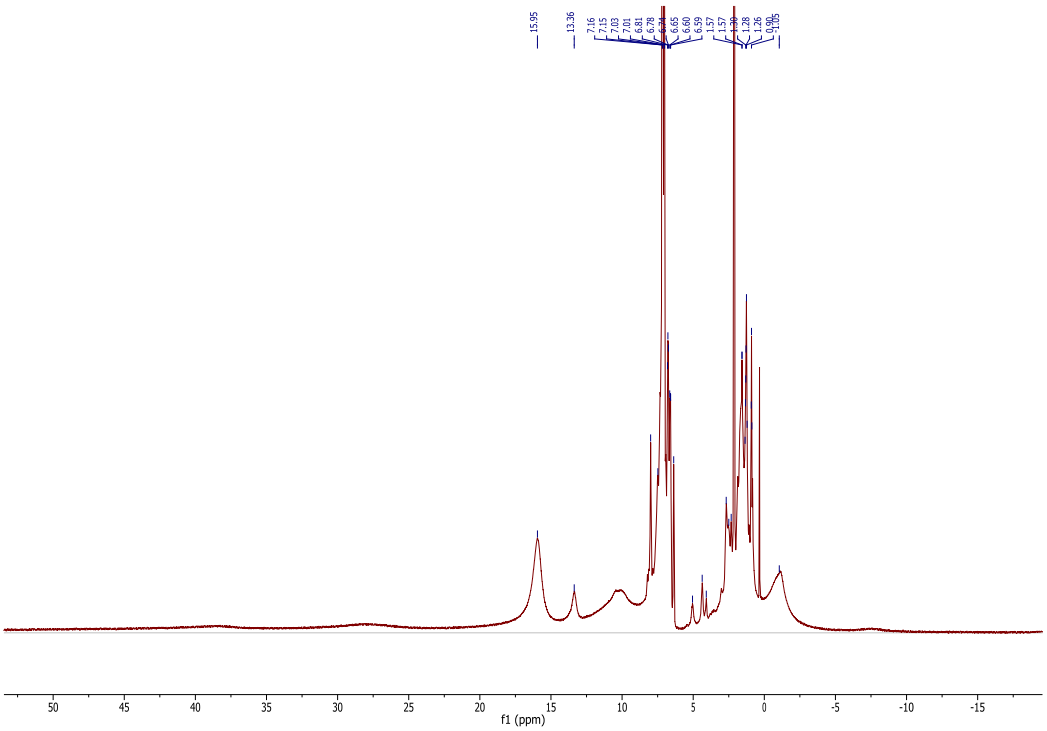


Figure S3 ^{1}H NMR (C_6D_6) spectrum of complex **3**

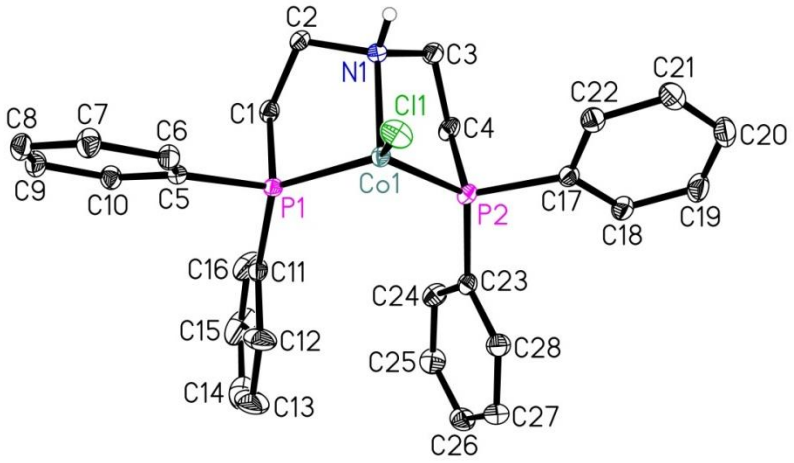
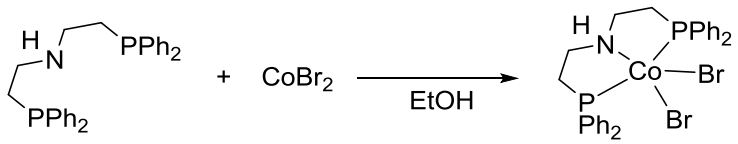


Figure S4 Molecular structure of complex **3** with thermal ellipsoids at 30% probability. All hydrogens except that attached to nitrogen and co-crystallized solvent (benzene) were eliminated for clarity.

Table S2. Selected bond lengths and angles of complex **3**:

Bond distances [Å]		**Bond Angles [°]**	
Cl1-Co1	2.2240(4)	N1-Co1-P2	86.17(4)
Co1-N1	2.1528(13)	N1-Co1-Cl1	113.03(4)
Co1-P2	2.2094(4)	P2-Co1-Cl1	127.384(17)
Co1-P1	2.2313(4)	N1-Co1-P1	86.04(4)
		P2-Co1-P1	102.380(15)
		Cl1-Co1-P1	126.349(17)

2.3 Preparation of Co(II) complex 5



$CoBr_2$ (109.4 mg, 0.5 mmol) was dissolved in 10 mL EtOH. To this solution the pincer ligand (220.7 mg, 0.5 mmol in 3 mL THF) was added at 60 °C, the color turned from blue to dark purple with precipitate. The system stirred at r.t. overnight and the resultant bluish green solvent was removed via syringe. The product was washed with EtOH (10 mL × 3) and heptane (10 mL × 3), dried under vacuum to give a purple solid. Yield: 284.9 mg, 86%.

Crystals suitable for X-ray analysis were grown by layering a DCM solution with EtOH.

Anal. Calc: C, 50.94; H, 4.43; N, 2.12. Observed: C, 51.02; H, 5.59; N, 1.79.

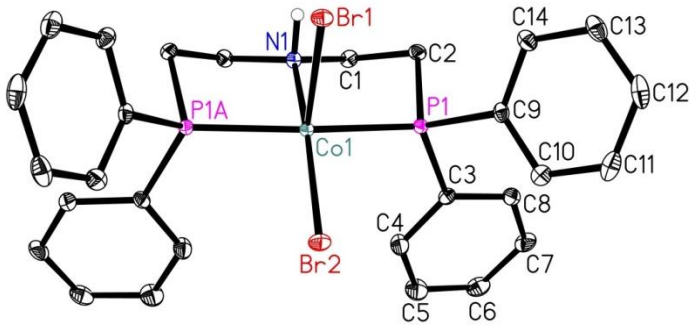
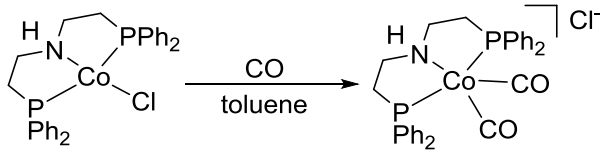


Figure S5 Molecular structure of complex **5** with thermal ellipsoids at 30% probability. All hydrogens except that attached to nitrogen were eliminated for clarity. Operator for generating equivalent atoms: x, -y+1/2, z

Table S3. Selected bond lengths and angles of complex **5**:

Bond distances [Å]		Bond Angles [°]	
Br1-Co1	2.5463(6)	N1-Co1-P1	84.44(2)
Br2-Co1	2.3754(6)	P1-Co1-P1	167.28(4)
Co1-N1	2.014(3)	N1-Co1-Br2	165.45(10)
Co1-P1	2.2082(6)	P1-Co1-Br2	94.60(2)
		N1-Co1-Br1	89.37(9)
		P1-Co1-Br1	93.02(2)
		Br2-Co1-Br1	105.18(2)

2.3 Preparation of Co(I) complex 9



(^{Ph}PNP)CoCl (200 mg, 0.37 mmol) was dissolved in 10 mL toluene and the solution was stirred under CO atmosphere overnight to give a precipitate. After removal of the solvent through filtered cannula, the resulting solid was washed with toluene (8 mL × 4) and ether (4 mL × 2), dried under vacuum to give the pale pink product. Yield: 144.6 mg, 66%.

^{1}H NMR (300 MHz, Methylene Chloride-d_2) δ 8.51 (s, 1H), 7.84 – 7.65 (m, 8H), 7.65 – 7.55 (m, 6H), 7.54 – 7.43 (m, 6H), 3.55 (br, s, 2H), 2.99 (br, s, 4H) , 2.52 (br, s, 2H). {^{1}H}^{13}C NMR (101 MHz, Methylene Chloride-d_2) δ 133.58 (t, *J* = 25.9 Hz), 132.19 (t, *J* = 5.4 Hz), 131.17 (d, *J* = 31.5 Hz), 129.02 (dt, *J* = 32.1, 5.3 Hz), 52.15 , 33.76 (t, *J* = 12.2 Hz). {^{1}H}^{31}P NMR δ 72.82 (s).

Anal. Calc: C, 60.88; H, 4.94; N, 2.37. Observed: C, 61.49; H, 4.98; N, 3.21.

IR (ATR): 2004 cm^{-1}(CO), 1926 cm^{-1}(CO)

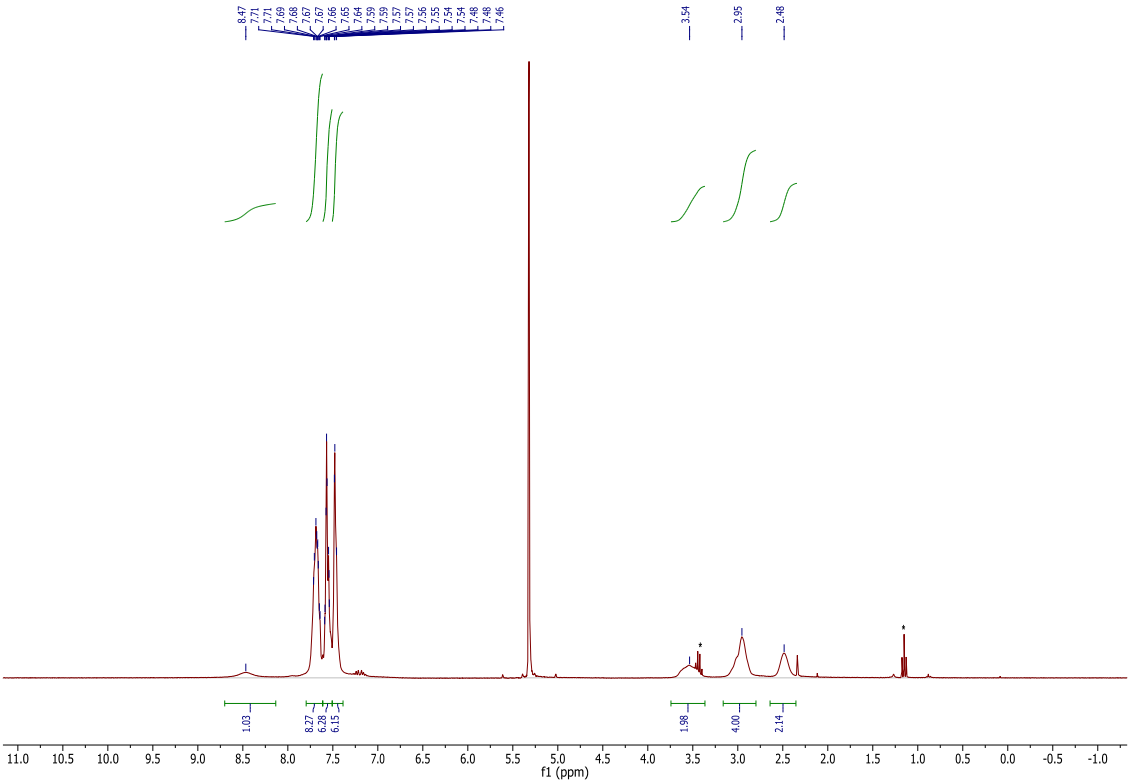


Figure S6 ^{1}H NMR (CD_2Cl_2) spectrum of complex **9** (asterisk denote residual ether peaks)

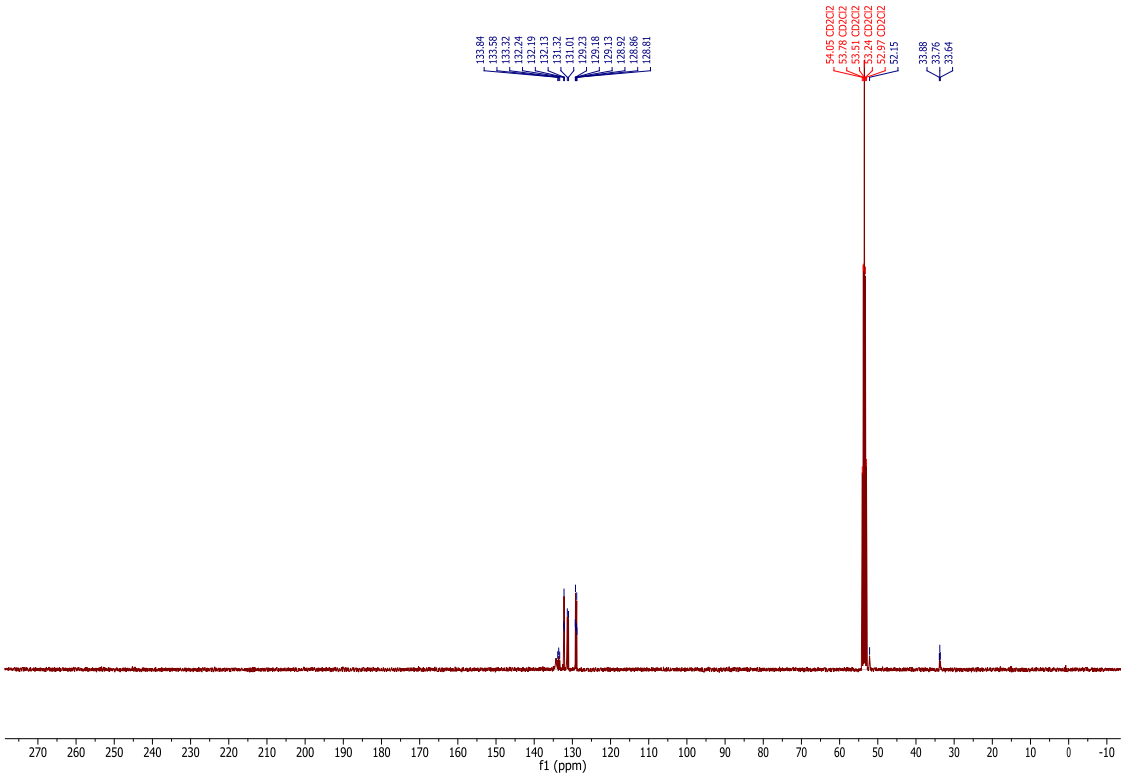


Figure S7 $\{^{1}H\}^{13}C$ (CD_2Cl_2) spectrum of complex **9**

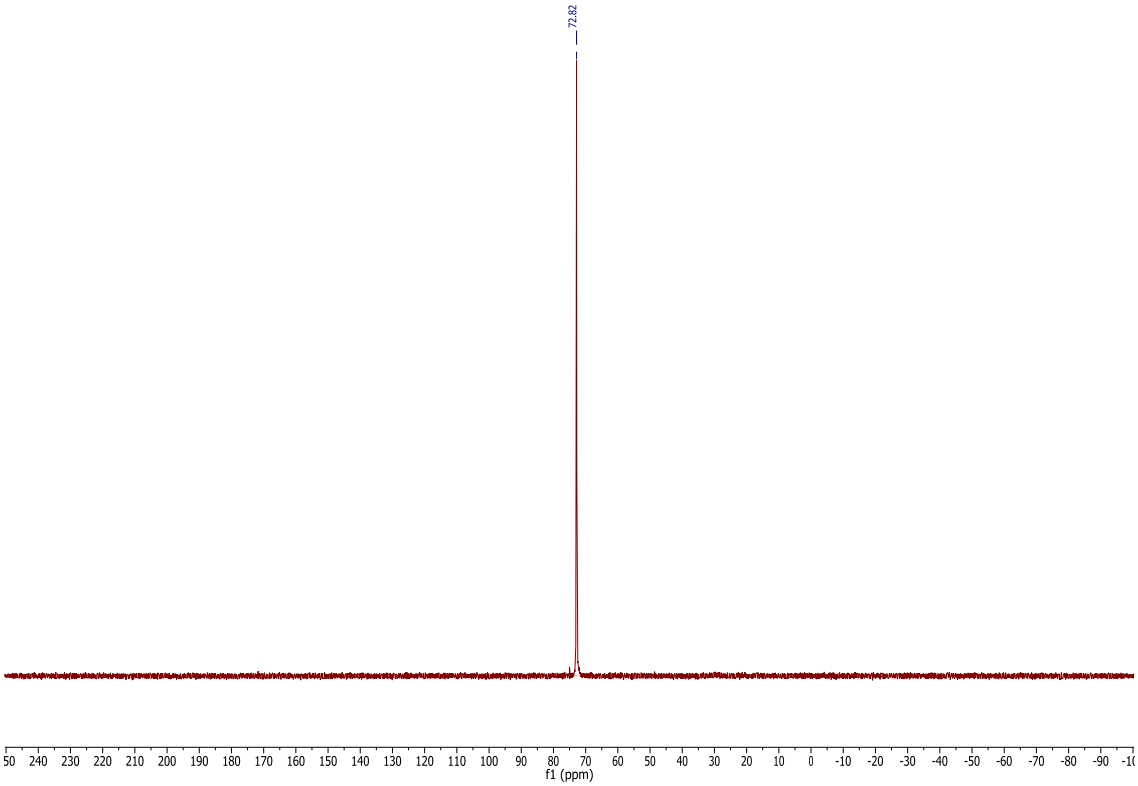
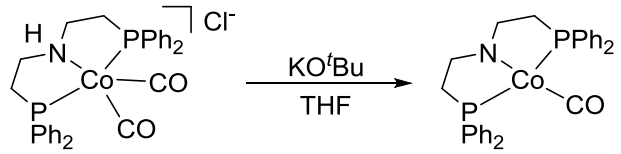


Figure S8 ^{31}P (CD_2Cl_2) spectrum of complex **9**

2.4 Preparation of Co(I) complex 10



(^{Ph}PNP)Co(CO)$_2$Cl (118.4 mg, 0.20 mmol) was dissolved in 5 mL THF (not completely dissolved). KO^{t}Bu (22.4 mg, 0.20 mmol) in 2 mL THF was added to this suspension at -40 °C, and the solid dissolved gradually and the solution turned to dark red. After one hour, the cooling bath was removed and the system was stirred for another hour at r.t. before the solvent was removed under vacuum. The resulting solid was extracted with toluene (4 mL × 4), filtered through Celite, the solvent removed under vacuum to give a red solid product. Yield: 75.6 mg, 72%.

Crystals suitable for X-ray analysis were obtained by vaper diffusion of hexane into a concentrated benzene solution.

^{1}H NMR (400 MHz, Benzene-d_6) (400 MHz, Benzene-d_6) δ 8.03 – 7.77 (m, 8H), 7.11 – 6.95 (m, 12H), 3.42 – 3.03 (m, 4H), 2.67 – 2.52 (m, 4H). {^{1}H}^{13}C NMR (101 MHz, Benzene-d_6) δ 135.05 (t, J = 20.2 Hz), 132.66 (t, J = 6.1 Hz), 129.43 , 128.25 (t, J = 4.7 Hz), 57.71 (t, J = 8.6 Hz), 33.54 (t, J = 11.7 Hz). carbonyl carbon resonance not observed. {^{1}H}^{31}P NMR δ 76.17 (s, br).

Anal. Calc: C, 66.04; H, 5.35; N, 2.66. Observed: C, 65.78; H, 5.31; N, 2.31.

IR (ATR): 1873 cm^{-1}(CO)

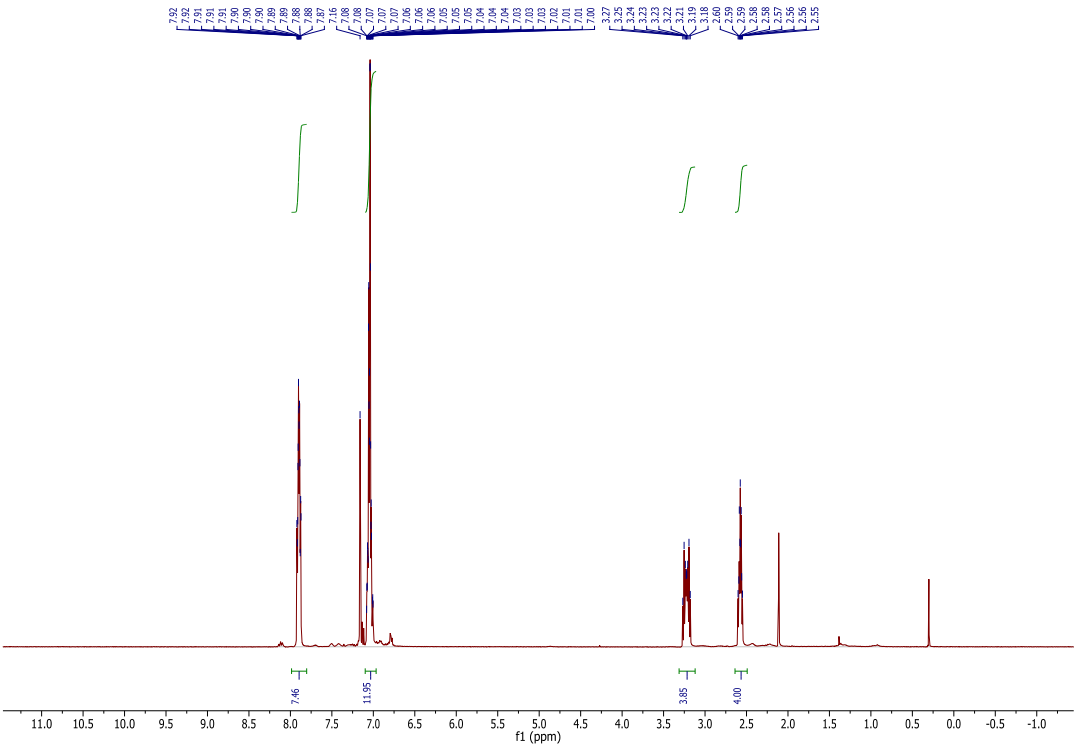


Figure S9 ^{1}H NMR (C_6D_6) spectrum of complex **10**

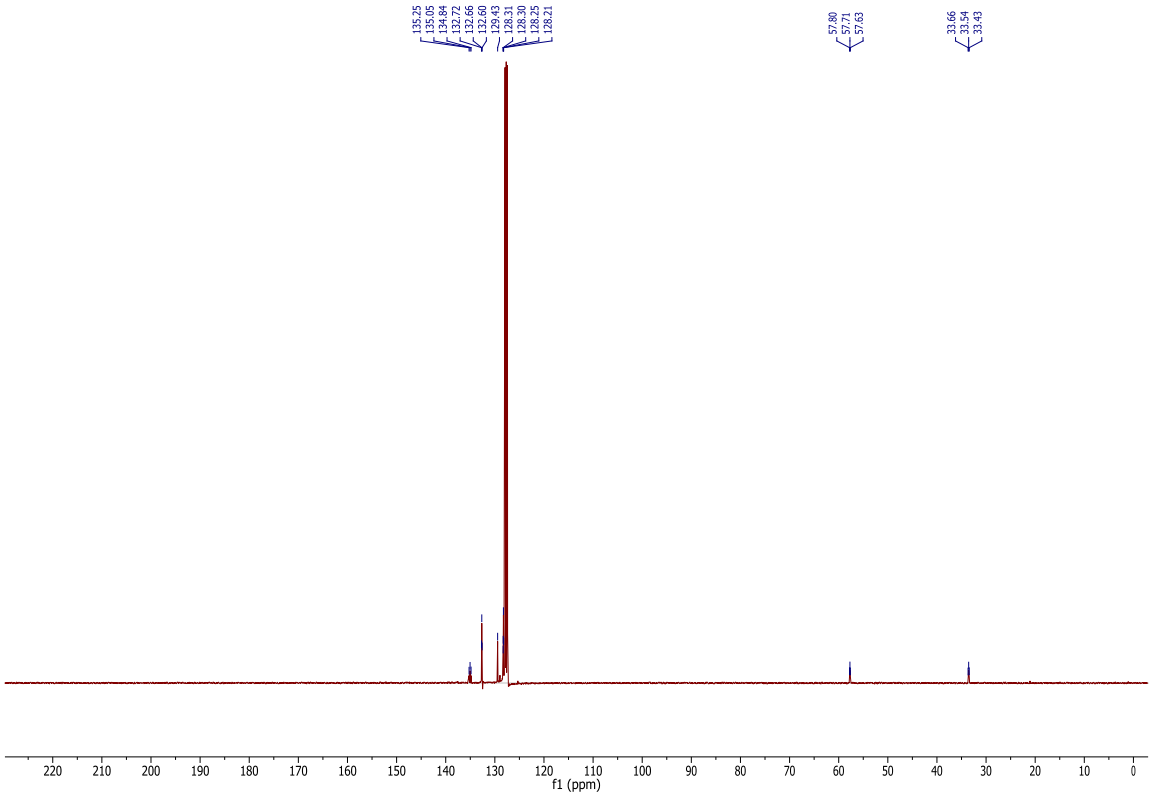


Figure S10 $\{^{1}H\}^{13}C$ (C_6D_6) spectrum of complex **10**

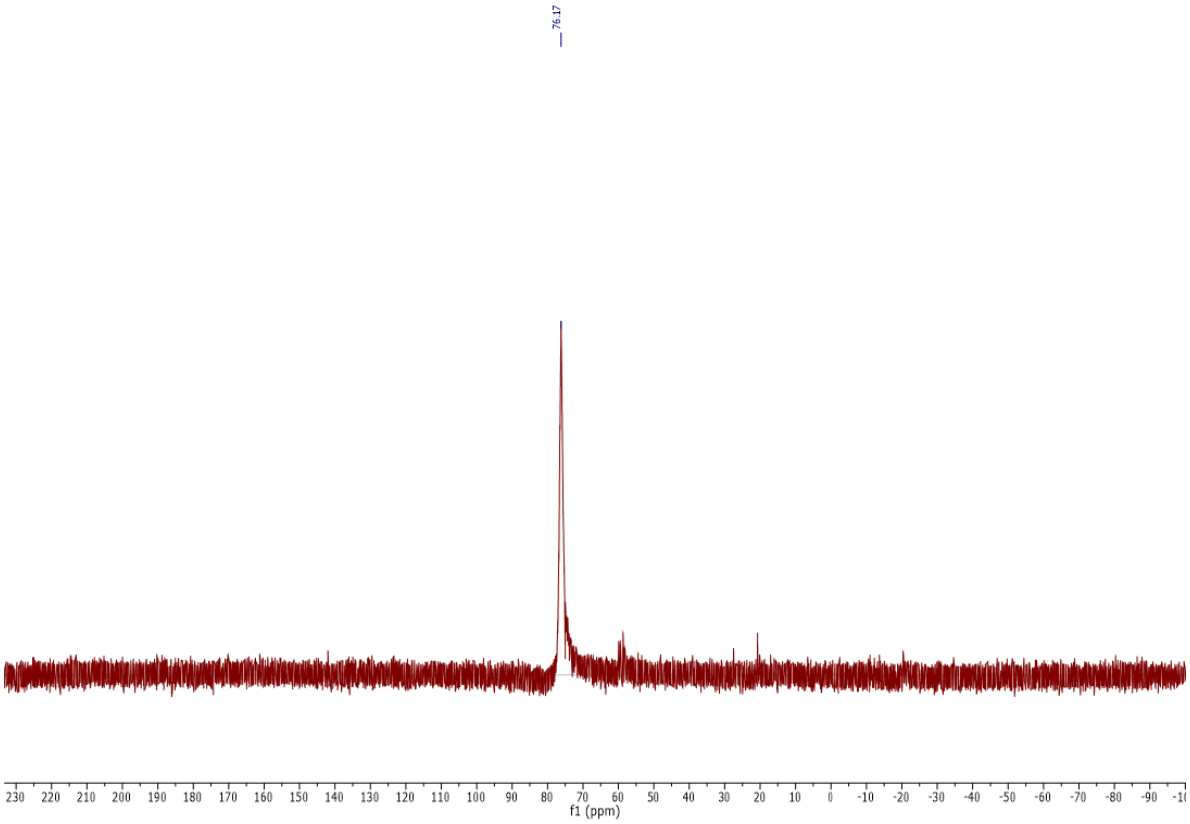


Figure S11 ^{31}P (C_6D_6) spectrum of complex **10**

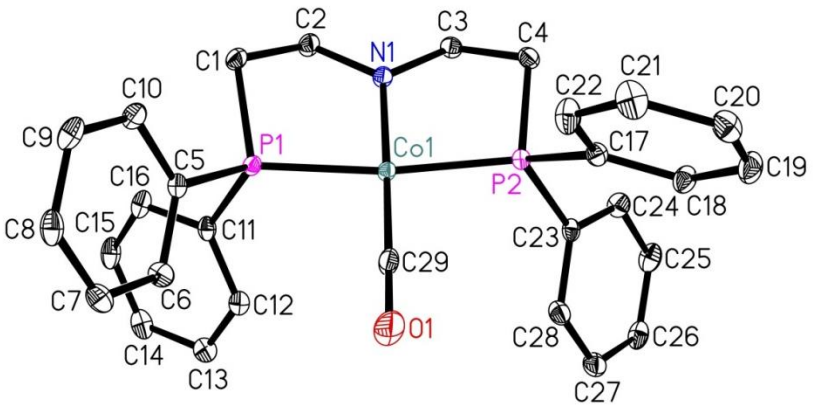


Figure S12 Molecular structure of complex **10** with thermal ellipsoids at 30% probability. All hydrogens were eliminated for clarity.

Table S4. Selected bond lengths and angles of complex **10**:

Bond distances [Å]		**Bond Angles [°]**	
C29-Co1	1.7032(18)	O1-C29-Co1	178.3(3)
Co1-N1	1.8615(14)	C29-Co1-N1	178.03(10)
Co1-P1	2.1589(5)	C29-Co1-P1	94.43(6)
Co1-P2	2.1742(5)	N1-Co1-P1	84.59(5)
C29-O1	1.165(2)	C29-Co1-P2	95.56(6)
		N1-Co1-P2	85.47(5)
		P1-Co1-P2	169.934(19)

3. General procedure for dehydrogenation of formic acid

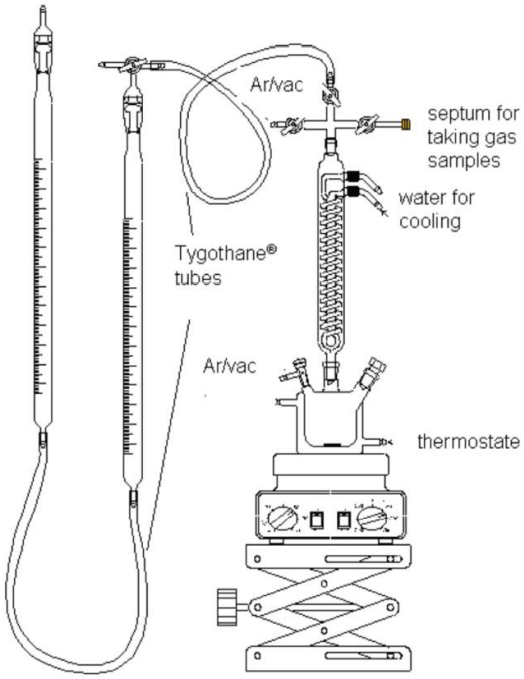


Figure S13 Manual burette setup for measuring gas evolution

Substrates (11FA/10DMOA or HCOOK, FA, H_2O) were given into a double walled reaction vessel. The system was heated to the desired reaction temperature and let equilibrate for 25 minutes. Then, the cobalt complex **3** (5.4 mg, 10µmol), dissolved in 0.4 mL toluene, was added to the reaction mixture and immediately the gas evolution was started to be recorded in dependence of time.

In the case of the *in-situ* formed Co(I) catalyst, the corresponding Co(II) complex (10µmol), suspended in 0.2 mL of toluene, and $NaBEt_3H$ (0.2 mL, 1.0 M in toluene) were mixed at room temperature and stirred for 15 minutes before adding it to the system for dehydrogenation reaction. All experiments (except the experiment applying catalyst **2** in Figure 2) were performed at least twice. The standard deviation/average value was in general less than 10%, except for entries 2 (17% and 7 % after 1 and 3 hours, respectively), 7 (14%, 12%), 9 (23%, 21%), 10 (18%, 28%) and 15 (39%, 16%) in Table 1.

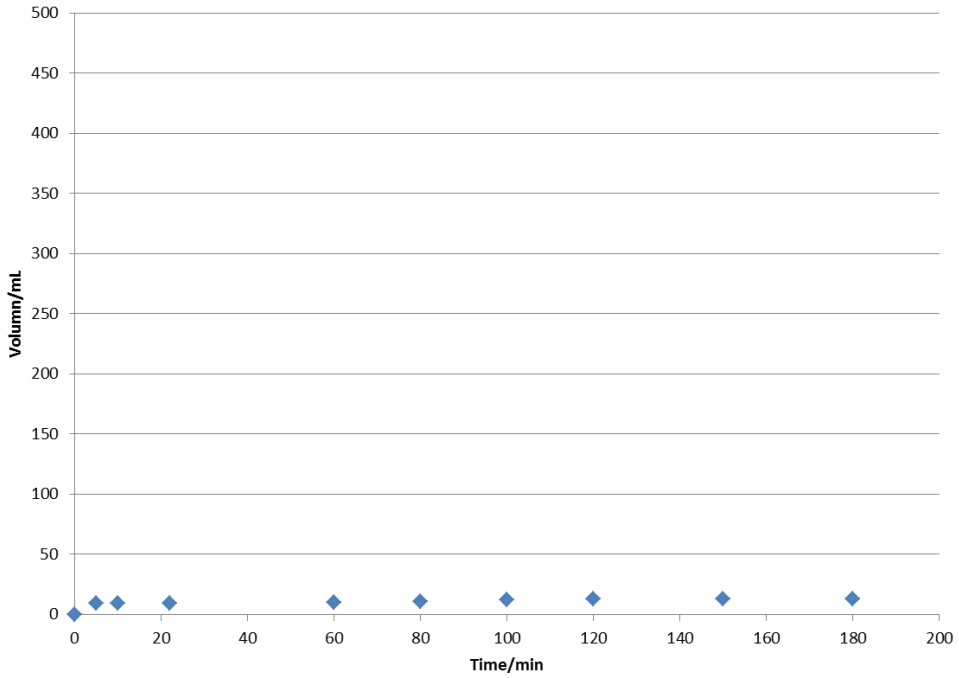


Figure S14. Gas volume measured in blank reaction in aqueous system at 60 °C in the absence of any catalyst.

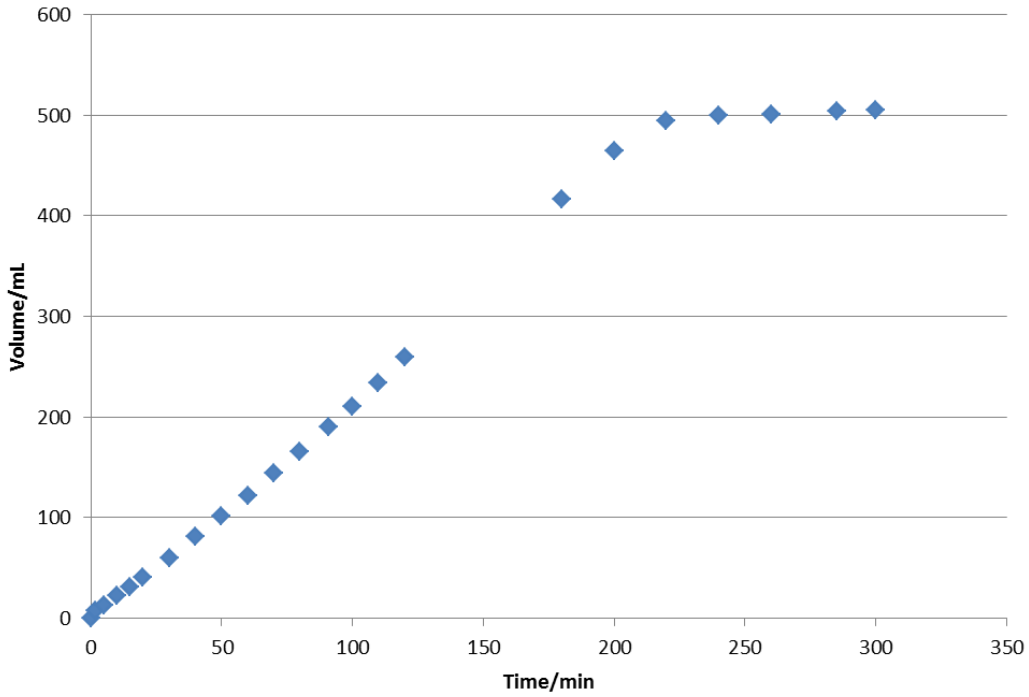


Figure S15 Gas evolution curve at 60 °C. Conditions: formic acid (10 mmol), potassium formate (10 mmol), water (3.62 mL), complex **4** (10 µmol) with *in-situ* treatment with two equivalent of $NaBEt_3H$.

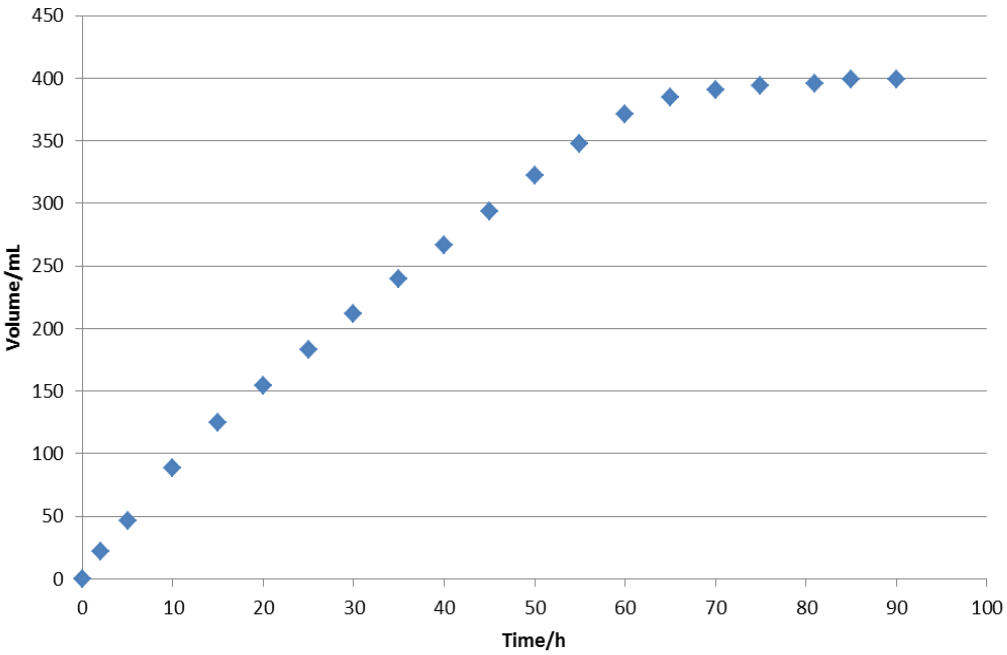
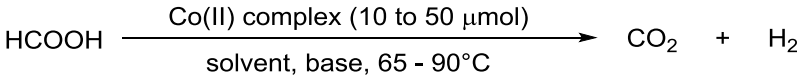


Figure S16 Gas evolution curve at 80 °C. Conditions: formic acid (10 mmol), potassium formate (40 mmol), water (3.62 mL), complex **3** (10 µmol).

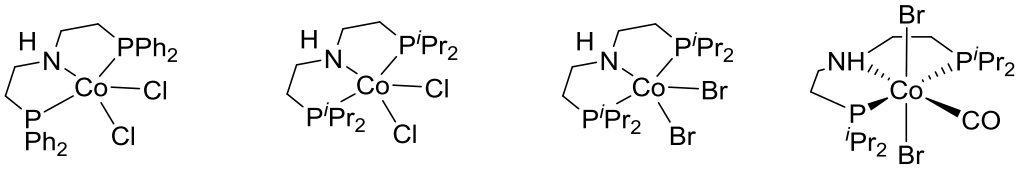
Table S5. Summary of initial TOF at different pH value. All reactions were conducted at 60 °C, with complex **4** (10 µmol) under *in-situ* treatment with two equivalents of $NaBEt_3H$, the volume of formic acid and water is 4 mL in all cases. Initial TOF was measured as the first 20 minutes of the reaction.

Entry	HCO_2H (mmol)	HCO_2K (mmol)	Initial pH	Initial TOF (/h)	V_{1h} (mL)	V_{3h} (mL)
1	10	40	5.4	246	134	426
2	10	20	4.8	240	133	448
3	10	10	3.8	240	125	436
4	20	10	3.6	148	69	168
5	10	5	3.5	166	71	200
6	20	20	4.0	185	102	292
7	10	0	1.1	49	14	26
8	0	10	11.7	43	12	22

4. Summary of tested dehydrogenation of formic acid using Co(II) complexes

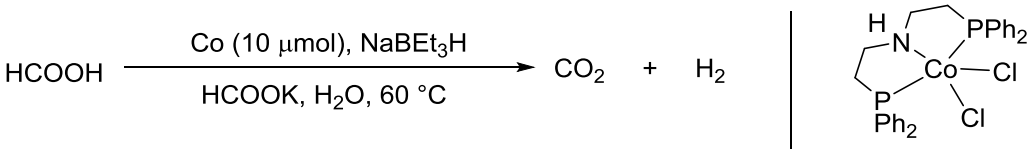


Tested Co(II) complexes



Tested solvent: toluene, triglyme, proplene, propylene carbonate
Tested base: trimethylamine, N,N-dimethyloctylamine

5. Long term experiments



Initial conditions: HCOOH (50 mmol), HCOOK (50 mmol), H_2O (18.1 mL), PNP-Ph-CoCl2 (5.7 mg, 10 µmol) under *in-situ* treatment with two equivalent of $NaBEt_3H$. 1.5 mL (39.8 mmol) FA was added to the system to restore the FA concentration after 16.5h.

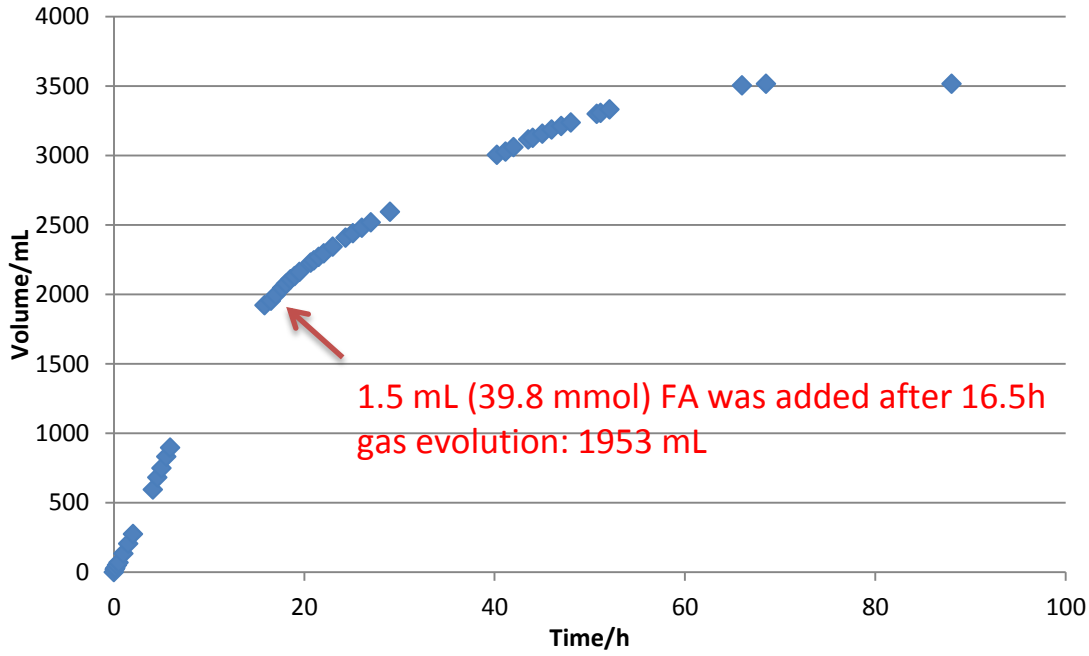


Figure S17 Gas evolution of a long term experiment

6. KIE experiments

KIE experiments were conducted either under optical aqueous conditions or in 11FA/10DMOA mixture

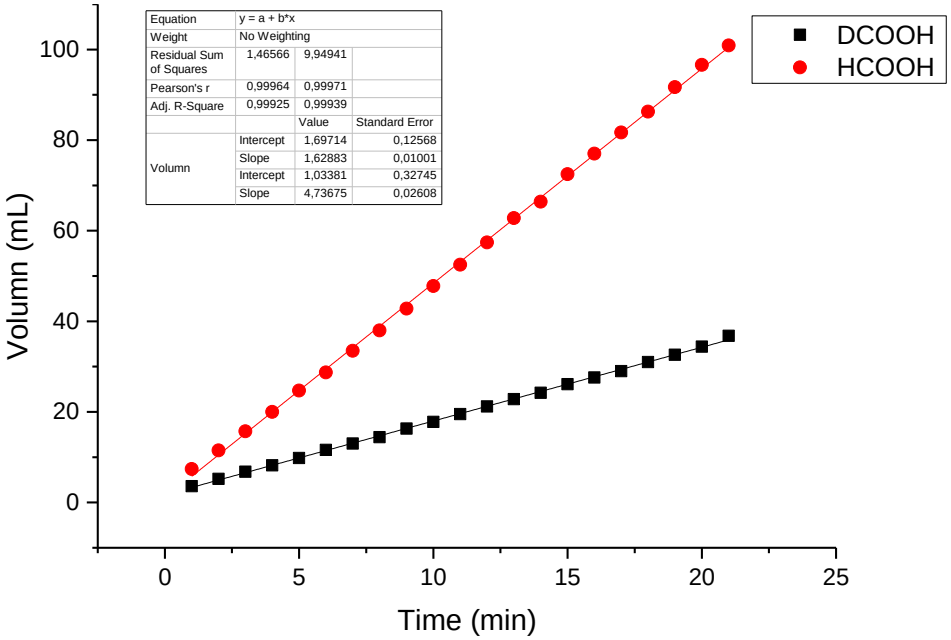


Figure S18. KIE experiment in 11FA/10DMOA mixture; conditions: 11FA/10DMOA (5 mL), complex **4** (10 µmol) with *in-situ* treatment with two equivalents of $NaBEt_3H$.

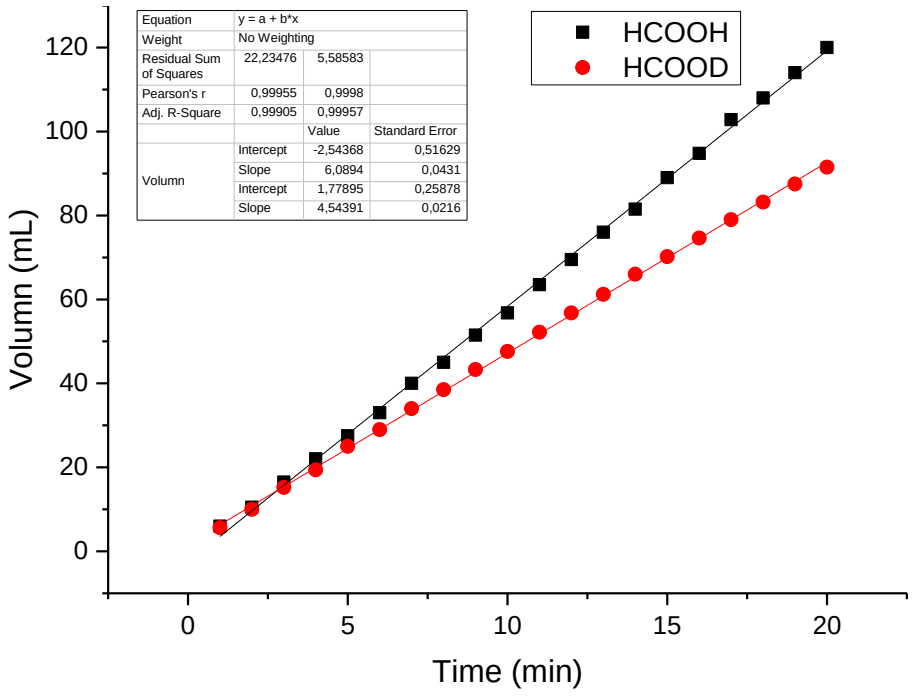


Figure S19. KIE experiment in 11FA/10DMOA mixture; conditions: 11FA/10DMOA (5 mL), complex **4** (10 µmol) with *in-situ* treatment with two equivalents of $NaBEt_3H$.

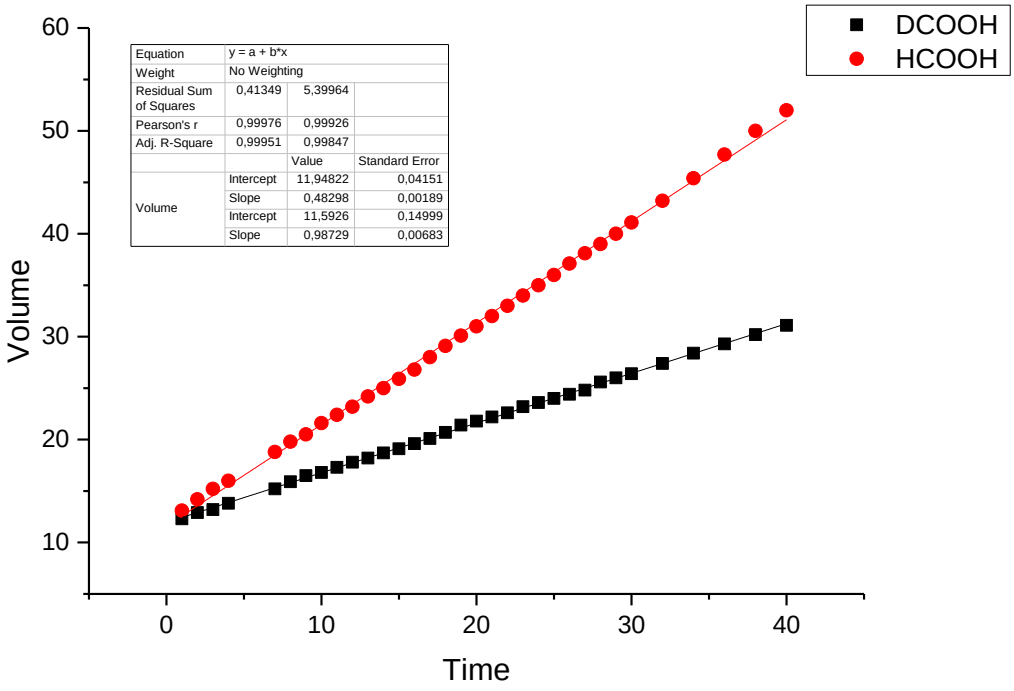


Figure S20. KIE experiment in aqueous system; conditions: formic acid (10 mmol), potassium formate (10 mmol), water (3.62 mL), complex **4** (10 µmol) with *in-situ* treatment with two equivalents of $NaBEt_3H$.

7. Additional experiment regarding mechanism study

7.1 CO poisoning experiment

A typical dehydrogenation reaction was performed at 60 °C. Conditions: formic acid (10 mmol), potassium formate (10 mmol), water (3.62 mL), complex **4** (10 µmol) with *in-situ* treatment with two equivalents of $NaBEt_3H$. After one hour 10 mL of CO was bubbled through the system with an air tight syringe within one minute (the gas collection was stopped during this time and continued afterwards.) The curve of gas evolution is shown below:

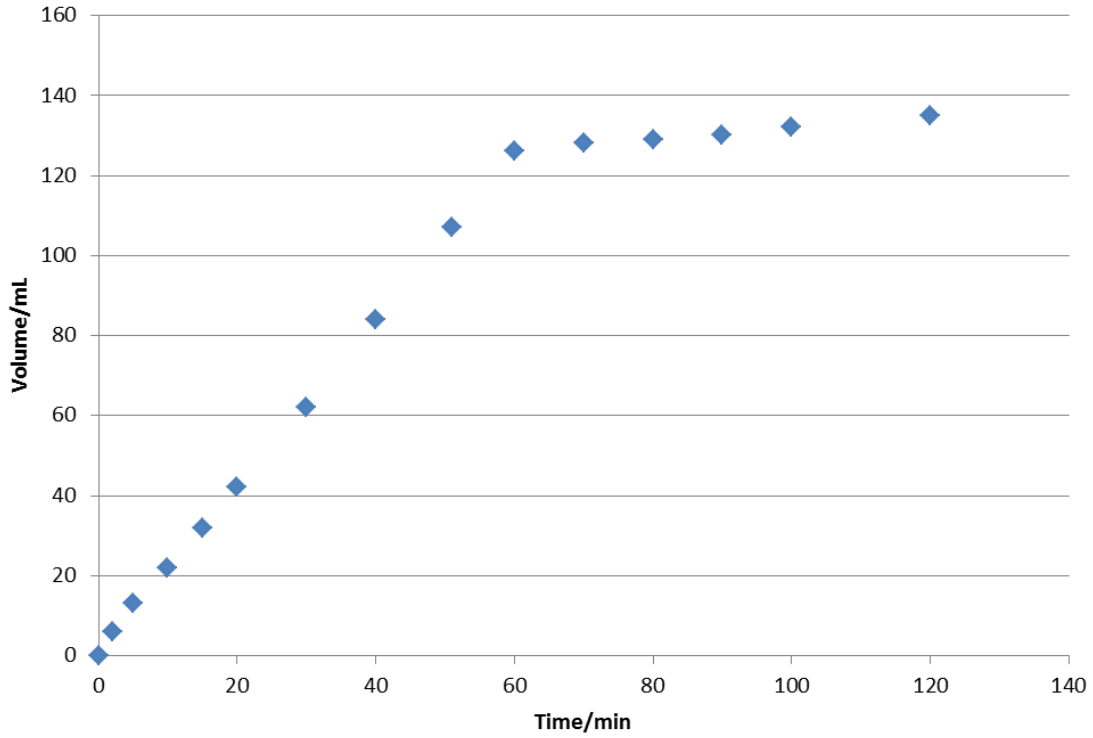


Figure S21 FA dehydrogenation reaction with CO poisoning

7.2 Thiourea poisoning experiment[4]

A typical dehydrogenation reaction was performed at 60 °C using *N*,*N*'-dibutylthiourea as a strongly binding catalyst poison. Applying 0.2 eq. or 0.5 eq. of *N*,*N*'-dibutylthiourea the system only partially deactivated the system. Conditions: formic acid (10 mmol), potassium formate (10 mmol), water (3.62 mL), complex 4 (10 µmol) with in-situ treatment with two equivalents of $NaBEt_3H$, *N*,*N*'-dibutylthiourea (0.2 or 0.5 eq).

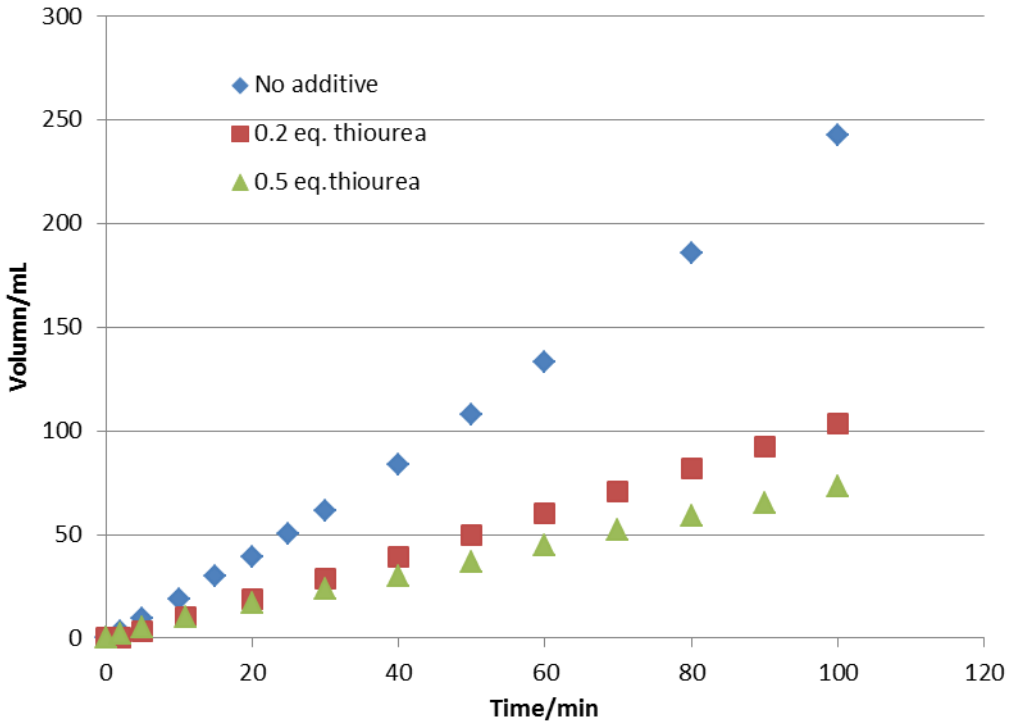


Figure S22 Thiourea poisoning experiment

8. Computational Details

All calculations were carried out by using the Gaussian 16 program.[5] All structures were optimized at the B3PW91[6] level of density functional theory (DFT) with the TZVP[7] basis set. All optimized structures were characterized either as energy minimums without imaginary frequencies or transition states with only one imaginary vibrational mode by frequency calculations. The thermal correction to Gibbs free energy at 298 K from frequency analysis was added to the total electronic energy, and the corrected Gibbs free energy (ΔG) at 298 K was used for discussion and comparison.

In addition, we carried out self-consistent reaction field (SCRF) structure optimization and frequency calculation at the M06L[8-9]/TZVP level using the solvation model based on solute electron density (SMD)[10] and water as solvent to estimate the solvation effect (M06L-SCRF). At first we have scaled the computed results on the basis of the experimental results; and this is because that recently computational study for the structures and stability as well as catalytic activity of cobalt PNP pincer in acetophenone hydrogenation used the M06L method under the consideration of solvation effect.[11] In our benchmark computation, we used the reaction in in Figure 3 with the formation of either the monocarbonyl complex **10** or the dicarbonyl complex **10a**. It is found that M06L favors the dicarbonyl amido complex (**10a**, trigonal bipyramidal) instead of the monocarbonyl complex **10** (square planar) [**10a** = **10** + CO] both in gas phase and solution by 6.09 and 8.94 kcal/mol, respectively, and this disagrees with the experiment. In contrast, B3PW91 prefers complex **10** instead of the dicarbonyl complex **10a** by 2.90 and 1.20 kcal/mol in gas phase and in solution, respectively, and this agrees with the experiment. Indeed, monocarbonyl complex has been found for the *i*-Pr[12] and *t*-Bu[13] substituted counterpart. This rationalized the use of B3PW91 in our computations.

Nevertheless, we also computed the potential energy surface by using M06L-SCRF and the computed Gibbs free energy surface is shown in Figure S1 for comparison. Despite some minor differences, both B3PW91 and M06L-SCRF gave very similar results.

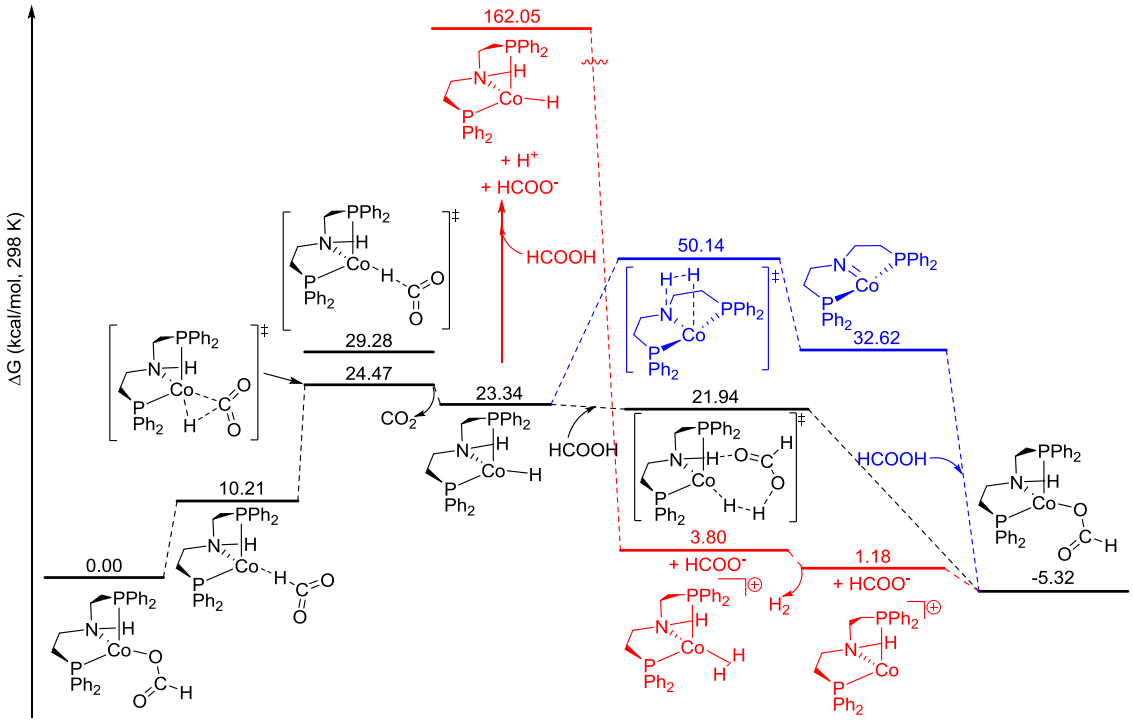
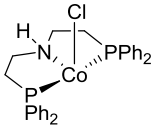
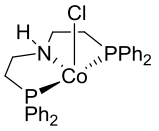
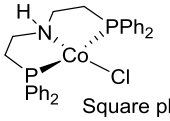
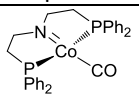
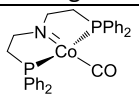
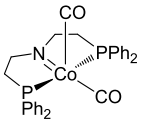
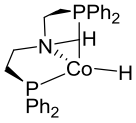
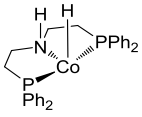
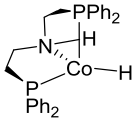


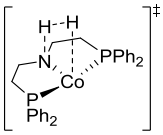
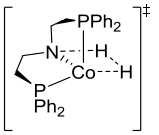
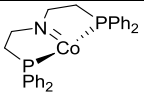
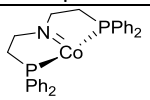
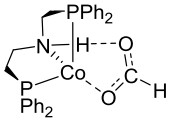
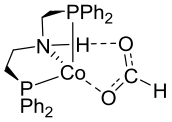
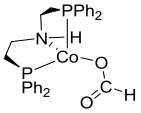
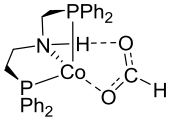
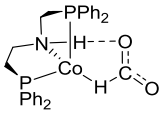
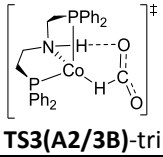
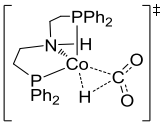
Figure S23. Gibbs free energy profile for formic acid dehydrogenation at M06L/TZVP-SCRF(SMD/H_2O) level.

Interestingly, for the O-coordinated formate species, the H-bonding between the second O atom and the H atom of the amine functionality cannot be located by using M06L functional. The H coordinated **3A2** is high in energy than **3A1** by 10.21 kcal/mol. It is worth noted that the C-H activation involving H-bonding between the O atom of formate and the H atom of the amine functionality cannot be located, instead the two configurations of transition state in the absence of H-bond were found. The corresponding transition states for the C-H activation (**TS3A2/3B)** has free energy barrier of 24.47 and 29.28 kcal/mol, respectively. The formation of CO_2 and amine complex **3B** is endergonic by 23.34 kcal/mol.

Starting from the parent amine complex **3B**, the direct H_2 elimination via the non-innocent mechanism has free energy barrier of 26.80 kcal/mol and is exergonic by 9.27 kcal/mol. The H_2 elimination via innocent mechanism has negative Gibbs free energy barrier of -14.07 kcal/mol and is highly exergonic (-37.93 kcal/mol). The third one involves the protonation of the Co-H group by formic acid and this step is very exergonic by 19.54 kcal/mol. As a result, the rate-determining step for formic acid dehydrogenation is the hydride transfer from formate to Co center.

Table S6. Energies for All Optimized Structures at B3PW91/TZVP level

	Ee	ZPE	H(298.15)	G(298.15)
HCOOH	-189.762022	0.033913	-189.724004	-189.75218
CO_2	-188.580271	0.010286	-188.566078	-188.585337
H_2	-1.178636	0.010066	-1.165265	-1.180063
CO	-113.304331	0.005076	-113.29595	113,318374
proton	0.000000	0	0.00236	-0.01
HCOO-Anion	-189.198628	0.02009	-189.174623	189.202331
H_2O	-76.430962	0.021369	-76.405814	-76.427232
 **3**-triplet	-3664.8206097	0.499848	-3664.287584	-3664.390742
 **3**-singlet	-3664.759033	0.500736	-3664.2255	-3664.325381
 **3**-Square-Planar-singlet	-3664.786629	0.500645	-3664.253304	-3664.353472
 **10**-singlet	-3317.314342	0.494726	-3316.786847	-3316.887914
 **10**-triplet	3317.3047093	0.492373	-3316,778633	-3316.88425
 **10a**-singlet	-3430.63398	0.502223	3430.096512	-3430.20167
 **3B**-triplet	-3205.147625	0.502872	-3204.612494	-3204.713843
 ***mer*-3B**-triplet	-3205.145198	0.503968	-3204.609595	-3204.708329
 **3B**-singlet	-3205.103015	0.505967	-3204.565943	-3204.661101

 *mer*-TS(**3B/3A1)**-triplet (favored)	-3205.11627	0.497772 NImag= 1 (-1048 cm^{-1})	-3204.587084	-3204.685731
 TS(**3B/3A1)**-triplet	-3205.107662	0.497442 NImag= 1 (-755 cm^{-1})	-3204.578568	-3204.678065
 **3C**-triplet	-3203.956708	0.484463	-3203.441253	-3203.540106
 **3C**-singlet	-3203.9195689	304.28563	-3203.403834	-3203.500577
 **3A1**-triplet (favored)	-3393.786027	0.522091	-3393.228841	-3393.336026
 **3A1**-singlet	-3393.728782	0.523018	-3393.171289	-3393.274523
 **3A1'**-triplet	-3393.779491	0.521781	-3393.222324	-3393.330094
 **3A1**-singlet	-3393.728782	0.523018	-3393.171289	-3393.274523
 **3A2**-triplet	-3393.741847	0.519517	-3393.18692	-3393.295747
 **TS3(A2/3B)**-triplet	-3393.731215	0.515726 NImag=1 (-240 cm^{-1})	-3393.179945	-3393.290165
 **TS3'(A2/3B)**-triplet	Not located at B3PW91			

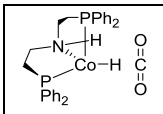
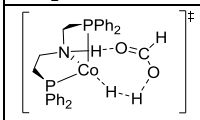
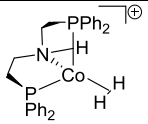
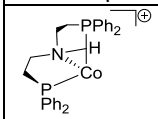
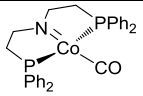
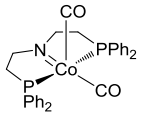
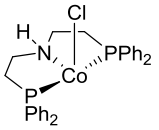
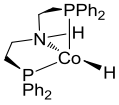
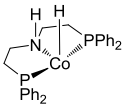
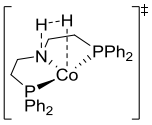
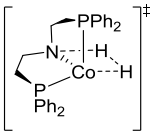
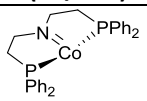
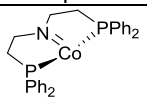
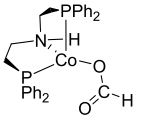
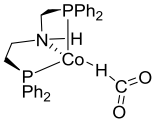
 CO_2 dissociated	-3393.733309	0.515905	-3393.180947	-3393.293888
 TS**3(3B/3A1)**-triplet	-3394.932905	0.535719 NImag = 1 (-523 cm^{-1})	-3394.361326	-3394.470813
 **3BH**$^{+}$-triplet	-3205.58586	0.514925	3205.039266	-3205.136723
 **3BH$_2$**$^{+}$-triplet	3204.39546	0.499499	3203.86456	-3203.965378
CO-SCRF	113.295698	0.005049	-113.287344	113.309768
 **10**-singlet-SCRF	-3317.328055	0.494513	-3316.800799	-3316.901463
 **10a**-singlet-SCRF	-3430.642299	0.502075	-3430.105153	-3430.209317

Table S7. Energies for All Optimized Structures at M06L-SCRF/TZVP-SCRF(SMD,H_2O) level

	Ee	ZPE	H(298.15)	G(298.15)
HCOOH	-189,815295	0.033524	-189.777668	-189.805843
CO_2	-188,637958	0.010195	-188.623851	-188.64359
H_2	-1,169050	0.009819	-1.155926	-1.170723
CO	-113,329746	0.005009	-113.321432	-113,343861
proton	-0,215180	0	-0.21282	-0.22518
HCOO-Anion	-189.356146	0.020345	-189.331882	-189.359617
H_2O	-76.4544348	0.021206	76.429449	-76.450879
 **3**-triplet-M06L-SCRF	-3665.1863981	0.499972	-3664.653609	-3664.753213
 **3B**-triplet-M06L-SCRF	-3205.480223	0.503767	-3204.945043	-3205.040728
 ***mer*-3B**-triplet-M06L-SCRF	-3205.471709	0.503427	-3204.936581	-3205.034669
 ***mer*-TS(3B/3A1)**-triplet-M06L-SCRF (favored)	-3205.429823	0.497036 NImag = 1 (-1444 cm^{-1})	-3204.9015	-3204.99803
 **TS(3B/3A1)**-triplet-M06L-SCRF	-3205.429611	0.4971	-3204.901304	-3204.996878
 **3C**-triplet-M06L-SCRF	-3204.273527	0.483096	3203.760121	-3203.855226
 **3C**-singlet-M06L-SCRF	3204.2431555	0.484823	3203,727848	-3203,822070
 **3A1**-triplet-M06L-SCRF	-3394.173253	0.521512	3393.616745	3393.721516
 **3A2**-triplet-M06L-SCRF	-3394.156543	0.521382	-3393.600183	-3393.705253

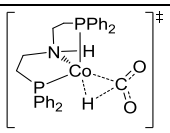
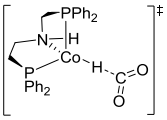
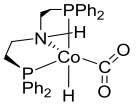
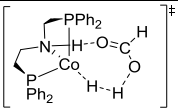
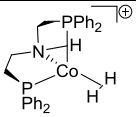
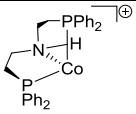
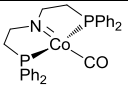
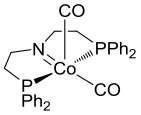
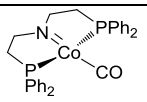
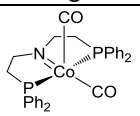
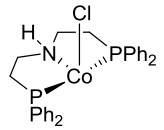
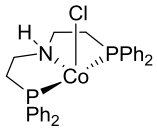
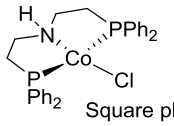
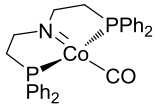
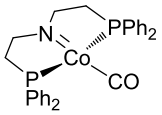
 **TS(3A2/3B)**-triplet-M06L-SCRF (favored)	-3394.131605	0.516661 NImag = 1 (-468 cm^{-1})	-3393.580593	-3393.682521
 **TS(3A2/3B)'**-triplet-M06L-SCRF	-3394.120904	0.515991 NImag = 1 (-546 cm^{-1})	-3393.569986	-3393.674848
 **3B-CO_2-**triplet-M06L-SCRF	-3394.133254	0.5177	-3393.581045	-3393.682791
 **TS(3B/3A1)**-triplet-M06L-SCRF	-3395.312665	0.534513 NImag = 1 (-1156 cm^{-1})	-3394.742651	-3394.8488
 **3B**H^+-M06L-SCRF-Cation	-3205.966749	0.514621	-3205.42001	-3205.518099
 **3B-H_2**$^+$-M06L-SCRF-Cation	-3204,786178	0.499179	-3204,256162	-3204,351549
 **10**-singlet-M06L-SCRF	-3317.675069	0.49441	-3317.148089	-3317,247064
 **10a**-singlet-M06L-SCRF	-3431.037404	0.501352	-3430.500841	-3430,605176
CO-M06L	-113.33834	0.00503	-113.330005	-113,352435
 **10**-singlet-M06L	-3317.666731	0.494885	3317.139326	-3317,238046
 **10a**-singlet-M06L	-3431.032622	0.502027	-3430.4954	-3430,600182

Table S8. The Cartesian Coordinates (xyz) for All Optimized Structures at B3PW91/TZVP level

HCOOH C 0.00000000 0.41956600 0.00000000 H -0.38102000 1.44953600 0.00000000 O 1.15729400 0.11335100 0.00000000 O -1.02731900 -0.44182100 0.00000000 H -0.65878100 -1.33917900 0.00000000	**CO_2** C 0.00000000 -0.00012600 0.00000000 O -0.66403500 -0.94978700 0.00000000 O 0.66403500 0.94988200 0.00000000
H_2 H 0.00000000 0.00000000 0.37255500 H 0.00000000 0.00000000 -0.37255500	**CO** C 0.00000000 0.00000000 -0.64366200 O 0.00000000 0.00000000 0.48274700
H^+ H 0.00000000 0.00000000 0.00000000	**$HCOO^-$** C 0.00000000 0.31236700 0.00000000 H -0.00125000 1.45602800 0.00000000 O 1.13448500 -0.20737600 0.00000000 O -1.13432800 -0.20890200 0.00000000
H_2O O 0.00000000 0.00000000 0.11710900 H 0.00000000 0.76127400 -0.46843500 H 0.00000000 -0.76127400 -0.46843500	
 **3**-triplet C -1.76103000 -0.25142300 2.10147100 H -1.08463200 0.51349500 2.48939300 H -2.74191400 -0.09403400 2.55748300 C -1.25217000 -1.64916100 2.44398700 H -1.13406100 -1.74498500 3.53239000 H -2.00388300 -2.38039900 2.13656100 C 1.25241300 -1.64814600 2.44426600 H 2.00462100 -2.37917000 2.13754300 H 1.13392100 -1.74344900 3.53267000 C 1.76076900 -0.25033700 2.10122100 H 2.74148700 -0.09236500 2.55739500 H 1.08397900 0.51450000 2.48861800 C -3.47631200 -0.80162600 -0.15704500 C -3.51153000 -2.02033200 -0.83394600 H -2.58212400 -2.49471400 -1.13772000 C -4.73080500 -2.62486800 -1.12324100 H -4.74546300 -3.57211300 -1.65102400 C -5.91968400 -2.01537900 -0.74748200 H -6.86958300 -2.48527800 -0.97835100 C -5.89118500 -0.79476400 -0.07997700 H -6.81816100 -0.30995900 0.20706000 C -4.67678300 -0.19072900 0.21245100 H -4.66555200 0.77009400 0.71638800 C -2.13564900 1.72999300 -0.01812000	 **3**-singlet C -1.89267100 -0.46543300 2.07190000 H -1.32589400 0.33385300 2.55566500 H -2.89449000 -0.49088900 2.50623300 C -1.20257000 -1.80486400 2.25349200 H -1.06640000 -2.04425500 3.31455200 H -1.81899100 -2.59210800 1.81381200 C 1.28313100 -1.43959100 2.37798200 H 2.07935400 -2.15896100 2.17332700 H 1.03202400 -1.52396300 3.44051400 C 1.78237200 -0.04490700 2.03908400 H 2.73610100 0.14660300 2.53604900 H 1.07303200 0.72106900 2.35644100 C -3.51946900 -0.94730700 -0.27613900 C -3.43399700 -2.19189000 -0.90122600 H -2.45655300 -2.62343200 -1.10301200 C -4.59159800 -2.87012400 -1.26908300 H -4.51347700 -3.83639900 -1.75534200 C -5.83777900 -2.30793400 -1.02823900 H -6.73929900 -2.83476300 -1.32187000 C -5.92835100 -1.06134300 -0.41701500 H -6.89988600 -0.61377500 -0.23610800 C -4.77599800 -0.38310500 -0.04478300 H -4.85680200 0.59559600 0.41584900 C -2.36861400 1.64802300 0.10508600

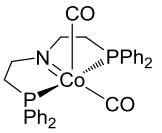
C -2.07148900 2.19992100 -1.33224600	C -2.22252300 2.25645500 -1.14433000
H -1.83225000 1.51058500 -2.13577600	H -1.85625700 1.67506100 -1.98456300
C -2.30877200 3.53554800 -1.61972600	C -2.53210000 3.59645600 -1.32303600
H -2.25979600 3.88213900 -2.64611200	H -2.41481400 4.04975800 -2.30109900
C -2.59823300 4.42936500 -0.59484000	C -2.97846200 4.35915800 -0.24940100
H -2.77702100 5.47530500 -0.81786100	H -3.21442700 5.40855600 -0.38661300
C -2.65299300 3.97656900 0.71581900	C -3.11757100 3.76991900 0.99983000
H -2.87627100 4.66779900 1.52136200	H -3.46665800 4.35695600 1.84264300
C -2.42728700 2.63457900 1.00273200	C -2.82032800 2.42234000 1.17506300
H -2.48534800 2.30218000 2.03267600	H -2.95094900 1.98057800 2.15640700
C 3.47654300 -0.80121500 -0.15672200	C 3.58688300 -0.76523600 -0.07938600
C 4.67685300 -0.18996400 0.21270000	C 4.76285600 -0.29435500 0.51244600
H 4.66538400 0.77109200 0.71619000	H 4.74580000 0.60915200 1.11359200
C 5.89139800 -0.79395200 -0.07923600	C 5.96278200 -0.96450100 0.32278300
H 6.81825300 -0.30887600 0.20773600	H 6.87006000 -0.59048800 0.78517900
C 5.92019700 -2.01487300 -0.74616600	C 6.00213900 -2.11301000 -0.46291700
H 6.87020700 -2.48473700 -0.97664800	H 6.94097500 -2.63542100 -0.61184500
C 4.73147600 -2.62471300 -1.12186400	C 4.83896200 -2.58834000 -1.05172100
H 4.74637800 -3.57219400 -1.64921600	H 4.86269900 -3.48516400 -1.66095300
C 3.51206200 -2.02022400 -0.83306800	C 3.63324000 -1.91996700 -0.85964600
H 2.58277400 -2.49485100 -1.13682600	H 2.71605500 -2.30419900 -1.29764400
C 2.13532100 1.73024500 -0.01916900	C 2.28058900 1.80892500 -0.17232400
C 2.42693600 2.63527700 1.00129200	C 1.44967900 2.79646000 0.36341000
H 2.48520400 2.30328300 2.03135700	H 0.63146000 2.52256100 1.02024700
C 2.65232800 3.97720400 0.71383200	C 1.64041400 4.13386700 0.04773300
H 2.87557600 4.66878900 1.51907900	H 0.98908200 4.88438500 0.48170700
C 2.59728500 4.42948400 -0.59699300	C 2.64879000 4.50828700 -0.83292800
H 2.77582300 5.47537500 -0.82044300	H 2.79398000 5.55287200 -1.08490200
C 2.30786200 3.53521400 -1.62149600	C 3.46130300 3.53285100 -1.39507800
H 2.25867600 3.88140000 -2.64800800	H 4.24395600 3.81170600 -2.09237500
C 2.07088200 2.19965000 -1.33346800	C 3.27966400 2.19440800 -1.06860300
H 1.83167100 1.50995500 -2.13670000	H 3.92692000 1.44632300 -1.51088100
Cl 0.00030000 -3.29355300 -1.37770300	Cl 0.13442100 -3.14001500 -1.23182300
Co 0.00010800 -1.29493900 -0.33085800	Co 0.04150100 -1.06611400 -0.24708900
N 0.00033100 -1.99899300 1.75020500	N 0.10694200 -1.84324200 1.55265100
H 0.00073900 -2.99592400 1.56809200	H 0.25575200 -2.80240800 1.24098800
P -1.82024900 -0.06929400 0.24267100	P -1.92468600 -0.14086000 0.23340600
P 1.82029000 -0.06899100 0.24236700	P 1.92993300 0.02871300 0.17860100
 Square planar **3**-Square-Planar-singlet	 **10**-singlet
C -1.76103000 -0.25142300 2.10147100	C -2.41207500 -0.10118900 2.35005800
H -1.08463200 0.51349500 2.48939300	H -3.35963900 0.36238000 2.63319000
H -2.74191400 -0.09403400 2.55748300	H -2.38421700 -1.13152300 2.71226100
C -1.25217000 -1.64916100 2.44398700	C -1.19931100 0.64862000 2.87891500
H -1.13406100 -1.74498500 3.53239000	H -1.36250000 1.73580800 2.76086000
H -2.00388300 -2.38039900 2.13656100	H -1.11382800 0.47653100 3.96439000
C 1.25241300 -1.64814600 2.44426600	C 1.17904700 0.69028100 2.88438800
H 2.00462100 -2.37917000 2.13754300	H 1.10019800 0.50061900 3.96780200
H 1.13392100 -1.74344900 3.53267000	H 1.29040600 1.78612100 2.78277400
	C 2.42245900 0.00153700 2.34621300

C	1.76076900	-0.25033700	2.10122100	H	2.46552900	-1.02877000	2.70736800
H	2.74148700	-0.09236500	2.55739500	H	3.35587700	0.49539600	2.62392300
H	1.08397900	0.51450000	2.48861800	C	-3.37639100	-1.36373900	-0.14635000
C	-3.47631200	-0.80162600	-0.15704500	C	-3.47301500	-1.51312500	-1.53245100
C	-3.51153000	-2.02033200	-0.83394600	H	-2.84922800	-0.91448100	-2.18672000
H	-2.58212400	-2.49471400	-1.13772000	C	-4.36054000	-2.42512500	-2.08344300
C	-4.73080500	-2.62486800	-1.12324100	H	-4.42166600	-2.53009600	-3.16092200
H	-4.74546300	-3.57211300	-1.65102400	C	-5.16206000	-3.20675800	-1.25888800
C	-5.91968400	-2.01537900	-0.74748200	H	-5.85348100	-3.92204600	-1.69020200
H	-6.86958300	-2.48527800	-0.97835100	C	-5.07091300	-3.06826500	0.11890500
C	-5.89118500	-0.79476400	-0.07997700	H	-5.69256300	-3.67355100	0.76960100
H	-6.81816100	-0.30995900	0.20706000	C	-4.18308800	-2.15272400	0.67299000
C	-4.67678300	-0.19072900	0.21245100	H	-4.12949000	-2.05851100	1.75081100
H	-4.66555200	0.77009400	0.71638800	C	-2.80558400	1.45894900	-0.07790100
C	-2.13564900	1.72999300	-0.01812000	C	-1.89462300	2.44264700	-0.45768800
C	-2.07148900	2.19992100	-1.33224600	H	-0.83387800	2.21238000	-0.43137100
H	-1.83225000	1.51058500	-2.13577600	C	-2.34260800	3.69290200	-0.86821000
C	-2.30877200	3.53554800	-1.61972600	H	-1.62575100	4.45132100	-1.16311500
H	-2.25979600	3.88213900	-2.64611200	C	-3.70335800	3.96622100	-0.90659000
C	-2.59823300	4.42936500	-0.59484000	H	-4.05387800	4.93984800	-1.23134100
H	-2.77702100	5.47530500	-0.81786100	C	-4.61807400	2.98716200	-0.53274100
C	-2.65299300	3.97656900	0.71581900	H	-5.68191000	3.19573400	-0.56674200
H	-2.87627100	4.66779900	1.52136200	C	-4.17248400	1.73925300	-0.12016500
C	-2.42728700	2.63457900	1.00273200	H	-4.89235300	0.97679300	0.15785700
H	-2.48534800	2.30218000	2.03267600	C	3.35861100	-1.44426700	-0.01157000
C	3.47654300	-0.80121500	-0.15672200	C	4.68572300	-1.15778500	-0.33164300
C	4.67685300	-0.18996400	0.21270000	H	5.03623900	-0.13177000	-0.32433500
H	4.66538400	0.77109200	0.71619000	C	5.56024600	-2.18154300	-0.67213900
C	5.89139800	-0.79395200	-0.07923600	H	6.58938200	-1.94882800	-0.92317600
H	6.81825300	-0.30887600	0.20773600	C	5.11785900	-3.49882500	-0.69639000
C	5.92019700	-2.01487300	-0.74616600	H	5.80138900	-4.29643600	-0.96593700
H	6.87020700	-2.48473700	-0.97664800	C	3.79657800	-3.79040900	-0.38158400
C	4.73147600	-2.62471300	-1.12186400	H	3.44342100	-4.81532200	-0.40851700
H	4.74637800	-3.57219400	-1.64921600	C	2.91923000	-2.76782800	-0.04509100
C	3.51206200	-2.02022400	-0.83306800	H	1.88229600	-2.99018600	0.18491000
H	2.58277400	-2.49485100	-1.13682600	C	2.82102600	1.39116400	-0.24808600
C	2.13532100	1.73024500	-0.01916900	C	3.48403500	2.38748100	0.46733600
C	2.42693600	2.63527700	1.00129200	H	3.65857100	2.27661300	1.53044700
H	2.48520400	2.30328300	2.03135700	C	3.92927100	3.54001300	-0.17225800
C	2.65232800	3.97720400	0.71383200	H	4.43923500	4.30757400	0.39962700
H	2.87557600	4.66878900	1.51907900	C	3.72510400	3.70580600	-1.53447600
C	2.59728500	4.42948400	-0.59699300	H	4.07591600	4.60257700	-2.03302400
H	2.77582300	5.47537500	-0.82044300	C	3.06589800	2.71657700	-2.25706800
C	2.30786200	3.53521400	-1.62149600	H	2.89927300	2.83939600	-3.32155700
H	2.25867600	3.88140000	-2.64800800	C	2.60782300	1.57458800	-1.61786200
C	2.07088200	2.19965000	-1.33346800	H	2.07989600	0.81736600	-2.18722900
H	1.83167100	1.50995500	-2.13670000	C	0.01899500	-1.04788500	-1.17830200
Cl	0.00030000	-3.29355300	-1.37770300	Co	0.00887300	-0.40048500	0.40804400
Co	0.00010800	-1.29493900	-0.33085800	N	-0.00016200	0.19206100	2.20169900
N	0.00033100	-1.99899300	1.75020500	O	0.03187600	-1.47008800	-2.25837400
H	0.00073900	-2.99592400	1.56809200	P	-2.15502600	-0.16155600	0.52442800
P	-1.82024900	-0.06929400	0.24267100	P	2.16413300	-0.14830700	0.52616000
P	1.82029000	-0.06899100	0.24236700				



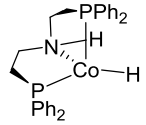
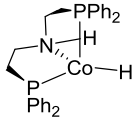
10-triplet

C	-2.43709200	-0.23707700	2.18343600
H	-3.32528700	0.31163700	2.50533600
H	-2.56110700	-1.29330800	2.43727300
C	-1.17384400	0.31360700	2.83748100
H	-1.23672500	1.41807300	2.86996500
H	-1.16368700	-0.00815700	3.89463500
C	1.20727100	0.29882000	2.82562300
H	1.20688300	-0.02727500	3.88173700
H	1.27950600	1.40305200	2.86135700
C	2.45211900	-0.26441400	2.15038700
H	2.56100900	-1.32525700	2.39045800
H	3.36901000	0.23813000	2.46707200
C	-3.62840400	-1.14420500	-0.33727000
C	-3.48906800	-1.70570300	-1.60775800
H	-2.55839900	-1.57461600	-2.15014200
C	-4.52227100	-2.43824000	-2.17602900
H	-4.39838500	-2.86820800	-3.16375400
C	-5.70490100	-2.63360300	-1.47315700
H	-6.50910200	-3.21402300	-1.91157200
C	-5.85059500	-2.08932000	-0.20344700
H	-6.76939100	-2.24285800	0.35202500
C	-4.82047900	-1.34622200	0.36024100
H	-4.95224600	-0.92447200	1.34991300
C	-2.59652000	1.55669200	-0.10938000
C	-1.59038700	2.50976800	0.06730600
H	-0.61783100	2.19447500	0.43135000
C	-1.82549400	3.84576000	-0.22819200
H	-1.03530300	4.57401100	-0.08269900
C	-3.06213500	4.24472300	-0.72112000
H	-3.24350700	5.28695900	-0.95979900
C	-4.06286700	3.30070300	-0.91388300
H	-5.02827400	3.60349900	-1.30494500
C	-3.83426600	1.96463400	-0.60769400
H	-4.62259800	1.23756500	-0.76390300
C	3.66435800	-1.18390500	-0.31144500
C	4.78715200	-0.58225200	-0.87950800
H	4.83461000	0.49611500	-0.97459400
C	5.84971400	-1.35733500	-1.32930100
H	6.71524600	-0.87514600	-1.77074900
C	5.80637100	-2.74034900	-1.21405400
H	6.63632100	-3.34327000	-1.56545200
C	4.68975500	-3.34845200	-0.65215700
H	4.64243200	-4.42841700	-0.56587600
C	3.62319500	-2.57712400	-0.21275500
H	2.74695000	-3.06357200	0.20204700
C	2.56750500	1.49443200	-0.22404000
C	3.28376600	2.41192000	0.54520900
H	3.67528100	2.12580400	1.51406600



10a-singlet

C	-2.46962300	-0.39826000	2.23731000
H	-3.39184700	0.11033800	2.52536700
H	-2.58184800	-1.46798000	2.42235600
C	-1.24943400	0.14884900	2.95259300
H	-1.27870200	1.25706500	2.88401800
H	-1.32446600	-0.08252900	4.02897500
C	1.08739500	0.36411500	2.91376200
H	1.18527300	0.21177500	4.00279800
H	0.94077900	1.45808400	2.78246500
C	2.38373600	-0.04246700	2.24145900
H	2.64578300	-1.07076900	2.50143600
H	3.22929500	0.59935500	2.49934000
C	-3.36183500	-1.07553500	-0.49896300
C	-3.95141500	-0.52850000	-1.63910700
H	-3.69857100	0.47857600	-1.94919300
C	-4.86873800	-1.26245800	-2.38096900
H	-5.31805600	-0.82183600	-3.26419600
C	-5.20794100	-2.55251900	-1.99623800
H	-5.92522800	-3.12385300	-2.57477000
C	-4.61675800	-3.11035300	-0.86887000
H	-4.86931700	-4.12006800	-0.56444600
C	-3.69461000	-2.38174000	-0.13111100
H	-3.22744100	-2.84181300	0.73226700
C	-2.46839300	1.60131000	0.13677600
C	-1.47823400	2.44970700	-0.34936500
H	-0.49101200	2.04925100	-0.55076100
C	-1.74748600	3.79750700	-0.56317200
H	-0.96612800	4.44707600	-0.94108300
C	-3.00889500	4.30615600	-0.28832500
H	-3.21988200	5.35720300	-0.45265200
C	-4.00432000	3.46536200	0.20037200
H	-4.99142100	3.85929800	0.41660900
C	-3.73639100	2.12091100	0.41155200
H	-4.52273900	1.47177900	0.78193100
C	3.44624500	-1.02794700	-0.28401300
C	4.70206400	-0.44244800	-0.45911500
H	4.84581000	0.60894500	-0.23681900
C	5.77011400	-1.19569700	-0.92639800
H	6.74023200	-0.72906800	-1.05833100
C	5.59685200	-2.54168600	-1.22821600
H	6.43125300	-3.12812800	-1.59673300
C	4.35124500	-3.13077100	-1.05913200
H	4.20669400	-4.17883200	-1.29682300
C	3.28162700	-2.37745400	-0.59061000
H	2.30955500	-2.83866700	-0.46191600
C	2.36978500	1.61926700	-0.21611800
C	2.64832400	2.70803000	0.60870500

C 3.50794100 3.70245100 0.07960700 H 4.06334900 4.40522400 0.69116000 C 3.02664100 4.09006700 -1.16416800 H 3.20496800 5.09614800 -1.52738600 C 2.31153700 3.18442200 -1.93899100 H 1.92648800 3.48110900 -2.90824000 C 2.07634000 1.90052400 -1.46731300 H 1.50099400 1.20391500 -2.06867400 C -0.08539600 -2.68690400 0.00370700 Co -0.00933000 -0.92186300 0.38537400 N 0.01096200 -0.12787500 2.14505800 O -0.15183000 -3.82816800 -0.12762500 P -2.20681600 -0.19210700 0.34036000 P 2.20874400 -0.23301700 0.31176600	H 2.69644500 2.58278200 1.68353900 C 2.86270600 3.97070900 0.06570500 H 3.07901300 4.80619500 0.72258300 C 2.80359300 4.16127400 -1.30754100 H 2.97540400 5.14502700 -1.72999400 C 2.52230100 3.08195300 -2.13917800 H 2.47297100 3.22042000 -3.21363900 C 2.30002900 1.82481400 -1.59784800 H 2.07933400 0.99226000 -2.25797000 Co -0.00294200 -0.93676300 0.45066600 N -0.02771800 -0.39531900 2.40071200 P -2.06335100 -0.17199300 0.44689000 P 2.02866300 -0.07845900 0.42847300 C -0.01122400 -2.62866800 1.09376000 C -0.02111300 -1.23805800 -1.27250900 O -0.03904200 -3.64827700 1.61558700 O -0.03783900 -1.42018500 -2.40670400
 **3B**-triplet C -1.79340800 -0.62526200 1.98892900 H -1.14703500 0.11623600 2.46450000 H -2.78864400 -0.53561300 2.43226400 C -1.25636000 -2.03457300 2.21419200 H -1.15741500 -2.22718300 3.29212900 H -1.98213300 -2.75207700 1.82334900 C 1.24644400 -1.94421500 2.25646500 H 2.02135800 -2.64457100 1.93500700 H 1.10559500 -2.09153100 3.33652200 C 1.73515800 -0.52367300 1.98869300 H 2.71146400 -0.37527600 2.45805200 H 1.04413500 0.20951200 2.41090400 C -3.44963000 -0.98711800 -0.34963800 C -3.43827200 -2.14122900 -1.13149100 H -2.48125400 -2.55388000 -1.44550400 C -4.63314300 -2.74589900 -1.50784500 H -4.61232600 -3.64239300 -2.11820200 C -5.84646800 -2.19945400 -1.11216700 H -6.77834800 -2.66812500 -1.40971200 C -5.86507900 -1.04248500 -0.33941000 H -6.81113200 -0.60642400 -0.03652300 C -4.67364900 -0.43921100 0.03881200 H -4.69939400 0.47334400 0.62529100 C -2.16339800 1.54192600 0.06802800 C -2.03551100 2.15323400 -1.18181000 H -1.73305900 1.55887200 -2.03806000 C -2.28491800 3.50847600 -1.33813200 H -2.18402700 3.96505100 -2.31661900 C -2.65113100 4.28189200 -0.24234800 H -2.83907000 5.34308700 -0.36206800	 **3B**-singlet C -1.59079900 -0.62929200 1.89039600 H -0.91893500 0.13094200 2.29370000 H -2.55920600 -0.51123300 2.38812900 C -1.04760900 -2.02598600 2.19117000 H -0.95299500 -2.16291200 3.27791400 H -1.76275300 -2.76442800 1.82377200 C 1.47044300 -2.02423200 2.31806500 H 2.24027500 -2.72589700 1.98752700 H 1.29809100 -2.20362300 3.38793700 C 1.97163900 -0.60587300 2.08727500 H 2.99368100 -0.50457500 2.45978200 H 1.34973400 0.12737200 2.60716800 C -3.42321100 -1.01399000 -0.32694500 C -3.56029100 -2.11674000 -1.16719700 H -2.66385600 -2.56386900 -1.58344600 C -4.81739400 -2.63841500 -1.45341200 H -4.90726200 -3.49556600 -2.11243900 C -5.95386700 -2.06311400 -0.90062400 H -6.93497400 -2.46829800 -1.12411500 C -5.82887800 -0.96042600 -0.06209700 H -6.71283200 -0.50164700 0.36845400 C -4.57332900 -0.43859300 0.21872900 H -4.49045600 0.43558100 0.85635500 C -2.10421400 1.46966500 -0.06482500 C -2.42081900 1.97781000 -1.33008600 H -2.46583700 1.30018600 -2.17772700 C -2.68218300 3.32548500 -1.51761400 H -2.93739000 3.69206900 -2.50638900 C -2.61213900 4.20766400 -0.44284600 H -2.80896200 5.26416900 -0.58778900 C -2.28596700 3.72215600 0.81455500

C -2.76995900 3.68885000 1.00686300	H -2.22819200 4.39937200 1.66031000
H -3.05329200 4.28537400 1.86748300	C -2.03855000 2.36523900 1.00314800
C -2.53163700 2.32737300 1.16082500	H -1.80193800 2.01630700 2.00103700
H -2.63994400 1.88475800 2.14431000	C 3.38315800 -0.95027000 -0.46434300
C 3.43661100 -0.99742000 -0.29124200	C 4.60950100 -0.28608900 -0.46890200
C 4.65357300 -0.46084400 0.13374300	H 4.68447800 0.71804300 -0.06694200
H 4.67037900 0.46040000 0.70711900	C 5.73702600 -0.89627200 -1.00482900
C 5.84892400 -1.08676500 -0.19108600	H 6.68528700 -0.36947100 -1.00416100
H 6.78971900 -0.65990700 0.13991400	C 5.65092800 -2.17256100 -1.54847100
C 5.84124700 -2.25546800 -0.94642400	H 6.53198000 -2.64464500 -1.96933200
H 6.77632300 -2.74202200 -1.20223600	C 4.43057400 -2.83710800 -1.55954400
C 4.63541200 -2.79124700 -1.37789800	H 4.35305300 -3.82755200 -1.99478000
H 4.62387700 -3.69712300 -1.97444200	C 3.30359100 -2.22773800 -1.02321900
C 3.43666000 -2.16385100 -1.05445300	H 2.33996300 -2.73447600 -1.02947200
H 2.48619400 -2.56949400 -1.39597500	C 2.09854400 1.56590200 0.14617300
C 2.16947600 1.55535200 -0.02276000	C 2.80420700 2.30646400 1.09610700
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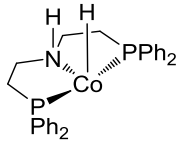
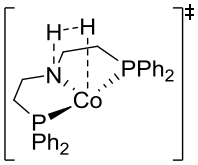
H 2.36684300 2.04732100 2.06842500	C 2.97428100 3.67688800 0.93849300
C 2.64769400 3.76783200 0.83333400	H 3.52100900 4.24161600 1.68607200
H 2.81495000 4.42523100 1.67981300	C 2.44587800 4.32098900 -0.17307800
C 2.69587700 4.27128900 -0.45878600	H 2.57805800 5.39039100 -0.29531500
H 2.89929000 5.32296600 -0.62710800	C 1.73851800 3.59261800 -1.12162400
C 2.47802700 3.41943300 -1.53619800	H 1.31009300 4.09198900 -1.98326000
H 2.51053100 3.80482100 -2.54945400	C 1.56048600 2.22583700 -0.95876900
C 2.20965300 2.07661200 -1.31908600	H 0.97975200 1.66104100 -1.68094300
H 2.02875400 1.42095700 -2.16507400	Co 0.06728900 -1.46637200 -0.25866500
Co -0.00078600 -1.45066600 -0.54391500	N 0.25179400 -2.33829400 1.53346800
N 0.01718200 -2.28697600 1.51923100	H 0.25357700 -3.33457100 1.35324100
H 0.05484900 -3.26362000 1.25984000	P -1.71469500 -0.34949700 0.02327800
P -1.81046300 -0.26948600 0.15376000	P 1.81960000 -0.25514300 0.25447500
P 1.79356200 -0.24522500 0.14260000	H -0.79024400 -2.66683200 -0.61439400
H -0.03541700 -2.82241700 -1.43577900	
	
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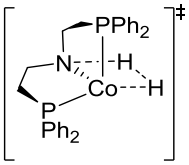
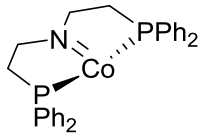
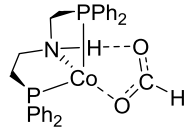
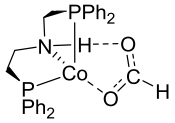
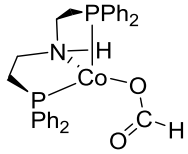
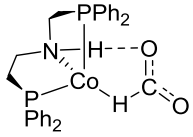
P 0.18409800 0.26387200 -2.17846000	P 2.23308000 -0.25104700 0.29748500
C 0.34645500 2.18861700 2.41806300	C -2.40389300 -0.27851200 2.17401800
C 0.17103800 2.11605400 -2.45065100	C 2.46729800 -0.36318600 2.14669900
H 1.41612300 2.41407100 2.43953700	H -2.51382500 -1.34052200 2.40960500
H 1.22185700 2.39390800 -2.57011000	H 2.53590600 -1.43041000 2.37264000
H -0.07824200 2.53993600 3.36045500	H -3.32052000 0.22265000 2.49540800
H -0.34011700 2.40339300 -3.37235900	H 3.39913900 0.10610400 2.46925600
C -0.31890100 2.87525500 1.23163400	C -1.16043400 0.27894400 2.86749100
C -0.42229800 2.82453200 -1.23796900	C 1.25396000 0.24423800 2.84785400
H -0.20051700 3.96678700 1.31135100	H -1.24354100 0.05201000 3.94654600
H -0.33425400 3.91524500 -1.36022900	H 1.34107500 0.02702300 3.92843900
H -1.39358200 2.66597700 1.23379600	H -1.16416400 1.38464200 2.79581800
H -1.48861800 2.59491500 -1.14635700	H 1.30266700 1.34745300 2.75997700
N 0.22954700 2.35356400 -0.01852500	

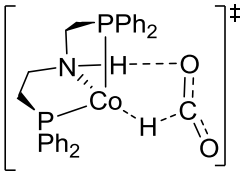
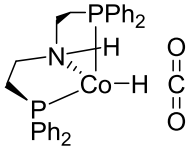
H 2.20148700 0.35663000 0.00558300	N 0.03392400 -0.27242700 2.28841100
H 1.22859100 2.53265200 -0.06297000	H 0.02758900 -2.22007000 0.91591300
Co 0.58953800 0.17383500 0.01132900	H 0.02482900 -1.57222600 1.64342300
C 1.40564800 -0.30756900 3.47043400	Co 0.01727100 -0.61454900 0.20163700
C 1.04983900 -0.68703600 4.76425600	C -3.49311700 -1.41201700 -0.26209800
C 2.73909900 -0.42272200 3.06945300	C -4.85135500 -1.09067500 -0.26670900
C 2.01500000 -1.15186600 5.65017400	C -3.09411300 -2.68392200 -0.67226000
H 0.01605100 -0.63268000 5.08412000	C -5.79246000 -2.02713000 -0.67253900
C 3.70160700 -0.87702300 3.96095200	H -5.17496100 -0.10092700 0.03674600
H 2.99679000 -0.16916200 2.04378800	C -4.03762900 -3.62213400 -1.07369300
C 3.34306400 -1.24202600 5.25345500	H -2.03751400 -2.93159400 -0.67347100
H 1.72514900 -1.44792200 6.65275500	C -5.38730600 -3.29494200 -1.07543800
H 4.73413400 -0.96037200 3.63886200	H -6.84537100 -1.76661100 -0.67558100
H 4.09446000 -1.60515400 5.94629600	H -3.71565900 -4.60787100 -1.39127100
C -1.44949600 -0.05899600 2.92715200	H -6.12376700 -4.02475200 -1.39348500
C -2.17192600 -1.08563600 2.31626400	C -2.84624500 1.39339200 -0.23662900
C -2.03191500 0.61551300 4.00272600	C -2.94729900 1.62163700 -1.61261700
C -3.43293700 -1.44259500 2.77541400	C -3.18161100 2.42560300 0.63782300
H -1.73925900 -1.59628500 1.46155800	C -3.39250200 2.84150000 -2.09853700
C -3.29901000 0.26913000 4.45623700	H -2.68113000 0.83236300 -2.30878500
H -1.49872600 1.41766900 4.50090100	C -3.61796500 3.65325100 0.15018500
C -4.00077300 -0.76339500 3.84602700	H -3.09984900 2.28346300 1.70878800
H -3.97660500 -2.24503000 2.28895900	C -3.72814000 3.86395900 -1.21680600
H -3.73792700 0.80596800 5.29045400	H -3.47373400 2.99736400 -3.16880800
H -4.98923700 -1.03351400 4.20100300	H -3.87359600 4.44568200 0.84525100
C -1.40830400 -0.32804900 -2.91945200	H -4.07085400 4.82035800 -1.59572100
C -1.61323400 -1.71115900 -2.97658700	C 3.52995500 -1.38594000 -0.36500100
C -2.44091100 0.51072400 -3.33798900	C 4.58442900 -0.96590900 -1.17441700
C -2.80325400 -2.23629000 -3.45546600	C 3.39396900 -2.75035300 -0.08996300
H -0.82683900 -2.38281800 -2.64622200	C 5.49491100 -1.88691800 -1.68105200
C -3.64047600 -0.01490500 -3.80772200	H 4.69916000 0.08436500 -1.41443400
H -2.32272400 1.58756100 -3.30450300	C 4.30911800 -3.66581400 -0.58819400
C -3.82526100 -1.38847400 -3.87138200	H 2.55375800 -3.09857100 0.50257200
H -2.93694700 -3.31177200 -3.50026300	C 5.36469200 -3.23670600 -1.38548500
H -4.43048500 0.65562200 -4.12881600	H 6.30978500 -1.54377700 -2.30941000
H -4.75904400 -1.79790800 -4.24017500	H 4.19207400 -4.71989500 -0.36111800
C 1.41472000 -0.30586200 -3.43596400	H 6.07673100 -3.95317000 -1.77981400
C 2.68416900 -0.66248100 -2.98270400	C 2.83129900 1.43889700 -0.13659700
C 1.13354900 -0.35956500 -4.80197300	C 3.99603300 1.99894700 0.39301900
C 3.66128600 -1.06213800 -3.88704500	C 2.06202000 2.19716400 -1.01851400
H 2.88311000 -0.61235000 -1.91498300	C 4.38187300 3.28593200 0.04396500
C 2.11180100 -0.76009200 -5.70239500	H 4.61273000 1.42783400 1.07832800
H 0.14400800 -0.10134700 -5.16378400	C 2.44784100 3.48489100 -1.37088800
C 3.37774600 -1.11144600 -5.24598900	H 1.14879100 1.77244200 -1.42333900
H 4.64557800 -1.34078800 -3.52614100	C 3.60826400 4.03106600 -0.83938600
H 1.88500300 -0.80129000 -6.76241200	H 5.28818000 3.70942200 0.46302600
H 4.13990700 -1.42685700 -5.95045600	H 1.83713100 4.06216400 -2.05614600
	H 3.90971100 5.03722300 -1.10926500
	 **3C**-triplet

TS(**3B/3A1)**-triplet

N	0.02747700	-2.32822100	1.46964200
Co	-0.01645900	-1.43678300	-0.43897500
P	-1.86780100	-0.29199800	0.19220100
P	1.84503900	-0.28132700	0.14514000
H	0.40568100	-3.11154600	-0.80979100
H	0.26161700	-3.02475600	0.10482500
C	-1.86318200	-0.74898400	2.00001100
H	-1.24492100	-0.01195000	2.51982500
H	-2.87221300	-0.71211800	2.42234500
C	-1.23901200	-2.15858200	2.13084500
H	-1.16713000	-2.39923700	3.20407300
H	-1.95775900	-2.87711300	1.71362700
C	1.21669700	-1.98585900	2.21101500
H	2.02620500	-2.67464300	1.93059700
H	1.06304600	-2.13098500	3.29185300
C	1.73956400	-0.54998000	1.98429500
H	2.70560500	-0.38621900	2.47219300
H	1.02507000	0.17841300	2.37721100
C	-3.47476200	-0.99595300	-0.40535800
C	-3.44456700	-2.19671900	-1.11452400
H	-2.48973700	-2.66733500	-1.33016900
C	-4.62171500	-2.79392800	-1.54922200
H	-4.58098900	-3.72909800	-2.09680200
C	-5.84392700	-2.18783900	-1.29145900
H	-6.76342800	-2.64782600	-1.63629400
C	-5.88419800	-0.98494700	-0.59523200
H	-6.83581600	-0.50336500	-0.39765000
C	-4.70830800	-0.39346700	-0.15388800
H	-4.75185000	0.55026300	0.37848700
C	-2.18661300	1.52228700	0.14417200
C	-1.94000300	2.19376100	-1.05474000
H	-1.55152300	1.64266700	-1.90489100
C	-2.17334600	3.55686300	-1.16371300
H	-1.97729100	4.06361800	-2.10208400
C	-2.64299900	4.27329300	-0.06906400
H	-2.81821600	5.34026200	-0.15101700
C	-2.87906300	3.61855800	1.13226600
H	-3.24074700	4.17229300	1.99195100
C	-2.65549600	2.25046000	1.23833300
H	-2.84960000	1.75401500	2.18205600
C	3.52227100	-0.95563700	-0.27274900
C	4.69977700	-0.32633100	0.13661600
H	4.65174400	0.60678700	0.68782900
C	5.93624000	-0.87650300	-0.16993700
H	6.84358000	-0.37674500	0.15197800
C	6.01283500	-2.06302700	-0.89204200
H	6.97973500	-2.49140800	-1.13251000
C	4.84796900	-2.69378800	-1.30625100
H	4.90008000	-3.61760900	-1.87211600
C	3.60914200	-2.14071400	-1.00064400
H	2.69742700	-2.63254000	-1.32318100
C	-2.43644600	-0.25262300	2.17448800
H	-3.38784100	0.17898600	2.49387100
H	-2.44080600	-1.31396600	2.43342600
C	-1.23587700	0.43007300	2.82720800
H	-1.41403100	1.52163400	2.86398700
H	-1.18922300	0.10363100	3.88212300
C	1.16398700	0.46244600	2.85260900
H	1.12025600	0.10235900	3.89693900
H	1.28268200	1.56061800	2.92967600
C	2.40612900	-0.14256800	2.19645600
H	2.47797300	-1.20074700	2.46034800
H	3.33508500	0.34202700	2.50866300
C	-3.37815500	-1.49081900	-0.29369800
C	-4.41338800	-1.23819400	-1.19276700
H	-4.61037000	-0.22454800	-1.52083300
C	-5.19976900	-2.27864300	-1.67557500
H	-6.00149500	-2.06378500	-2.37392000
C	-4.96404100	-3.58401500	-1.26736700
H	-5.57984700	-4.39362600	-1.64291800
C	-3.92652900	-3.84766700	-0.37955700
H	-3.72763600	-4.86537400	-0.06150700
C	-3.13573200	-2.81194200	0.09534300
H	-2.31030000	-3.03369600	0.76490500
C	-3.01644400	1.39904900	-0.18208700
C	-2.31817700	2.23781700	-1.04975700
H	-1.33958200	1.93428900	-1.40722500
C	-2.85753400	3.45573000	-1.44620400
H	-2.30151800	4.09775300	-2.12041200
C	-4.10132300	3.85125000	-0.97262600
H	-4.52222200	4.80325300	-1.27697900
C	-4.80492300	3.02511200	-0.10305400
H	-5.77575500	3.33106500	0.27144700
C	-4.26599300	1.80745700	0.28955100
H	-4.82879700	1.16953500	0.96241700
C	3.39621700	-1.45611700	-0.19434500
C	4.77956400	-1.27209200	-0.15945400
H	5.19048100	-0.31655500	0.14810500
C	5.63484300	-2.30072600	-0.53031200
H	6.70805600	-2.14608700	-0.50182000
C	5.11847500	-3.52597400	-0.93823300
H	5.78818100	-4.32780100	-1.22920800
C	3.74370500	-3.71808800	-0.97594000
H	3.33512300	-4.66990000	-1.29738800
C	2.88777500	-2.68666100	-0.60785400
H	1.81222900	-2.83066400	-0.64057400
C	2.98454900	1.39230600	-0.27901600
C	3.23390600	2.48897700	0.54558400
H	3.02131600	2.43294100	1.60641200
C	3.75129800	3.66746400	0.01868000
H	3.93982100	4.51031800	0.67478100
C	4.02665400	3.76589700	-1.33797100
H	4.43269300	4.68420500	-1.74735700

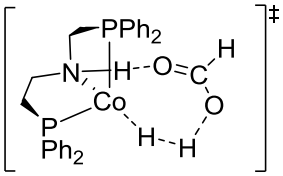
C 2.12905500 1.52919000 -0.07636500 C 2.24760100 2.43326700 0.97843000 H 2.18959600 2.08769300 2.00372800 C 2.44671300 3.78770400 0.73122900 H 2.53495900 4.47749600 1.56364500 C 2.53724600 4.25490300 -0.57206800 H 2.69588500 5.31038300 -0.76338100 C 2.42048800 3.36158700 -1.63169500 H 2.48822500 3.71817600 -2.65381000 C 2.21069700 2.01346700 -1.38489300 H 2.11163100 1.32448900 -2.21799500	C 3.77662900 2.67944400 -2.16979300 H 3.98746800 2.74740400 -3.23156800 C 3.25352000 1.50657400 -1.64617500 H 3.05968500 0.66634500 -2.30520900 Co -0.00665500 -0.28489000 0.25572400 N -0.02286800 0.09448300 2.12264500 P -2.22318300 -0.18736400 0.32637500 P 2.20055800 -0.15595400 0.34748700
 **3A1**-triplet (favored) H -0.00046700 -2.89744900 1.44152500 N -0.00020800 -1.89944500 1.69296200 Co -0.00010400 -1.16902700 -0.35687800 O 0.00024000 -2.87651000 -1.36466300 C 0.00009400 -4.05523600 -0.86652800 H 0.00041700 -4.86317400 -1.62566200 O -0.00035500 -4.37198700 0.32484100 P -1.81686600 0.05224200 0.22674700 P 1.81683800 0.05207300 0.22679100 C -1.77272800 -0.17101000 2.07886400 H -1.10344100 0.59137600 2.48497900 H -2.75802600 -0.02751000 2.52999400 C -1.24905000 -1.57220000 2.39215500 H -1.13018000 -1.68464400 3.47901100 H -1.99394400 -2.30757600 2.07689500 C 1.24895200 -1.57284300 2.39185800 H 1.99350700 -2.30835000 2.07610000 H 1.13041900 -1.68563400 3.47872100 C 1.77293000 -0.17171200 2.07888400 H 2.75835600 -0.02854600 2.52983300 H 1.10388800 0.59070400 2.48534300 C -3.46194300 -0.67639800 -0.22044100 C -3.47727600 -1.85080800 -0.97151500 H -2.53892800 -2.28859400 -1.29809000 C -4.68415000 -2.45600200 -1.30601400 H -4.68308500 -3.37018300 -1.88929600 C -5.88373400 -1.88915100 -0.89879800 H -6.82502300 -2.35908900 -1.16207400 C -5.87684800 -0.71240900 -0.15637400 H -6.81258200 -0.26177300 0.15655700 C -4.67345400 -0.10894300 0.17950500 H -4.67935000 0.81799500 0.74340800 C -2.13821500 1.85516200 -0.00383700 C -2.06869900 2.35332300 -1.30713500 H -1.82117600 1.68262200 -2.12384000 C -2.31136600 3.69342300 -1.56811000	 **3A1**-singlet H -0.06661000 -2.99956700 1.39195500 N -0.17574500 -1.98900700 1.59746600 Co -0.12433200 -1.24370700 -0.23816200 O 0.51850900 -2.83646400 -1.08614200 C 0.49161700 -4.04703400 -0.67712800 H 0.69531500 -4.78849100 -1.47300600 O 0.28046300 -4.44853800 0.47131300 P -1.85969600 -0.03906200 0.33495400 P 1.68806400 0.04990400 0.04518200 C -2.01639200 -0.41146100 2.15564500 H -1.44527800 0.34688700 2.69714500 H -3.05005800 -0.37090100 2.50526900 C -1.42472700 -1.79825900 2.35931600 H -1.25928400 -1.99562400 3.42657000 H -2.12832200 -2.54996700 1.99405900 C 1.06784100 -1.53800800 2.26954100 H 1.85212800 -2.23959000 1.97477400 H 0.95149100 -1.62499600 3.35767900 C 1.50782800 -0.11951200 1.90730200 H 2.44659300 0.10830600 2.42062300 H 0.76352100 0.60809000 2.23753400 C -3.43202200 -0.68281600 -0.40880800 C -3.40240000 -1.95709700 -0.97630200 H -2.46158500 -2.50053800 -0.99767700 C -4.55558200 -2.51784600 -1.51096300 H -4.51825900 -3.50864400 -1.95009800 C -5.74849000 -1.80694700 -1.48927600 H -6.64890900 -2.24166500 -1.90922100 C -5.78378600 -0.53231600 -0.93518200 H -6.71115200 0.03016100 -0.92483100 C -4.63187700 0.02940600 -0.40011400 H -4.66724300 1.03089600 0.01348800 C -2.09073300 1.78657300 0.22285000 C -1.62161600 2.42654400 -0.92499200 H -1.11539000 1.84833900 -1.69100000 C -1.77919900 3.79573200 -1.08497800 H -1.40520800 4.27901300 -1.98030300

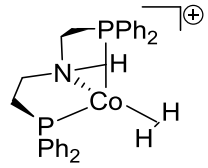
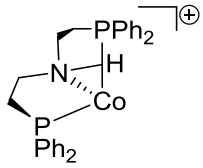
H -2.25792200 4.06200500 -2.58660400 C -2.61179700 4.56387900 -0.52640600 H -2.79482400 5.61334800 -0.72840400 C -2.67198600 4.08310500 0.77399300 H -2.90361200 4.75594000 1.59262900 C -2.44071100 2.73659000 1.03396000 H -2.50209000 2.38185800 2.05614900 C 3.46183800 -0.67652800 -0.22074400 C 4.67340600 -0.10918800 0.17917600 H 4.67938800 0.81769900 0.74316300 C 5.87674300 -0.71268900 -0.15685600 H 6.81252300 -0.26213600 0.15605500 C 5.88350500 -1.88934800 -0.89941000 H 6.82474400 -2.35932800 -1.16278700 C 4.68385600 -2.45606700 -1.30662400 H 4.68270000 -3.37017100 -1.89002900 C 3.47703900 -1.85084500 -0.97197500 H 2.53864300 -2.28852000 -1.29855900 C 2.13836600 1.85505800 -0.00319500 C 2.44065300 2.73618800 1.03491700 H 2.50182900 2.38117700 2.05701700 C 2.67203200 4.08277100 0.77538200 H 2.90350900 4.75535800 1.59426500 C 2.61214800 4.56392400 -0.52488800 H 2.79524400 5.61344600 -0.72654700 C 2.31194600 3.69376700 -1.56691000 H 2.25875600 4.06263500 -2.58531400 C 2.06919500 2.35360000 -1.30637000 H 1.82188100 1.68313700 -2.12333400	C -2.39703400 4.54680500 -0.09237900 H -2.51372300 5.61798700 -0.21376200 C -2.85768500 3.92236100 1.05935300 H -3.33695200 4.50375800 1.83956800 C -2.70824900 2.54921900 1.21543800 H -3.08103500 2.07797700 2.11797400 C 3.41466100 -0.59485100 -0.20656600 C 4.53359800 -0.00572200 0.38739900 H 4.41623800 0.87557000 1.00974100 C 5.80221200 -0.52402800 0.17080100 H 6.66381300 -0.05563100 0.63468300 C 5.96975900 -1.63728400 -0.64718500 H 6.96188000 -2.04090800 -0.81810500 C 4.86467300 -2.22573200 -1.24578100 H 4.98997600 -3.09192200 -1.88649800 C 3.59180100 -1.70669300 -1.02877600 H 2.72410500 -2.16557400 -1.48935900 C 2.01082800 1.86367200 -0.16695700 C 1.89815400 2.82104900 0.84141200 H 1.64529600 2.52853100 1.85324900 C 2.11680500 4.16850100 0.57105800 H 2.02429800 4.89627700 1.37019000 C 2.45744600 4.58098700 -0.70862900 H 2.63235500 5.63071800 -0.91662000 C 2.57223300 3.63560500 -1.72365200 H 2.83926400 3.94563700 -2.72833200 C 2.34139400 2.29565200 -1.45637000 H 2.42626700 1.56737700 -2.25744000
 **3A1'**-triplet N 0.00004900 -1.93724400 1.86329700 Co 0.00016000 -1.21307600 -0.27965000 P -1.82613000 -0.02500200 0.33023000 P 1.82623800 -0.02490600 0.33043400 O 0.00013600 -1.51657400 -2.64163900 C -1.75640200 -0.17221500 2.19126100 H -1.07915400 0.60057300 2.56164800 H -2.73430900 -0.01013500 2.65198100 C -1.24815900 -1.56590200 2.55375800 H -1.12663700 -1.64285300 3.64380300 H -2.00654800 -2.29766400 2.26409100 C 1.24842500 -1.56628700 2.55366200 H 2.00663600 -2.29811200 2.26369200 H 1.12705500 -1.64349100 3.64370700 C 1.75682300 -0.17258600 2.19143700 H 2.73483100 -0.01076300 2.65202700 H 1.07975400 0.60019700 2.56216900 C -3.46516100 -0.82026800 -0.02542500	 **3A2**-triplet N -0.05032000 -1.81452900 1.66431500 Co 0.00335600 -1.04034100 -0.32736500 P -1.89623300 0.09018900 0.17631900 P 1.86249200 0.12999300 0.25929600 O -0.15105200 -4.17956600 0.20537000 C -1.76824200 -0.01124500 2.03433500 H -1.07444700 0.77031300 2.35407900 H -2.73219200 0.16934400 2.51744300 C -1.24852400 -1.39945200 2.41378800 H -1.05902200 -1.43585600 3.49436700 H -2.02990800 -2.13474100 2.20642200 C 1.24152600 -1.59916700 2.33245000 H 1.93431800 -2.34568100 1.93581500 H 1.15757100 -1.78385200 3.41214800 C 1.81346500 -0.20254600 2.09691500 H 2.80648000 -0.12031000 2.54570900 H 1.17354000 0.55584000 2.55516000 C -3.47225000 -0.81498600 -0.16130500

C -3.46321200 -2.13817000 -0.48396800	C -3.39332800 -2.17843400 -0.45198200
H -2.51838700 -2.64182100 -0.66662100	H -2.42781400 -2.67340000 -0.50768300
C -4.66090300 -2.80331400 -0.72183600	C -4.54929300 -2.91864400 -0.66817100
H -4.64471300 -3.82676000 -1.08039300	H -4.47190400 -3.97728200 -0.88853800
C -5.87119200 -2.15478500 -0.51630300	C -5.79193900 -2.30134700 -0.61294700
H -6.80546100 -2.67025500 -0.71038800	H -6.69339500 -2.87704700 -0.79135100
C -5.88156400 -0.83729300 -0.07131900	C -5.87744100 -0.94186200 -0.33481700
H -6.82417100 -0.32232800 0.08049700	H -6.84554000 -0.45428000 -0.29742800
C -4.68656100 -0.17434500 0.17363100	C -4.72491200 -0.20181700 -0.10711000
H -4.70578500 0.85778400 0.50639100	H -4.80184800 0.85951900 0.10111600
C -2.18437600 1.75609700 0.02551100	C -2.32527800 1.84095800 -0.18570100
C -2.05752400 2.20326400 -1.29219900	C -2.27016700 2.25189400 -1.51967300
H -1.74853000 1.50625300 -2.06480100	H -1.97641600 1.54368600 -2.28789800
C -2.31590700 3.52722600 -1.61543300	C -2.58926800 3.55494100 -1.87142200
H -2.21789000 3.85856400 -2.64333200	H -2.54844500 3.85726300 -2.91196100
C -2.68535700 4.42932900 -0.62404800	C -2.94990000 4.47294800 -0.89155000
H -2.87876400 5.46627300 -0.87552600	H -3.19195100 5.49390500 -1.16469000
C -2.80022400 3.99835000 0.69054300	C -2.99557900 4.07817600 0.43837000
H -3.08460500 4.69749500 1.46961400	H -3.27411300 4.78972400 1.20790800
C -2.55594200 2.66801200 1.01358800	C -2.68990700 2.76821600 0.79020900
H -2.66090600 2.34942500 2.04444600	H -2.74168100 2.47725400 1.83274800
C 3.46535700 -0.81976200 -0.02570400	C 3.50929200 -0.54215000 -0.24310300
C 4.68665800 -0.17344800 0.17270800	C 4.70799000 0.08717500 0.10136900
H 4.70571800 0.85877200 0.50519200	H 4.69419700 1.02698000 0.64286200
C 5.88174700 -0.83613200 -0.07253300	C 5.92336500 -0.47418500 -0.26201000
H 6.82427300 -0.32086600 0.07876500	H 6.84865600 0.02425500 0.00608900
C 5.87156300 -2.15375000 -0.51715100	C 5.95528000 -1.67016700 -0.97270400
H 6.80590000 -2.66901700 -0.71144900	H 6.90645200 -2.10775700 -1.25538300
C 4.66137200 -2.80265800 -0.72205300	C 4.76862300 -2.29821300 -1.32276000
H 4.64532200 -3.82620000 -1.08033900	H 4.77891100 -3.22927500 -1.87764800
C 3.46358300 -2.13778100 -0.48391800	C 3.54846900 -1.73375200 -0.96661900
H 2.51882500 -2.64171500 -0.66615200	H 2.63285100 -2.23804900 -1.25776700
C 2.18396900 1.75635800 0.02610600	C 2.11042500 1.95115900 0.12820200
C 2.55605400 2.66798600 1.01425400	C 2.46939900 2.76650100 1.20190100
H 2.66182400 2.34903400 2.04491700	H 2.62042900 2.34261200 2.18788700
C 2.79985000 3.99849300 0.69152500	C 2.64417800 4.13422900 1.02258900
H 3.08463800 4.69740900 1.47065200	H 2.92163100 4.75554100 1.86715300
C 2.68398100 4.42992200 -0.62282800	C 2.46999500 4.70169600 -0.23211600
H 2.87699700 5.46699800 -0.87406900	H 2.60884300 5.76794400 -0.37141600
C 2.31403500 3.52810300 -1.61428900	C 2.11385900 3.89727500 -1.30844500
H 2.21524700 3.85980100 -2.64199800	H 1.97204000 4.33411600 -2.29065300
C 2.05613400 2.20397500 -1.29135900	C 1.92817000 2.53479800 -1.12742900
H 1.74674000 1.50717400 -2.06398900	H 1.63692000 1.91519000 -1.96936500
H -0.00009800 -2.93990600 1.72260700	H -0.13648100 -2.81002600 1.40614100
C 0.00064100 -2.71278000 -2.32129900	C 0.41633500 -3.81211500 -0.83208900
H 0.00081300 -3.48951900 -3.10886000	H 0.16417900 -2.64305100 -1.14087100
O 0.00096900 -3.12290000 -1.11319600	O 1.15977800 -4.32093100 -1.64724600
	 CO_2 dissociated

TS**3(A2/3B)**-triplet

N	-0.00004100	-1.78407800	1.76390100
Co	0.00003600	-1.12163400	-0.32645900
P	-1.81271500	0.12761500	0.23524000
P	1.81287200	0.12747400	0.23529400
O	-0.00022000	-4.50429700	0.45692800
C	-1.76651600	-0.03506400	2.09430300
H	-1.09517000	0.73769700	2.47589900
H	-2.75047100	0.12390600	2.54337700
C	-1.25076600	-1.42567600	2.45467900
H	-1.12917700	-1.50397300	3.54410000
H	-2.00034100	-2.16546500	2.16293000
C	1.25077500	-1.42595500	2.45465800
H	2.00019000	-2.16588900	2.16287000
H	1.12918100	-1.50427100	3.54407800
C	1.76681100	-0.03543100	2.09435200
H	2.75086400	0.12325100	2.54331000
H	1.09571300	0.73745500	2.47613000
C	-3.46022300	-0.61943300	-0.17794900
C	-3.47598500	-1.81648700	-0.89132700
H	-2.53334900	-2.25609100	-1.20656200
C	-4.68220900	-2.43626900	-1.20022700
H	-4.68094700	-3.36695900	-1.75693600
C	-5.88130100	-1.86119000	-0.80275400
H	-6.82263800	-2.34173000	-1.04610700
C	-5.87419000	-0.66172200	-0.09733100
H	-6.80979800	-0.20481500	0.20685000
C	-4.67099800	-0.04358700	0.21207500
H	-4.67707900	0.90132100	0.74550100
C	-2.14280900	1.92107900	-0.04998000
C	-2.09011300	2.37433300	-1.37059400
H	-1.85487300	1.67581700	-2.16734200
C	-2.33467400	3.70510000	-1.67390300
H	-2.29424300	4.03840000	-2.70507100
C	-2.62090200	4.61113800	-0.65885500
H	-2.80574800	5.65329000	-0.89426600
C	-2.66495500	4.17504500	0.65782500
H	-2.88597400	4.87566500	1.45584700
C	-2.43121500	2.83795100	0.96079100
H	-2.48028000	2.51905200	1.99542800
C	3.46038500	-0.61944100	-0.17810900
C	4.67117100	-0.04339200	0.21158100
H	4.67724800	0.90161400	0.74483400
C	5.87437200	-0.66145600	-0.09793400
H	6.80998700	-0.20439000	0.20598500
C	5.88147900	-1.86105700	-0.80313200
H	6.82282200	-2.34154200	-1.04657100
C	4.68237400	-2.43633500	-1.20027700
H	4.68110800	-3.36712400	-1.75681900
C	3.47614000	-1.81662400	-0.89127200
H	2.53348900	-2.25636900	-1.20626700
C	2.14283100	1.92099700	-0.04972700
N	-0.00007900	-1.76340800	1.73305100
Co	-0.00000300	-1.08331900	-0.38138800
P	-1.80056800	0.16551500	0.21892600
P	1.80059800	0.16545500	0.21894900
O	-0.00007600	-4.78557000	0.61237800
C	-1.76317400	-0.01422200	2.07699700
H	-1.09307600	0.75424600	2.46919300
H	-2.74855700	0.14000300	2.52474200
C	-1.25070000	-1.40801100	2.42654800
H	-1.12969400	-1.49613100	3.51555800
H	-2.00251000	-2.14245300	2.12708000
C	1.25063200	-1.40818000	2.42647600
H	2.00234600	-2.14267700	2.12690100
H	1.12969400	-1.49637100	3.51548700
C	1.76322600	-0.01441100	2.07700700
H	2.74863500	0.13970100	2.52473500
H	1.09320600	0.75408900	2.46927500
C	-3.44884200	-0.58253700	-0.20052400
C	-3.45896800	-1.76477900	-0.93834900
H	-2.51161000	-2.18849900	-1.26447500
C	-4.66292300	-2.38511300	-1.25584900
H	-4.65881000	-3.30316400	-1.83354900
C	-5.86454400	-1.82684200	-0.84185400
H	-6.80382100	-2.30806400	-1.09215700
C	-5.86248900	-0.64239900	-0.11140800
H	-6.79992600	-0.19799600	0.20564100
C	-4.66180900	-0.02298300	0.20577300
H	-4.67190200	0.91109400	0.75809000
C	-2.14589000	1.96063500	-0.04448300
C	-2.10358600	2.42753900	-1.36091700
H	-1.87049700	1.73758700	-2.16573200
C	-2.35476500	3.76031600	-1.64961100
H	-2.32198000	4.10375500	-2.67777400
C	-2.63758200	4.65566400	-0.62409400
H	-2.82749600	5.69944600	-0.84810800
C	-2.67135100	4.20636200	0.68843600
H	-2.88954200	4.89833300	1.49481900
C	-2.43085700	2.86715300	0.97666000
H	-2.47197700	2.53833900	2.00855300
C	3.44886900	-0.58255800	-0.20058500
C	4.66184100	-0.02303100	0.20573600
H	4.67194100	0.91099900	0.75813000
C	5.86251900	-0.64241600	-0.11151900
H	6.79995900	-0.19803500	0.20555000
C	5.86456600	-1.82679700	-0.84206600
H	6.80383700	-2.30799000	-1.09242900
C	4.66294000	-2.38503700	-1.25608800
H	4.65882000	-3.30303400	-1.83387300
C	3.45898800	-1.76473500	-0.93851400
H	2.51162400	-2.18842200	-1.26466800
C	2.14590700	1.96059900	-0.04433500
C	2.43099000	2.86702500	0.97685800

C 2.43126800 2.83774200 0.96115400 H 2.48048400 2.51868700 1.99573500 C 2.66484600 4.17490600 0.65837200 H 2.88589600 4.87542200 1.45647800 C 2.62058900 4.61120100 -0.65823400 H 2.80530200 5.65340800 -0.89350600 C 2.33432500 3.70529300 -1.67338900 H 2.29372400 4.03875400 -2.70449800 C 2.08992800 2.37445500 -1.37026200 H 1.85465100 1.67604300 -2.16709000 H -0.00015200 -2.78721100 1.60297700 C -0.00024600 -4.47218700 -0.72305900 H 0.00029300 -2.59357300 -1.09223700 O -0.00038800 -4.85966300 -1.82677700	H 2.47221600 2.53812000 2.00871700 C 2.67146800 4.20625700 0.68872700 H 2.88975100 4.89815500 1.49514800 C 2.63756600 4.65567500 -0.62375900 H 2.82746800 5.69947500 -0.84770100 C 2.35463300 3.76042100 -1.64932600 H 2.32174200 4.10395100 -2.67745500 C 2.10347000 2.42762100 -1.36072300 H 1.87028800 1.73774200 -2.16557400 H -0.00015300 -2.76384600 1.57544600 C -0.00001100 -5.01793900 -0.52802300 H 0.00012500 -2.48461700 -1.23363800 O -0.00000700 -5.34874000 -1.63626200
 TS**3(3B/3A1)**-triplet C -1.69028300 0.00859100 2.01733100 H -0.93549600 0.68720300 2.42168800 H -2.64292900 0.23251700 2.50446200 C -1.30361200 -1.44925200 2.26440200 H -1.15391000 -1.60991700 3.34057300 H -2.13508500 -2.09221200 1.96415400 C 1.16674500 -1.74673000 2.19657300 H 1.82611700 -2.52754100 1.80902400 H 1.05153500 -1.93549100 3.27292600 C 1.82362400 -0.38526000 1.98581700 H 2.81874800 -0.37216900 2.43764500 H 1.23187400 0.40575900 2.45255300 C -3.46019500 -0.32336500 -0.25038100 C -3.57348700 -1.56724400 -0.87145000 H -2.68555000 -2.13795700 -1.12728500 C -4.82626900 -2.09117000 -1.17068200 H -4.89756500 -3.06035700 -1.65122700 C -5.97342500 -1.37326000 -0.86243500 H -6.95014800 -1.77905600 -1.10209000 C -5.86779500 -0.12850900 -0.25035200 H -6.76147500 0.43893200 -0.01410300 C -4.61895600 0.39332800 0.05567900 H -4.54624800 1.37045800 0.52103100 C -1.95090200 2.11497300 -0.01779000 C -1.90217000 2.62838900 -1.31616800 H -1.75315900 1.95511700 -2.15431800 C -2.04575000 3.98844100 -1.54486600 H -2.01126800 4.37038700 -2.55918200 C -2.22414900 4.86050700 -0.47671200 H -2.33001300 5.92488000 -0.65421200 C -2.26314000 4.36246700 0.81796300 H -2.40073900 5.03650000 1.65640600	

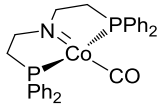
C -2.13140500 2.99714600 1.04701100 H -2.17493600 2.62838900 2.06502200 C 3.50631600 -0.82005700 -0.32312900 C 4.74130400 -0.23687800 -0.03196700 H 4.78373100 0.73428600 0.44888900 C 5.92156500 -0.88426600 -0.36982600 H 6.87482700 -0.41914200 -0.14283800 C 5.88311000 -2.12242900 -1.00217700 H 6.80619200 -2.62661000 -1.26638500 C 4.65967000 -2.70677000 -1.29934700 H 4.62084200 -3.66894300 -1.79800500 C 3.47664600 -2.05615500 -0.96717100 H 2.52013000 -2.50553000 -1.21275500 C 2.30527800 1.76025900 0.04771700 C 2.69106400 2.54078000 1.13775900 H 2.77020500 2.10298200 2.12603800 C 2.98636200 3.88962300 0.97288100 H 3.28297700 4.48328000 1.83080700 C 2.90796900 4.47305800 -0.28405000 H 3.14085800 5.52425900 -0.41212200 C 2.52585600 3.70379000 -1.37711600 H 2.45821400 4.15333300 -2.36160800 C 2.21999600 2.36131600 -1.21035900 H 1.90968100 1.77015900 -2.06602400 Co -0.04893900 -1.04028200 -0.47775100 N -0.12313700 -1.89478400 1.50394800 H -0.25056500 -2.90484600 1.30689700 P -1.76933100 0.29351400 0.17845500 P 1.89503700 -0.03473300 0.15453000 H 0.33500900 -2.31459800 -1.53343500 H -0.24811300 -3.00317900 -1.29176800 O -1.03158900 -4.11452900 -1.27300500 C -1.00191900 -4.85557700 -0.23754800 H -1.43935200 -5.86283800 -0.39027000 O -0.55703000 -4.57836100 0.88284600	
 **3BH**$^{+}$-triplet C -1.70124500 -0.54452800 1.96018900 H -0.98355100 0.17278100 2.36202500 H -2.64960500 -0.39196000 2.48042000 C -1.23526400 -1.97882200 2.18256900 H -1.07240700 -2.15854800 3.25135800 H -2.02707100 -2.65891900 1.85912900 C 1.27308100 -2.09473700 2.13214300 H 2.00579100 -2.79560800 1.72399900 H 1.15862900 -2.33101600 3.19645800 C 1.80148100 -0.67568000 1.96754100 H 2.78177700 -0.60218000 2.44330700	 **3BH$_2$**$^{+}$-triplet C -1.79780000 -0.51407800 1.96215300 H -1.12304000 0.23928000 2.37428300 H -2.75510800 -0.42058700 2.48056100 C -1.25652000 -1.92427500 2.17423900 H -1.10905600 -2.10726300 3.24499700 H -2.00443100 -2.64112200 1.82634200 C 1.25705400 -1.92461900 2.17381500 H 2.00481700 -2.64129800 1.82524000 H 1.11010400 -2.10808900 3.24456400 C 1.79818100 -0.51431700 1.96205700 H 2.75554000 -0.42087000 2.48037100

H 1.14522900 0.05046200 2.45084900	H 1.12339600 0.23886900 2.37445800
C -3.48665000 -1.00683500 -0.26827800	C -3.50693100 -1.08404700 -0.32236700
C -3.50683000 -2.18084100 -1.02077600	C -3.40111000 -2.20814500 -1.14167100
H -2.57773000 -2.59477200 -1.40212600	H -2.43089000 -2.50683000 -1.52929200
C -4.70915000 -2.81679200 -1.30711400	C -4.53070400 -2.94067100 -1.48582100
H -4.71358100 -3.72678900 -1.89609800	H -4.43818600 -3.81024600 -2.12628200
C -5.90220900 -2.27678700 -0.84740100	C -5.77698400 -2.54721600 -1.01810000
H -6.84217700 -2.76637400 -1.07449600	H -6.66107300 -3.11221500 -1.29002100
C -5.89250900 -1.10080100 -0.10405700	C -5.89326600 -1.42123000 -0.20944300
H -6.82498200 -0.67292100 0.24596500	H -6.86794400 -1.10762800 0.14648100
C -4.69256200 -0.46815500 0.18554400	C -4.76554800 -0.69168500 0.13737600
H -4.69822500 0.45816700 0.74991900	H -4.87092300 0.19567700 0.75215100
C -2.16497900 1.56539300 -0.04165600	C -2.38885300 1.59448300 -0.00645400
C -2.22588400 2.08114900 -1.33863800	C -2.27651500 2.18228200 -1.26813400
H -2.08263900 1.42541900 -2.19142500	H -1.92958100 1.59413600 -2.11152300
C -2.47733400 3.42850100 -1.54714800	C -2.60729500 3.51651800 -1.45174300
H -2.53091100 3.81623100 -2.55799200	H -2.52280600 3.96214200 -2.43617700
C -2.65792600 4.27954600 -0.46270500	C -3.03845200 4.28158600 -0.37433100
H -2.85195600 5.33337700 -0.62551300	H -3.29184400 5.32572200 -0.51681600
C -2.59070300 3.77654600 0.82896400	C -3.14214200 3.70728400 0.88542600
H -2.73280600 4.43573800 1.67771300	H -3.47643700 4.30124000 1.72836000
C -2.34915400 2.42416800 1.04152200	C -2.82291100 2.36760900 1.07083800
H -2.31299300 2.05260300 2.05866200	H -2.91680700 1.93796100 2.06134500
C 3.51032800 -0.97776700 -0.35175700	C 3.50701500 -1.08385500 -0.32269700
C 4.72785300 -0.39214900 0.00031700	C 4.76564600 -0.69172500 0.13720000
H 4.74528200 0.54611100 0.54370700	H 4.87108500 0.19544200 0.75224500
C 5.92354600 -0.99384400 -0.36464400	C 5.89332400 -1.42124700 -0.20980400
H 6.86438800 -0.52840400 -0.09391100	H 6.86801100 -1.10782000 0.14624900
C 5.91789500 -2.18597500 -1.08110400	C 5.77698900 -2.54697800 -1.01880600
H 6.85420300 -2.65126000 -1.36678200	H 6.66104400 -3.11196300 -1.29086500
C 4.71241400 -2.77309300 -1.43998800	C 4.53069500 -2.94019600 -1.48669100
H 4.70315900 -3.69587400 -2.00868900	H 4.43813500 -3.80956700 -2.12742300
C 3.51456500 -2.16723500 -1.08060400	C 3.40114500 -2.20769200 -1.14235500
H 2.57470400 -2.61802000 -1.38670200	H 2.43091600 -2.50617600 -1.53010900
C 2.14422600 1.55512900 0.08877500	C 2.38873100 1.59465200 -0.00633800
C 2.56156400 2.30863200 1.18693700	C 2.82387600 2.36735100 1.07083800
H 2.73588000 1.83971600 2.14839300	H 2.91870900 1.93729800 2.06108100
C 2.76515300 3.67721700 1.05964000	C 3.14293300 3.70708600 0.88564300
H 3.08864600 4.25421400 1.91847400	H 3.47806500 4.30071900 1.72847300
C 2.56225800 4.30201300 -0.16362400	C 3.03798700 4.28188700 -0.37379200
H 2.72623700 5.36893000 -0.26146100	H 3.29125300 5.32607600 -0.51611200
C 2.14713200 3.55775000 -1.26132900	C 2.60572400 3.51726500 -1.45106600
H 1.98494000 4.04221700 -2.21721600	H 2.52023100 3.96328300 -2.43523400
C 1.93306400 2.19320500 -1.13514200	C 2.27510300 2.18295200 -1.26765800
H 1.59663000 1.62108400 -1.99320600	H 1.92727200 1.59515700 -2.11091800
H -0.38606200 -1.41152100 -2.19663800	Co 0.00003800 -1.16055200 -0.44514900
Co 0.00734900 -1.41873900 -0.52069900	N 0.00011700 -2.21669800 1.43056000
H 0.42127200 -1.43290200 -2.19298000	P -1.97197000 -0.18222100 0.13726800
N -0.00953000 -2.34912100 1.41860800	P 1.97207300 -0.18210500 0.13718000
P -1.86420400 -0.23346900 0.13263200	H -0.00005100 -3.21849100 1.26806400
P 1.89174700 -0.25759500 0.15292300	
H -0.05789200 -3.35546000 1.29109400	
SMD-H_2O	

CO-B3PW91-SCRF

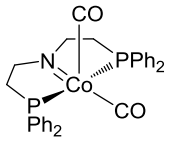
C 0.00000000 0.00000000 -0.64356100

O 0.00000000 0.00000000 0.48267100



10-singlet-SCRF

C	-2.42214800	-0.08271900	2.38772700
H	-3.35071700	0.42385400	2.65675400
H	-2.45637400	-1.10936200	2.75815000
C	-1.18378800	0.61363000	2.92498000
H	-1.29732000	1.70528900	2.80988500
H	-1.10954400	0.43472600	4.00806100
C	1.20267400	0.60958800	2.93078200
H	1.13778000	0.39734400	4.00881400
H	1.29739800	1.70568300	2.84827100
C	2.44639900	-0.04912500	2.36302300
H	2.52067700	-1.08498300	2.70465300
H	3.37161500	0.46256400	2.63240500
C	-3.36387100	-1.36507100	-0.12748200
C	-3.59134700	-1.35920900	-1.50713800
H	-3.09878100	-0.62502600	-2.13604500
C	-4.45058300	-2.28435300	-2.08402800
H	-4.61949200	-2.26570800	-3.15513000
C	-5.09133600	-3.23163300	-1.29169500
H	-5.76313600	-3.95401500	-1.74192100
C	-4.86744300	-3.24611600	0.07915000
H	-5.36478400	-3.97949000	0.70449800
C	-4.00652200	-2.32070100	0.66042800
H	-3.84928700	-2.35151100	1.73182800
C	-2.77756400	1.45607000	-0.07194700
C	-1.90365200	2.30610700	-0.74673800
H	-0.87454700	1.99601700	-0.90049700
C	-2.34557600	3.53867600	-1.21753000
H	-1.65856400	4.19292000	-1.74297900
C	-3.66339300	3.92801000	-1.01467200
H	-4.00937800	4.88824100	-1.38129500
C	-4.54136700	3.08328700	-0.34049600
H	-5.57096500	3.38458600	-0.18095200
C	-4.10230500	1.85260200	0.12846600
H	-4.79497700	1.19912000	0.64850900
C	3.36874300	-1.42152600	-0.05723800
C	4.70083200	-1.10342300	-0.32730200
H	5.04857900	-0.08122100	-0.22719700
C	5.58913200	-2.09385400	-0.72832800
H	6.62194900	-1.83718500	-0.93726500
C	5.15585900	-3.40869900	-0.86355800
H	5.85003300	-4.17962700	-1.17949700
C	3.83052400	-3.73159400	-0.59602700
H	3.48635900	-4.75438700	-0.70348000
C	2.93942800	-2.74187800	-0.19765000
H	1.90346600	-2.99489800	0.00319500



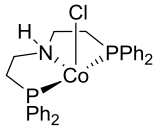
10a-singlet-SCRF

Co-4Ph-N-2CO-c4v-singlet-B3PW91-SCRF

C	-2.46559800	-0.31366600	2.30251000
H	-3.37881100	0.21179400	2.58781300
H	-2.58774300	-1.37769700	2.51530900
C	-1.22924400	0.24126500	2.97794200
H	-1.21949700	1.34052500	2.83181500
H	-1.31273200	0.09206600	4.06715400
C	1.11110800	0.40214800	2.93740400
H	1.21197700	0.31191700	4.03207900
H	0.97043500	1.48389700	2.74347300
C	2.40135000	-0.04415200	2.28393200
H	2.64192500	-1.07522300	2.55616900
H	3.25588300	0.58564100	2.53867800
C	-3.35113000	-1.10686300	-0.41812900
C	-3.94938900	-0.60705400	-1.57579600
H	-3.72482400	0.39725300	-1.91576400
C	-4.84288200	-1.38829300	-2.30047300
H	-5.30136500	-0.98534200	-3.19695100
C	-5.14787900	-2.67653700	-1.87883200
H	-5.84754900	-3.28365100	-2.44253600
C	-4.54832700	-3.18485200	-0.73110800
H	-4.77790100	-4.19067400	-0.39669200
C	-3.64920000	-2.41021600	-0.00982100
H	-3.17982600	-2.82888800	0.87344900
C	-2.50857400	1.61262100	0.10846100
C	-1.58371300	2.40595000	-0.56625100
H	-0.62374200	1.98637700	-0.84792900
C	-1.88259900	3.72994700	-0.87240700
H	-1.15576600	4.33827200	-1.39915200
C	-3.10661700	4.27019500	-0.49979500
H	-3.33920200	5.30317700	-0.73426400
C	-4.03497800	3.48392500	0.17707300
H	-4.99172100	3.90240500	0.46993800
C	-3.74012500	2.16119600	0.47790200
H	-4.47408000	1.55569800	0.99880200
C	3.41616400	-1.08729500	-0.25120300
C	4.73489500	-0.62584700	-0.20711600
H	4.95810000	0.34797500	0.21548300
C	5.76886700	-1.40780100	-0.70420700
H	6.78876400	-1.04139300	-0.66174900
C	5.49744300	-2.65592200	-1.25714900
H	6.30551800	-3.26392300	-1.64885700
C	4.18894700	-3.11881100	-1.30750700
H	3.97019400	-4.08896300	-1.74011100

C 2.76383400 1.41118800 -0.20466400 C 3.43728700 2.39376200 0.52119500 H 3.65894400 2.25026300 1.57160600 C 3.83906300 3.57368000 -0.09845500 H 4.35897400 4.33070900 0.47848900 C 3.58069800 3.77971400 -1.44713300 H 3.89778400 4.69820500 -1.92858400 C 2.91237200 2.80221000 -2.17879700 H 2.70598300 2.95609800 -3.23229800 C 2.49734600 1.63153700 -1.56007600 H 1.96663600 0.88160200 -2.13723700 C -0.00302100 -1.05920600 -1.13102100 Co 0.00534200 -0.43224600 0.44742600 N 0.01004800 0.11885300 2.24975100 O -0.00935900 -1.48757400 -2.21888300 P -2.15900400 -0.16016000 0.56794600 P 2.16902500 -0.16225800 0.54664700	C 3.15234500 -2.33871500 -0.80446200 H 2.13409800 -2.70805000 -0.84449600 C 2.44097300 1.60016700 -0.18696800 C 2.76246100 2.68424900 0.62928100 H 2.81672300 2.56852700 1.70501500 C 3.02177700 3.93256800 0.07081300 H 3.27202600 4.76609400 0.71813200 C 2.96562000 4.11075700 -1.30522800 H 3.17088600 5.08355800 -1.73816300 C 2.64499900 3.03341800 -2.12634400 H 2.59952000 3.16314700 -3.20215100 C 2.37784100 1.78999800 -1.57139500 H 2.12646100 0.95864200 -2.22213400 Co -0.01306000 -0.86292200 0.47263100 N -0.01800400 -0.38374900 2.47083400 P -2.08862200 -0.13682100 0.50698300 P 2.05136500 -0.07807300 0.47519500 C -0.02959000 -2.59840000 0.92655100 C -0.06267200 -0.96885600 -1.25955100 O -0.05253300 -3.69194500 1.28519400 O -0.12045000 -1.04497900 -2.41027900

Table S9. The Cartesian Coordinates (xyz) for All Optimized Structures at M06L/TZVP-SCRF(SMD,H_2O) level

HCOOH C 0.00000000 0.41844900 0.00000000 H -0.36180200 1.45419800 0.00000000 O 1.16407800 0.09788500 0.00000000 O -1.03278200 -0.42644200 0.00000000 H -0.68856000 -1.33643400 0.00000000	**CO_2** C 0.00000000 -0.00012300 0.00000000 O -1.12776200 -0.27129700 0.00000000 O 1.12776200 0.27138900 0.00000000
H_2 H 0.00000000 0.00000000 0.37233000 H 0.00000000 0.00000000 -0.37233000	**CO** C 0.00000000 0.00000000 -0.64537600 O 0.00000000 0.00000000 0.48403200
H^+ H 0.00000000 0.00000000 0.00000000	**$HCOO^-$** C 0.00000000 0.33728700 0.00000000 H -0.00016700 1.45600400 0.00000000 O 1.12624400 -0.21746600 0.00000000 O -1.12622300 -0.21749900 0.00000000
H_2O O 0.00000000 0.00000000 0.11955100 H 0.00000000 0.75429200 -0.47820200 H 0.00000000 -0.75429200 -0.47820200	 **3**-triplet-M06L-SCRF C -1.82170400 -0.57512400 2.11453700 H -1.21797000 0.15665000 2.65220900 H -2.83816600 -0.49836100 2.50301900 C -1.27449500 -1.97177100 2.32835700 H -1.23972800 -2.20078400 3.40043300 H -1.93701000 -2.70583800 1.86196200

	C 1.17187700 -1.52867800 2.47148800 H 2.04549700 -2.16988800 2.33602300 H 0.94511600 -1.52181200 3.54364100 C 1.51285800 -0.12420600 2.00379400 H 2.42947700 0.22130400 2.48732800 H 0.72214100 0.58269000 2.26234500 C -3.50256700 -0.55516500 -0.21581300 C -3.75045200 -1.76305200 -0.86609600 H -2.91650400 -2.42283200 -1.09196200 C -5.04460000 -2.11558300 -1.22658000 H -5.22658200 -3.05712800 -1.73062400 C -6.10069000 -1.25897200 -0.95037300 H -7.10934800 -1.52956500 -1.23739100 C -5.86132000 -0.05051000 -0.30731500 H -6.68366700 0.62084800 -0.09129900 C -4.57062500 0.29885800 0.06063500 H -4.39243300 1.24215000 0.56622500 C -1.72381000 1.65306700 0.22451900 C -1.41428300 2.23761600 -1.00693000 H -1.21405200 1.60182100 -1.86397500 C -1.34327400 3.61501100 -1.14011800 H -1.09940500 4.05204800 -2.10098000 C -1.56641000 4.43207400 -0.03808400 H -1.49802700 5.50842400 -0.13728700 C -1.86587000 3.86346100 1.19136900 H -2.04118900 4.49541100 2.05352400 C -1.95043700 2.48263800 1.32268700 H -2.20131800 2.05766000 2.28706800 C 3.36128100 -0.83212700 -0.06904000 C 4.52586700 -0.13690300 0.25794500 H 4.46139600 0.88048200 0.63001800 C 5.76604900 -0.73908200 0.10825200 H 6.66576200 -0.19136700 0.36131000 C 5.85577200 -2.04338600 -0.36361500 H 6.82555300 -2.51119800 -0.48025600 C 4.70247000 -2.74395400 -0.68718200 H 4.76899800 -3.75995800 -1.05672600 C 3.46122300 -2.13813900 -0.54447100 H 2.55171500 -2.67665800 -0.80236700 C 1.94743000 1.65203600 -0.25364700 C 1.83479300 2.68530700 0.67664200 H 1.61595800 2.46952600 1.71496300 C 2.00600700 4.00732900 0.28411500 H 1.91196700 4.79866600 1.01816400 C 2.29398100 4.31495000 -1.03725200 H 2.42584000 5.34623700 -1.34014800 C 2.40834700 3.29221100 -1.97176700 H 2.63152100 3.52352100 -3.00613300 C 2.23064900 1.97411400 -1.58434600 H 2.31271000 1.18166500 -2.32153600 Cl -0.38840500 -3.46001600 -1.57468400 Co -0.04066700 -1.46509600 -0.39799900 N 0.05768800 -2.14971200 1.71295400

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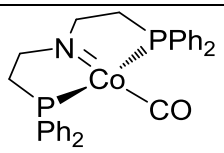
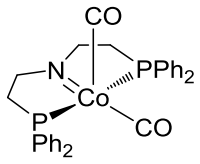
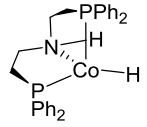
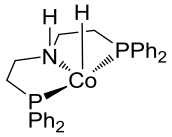
 **10**-singlet-M06L-SCRF C -2.42778200 -0.20675200 2.37502600 H -3.35397200 0.32375600 2.60067000 H -2.50449800 -1.22521700 2.76070200 C -1.20067300 0.48122800 2.92955200 H -1.28029700 1.56843500 2.74930700 H -1.16282900 0.37064300 4.02267400 C 1.16404000 0.60191600 2.93011100 H 1.13908300 0.48217500 4.02303700 H 1.12150600 1.69175400 2.75744600 C 2.45990200 0.05366700 2.37455000 H 2.67653000 -0.93312600 2.78894500 H 3.32159000 0.69370400 2.57001500 C -3.40325600 -1.35346400 -0.16967500 C -3.44147600 -1.47124500 -1.56139900 H -2.71442300 -0.94014200 -2.16705900 C -4.40469500 -2.25700600 -2.17264500 H -4.42635700 -2.33907900 -3.25223300 C -5.33935700 -2.93793600 -1.40215400 H -6.09179500 -3.55278000 -1.87992100 C -5.30713500 -2.82632900 -0.02003600 H -6.03642200 -3.35136900 0.58441500 C -4.34432900 -2.03817900 0.59677800 H -4.33599600 -1.95609800 1.67661700 C -2.48284900 1.36413000 -0.05484400 C -1.45370100 2.17482100 -0.52810000 H -0.44085000 1.77960100 -0.55130100 C -1.72076400 3.46525000 -0.96569300 H -0.91271800 4.08607700 -1.33401800 C -3.01942800 3.95250700 -0.93296300 H -3.23081300 4.95807800 -1.27503700 C -4.05159000 3.14869500 -0.46294700 H -5.06573500 3.52808300 -0.43786400 C -3.78666200 1.86001900 -0.02556200 H -4.59605400 1.23585100 0.33888200 C 3.51891000 -1.26078300 -0.03580900 C 4.78685900 -0.72470400 -0.26290800 H 4.96423000 0.33271000 -0.09814100 C 5.81980800 -1.53963800 -0.69943700 H 6.80191200 -1.11769100 -0.87348800 C 5.59505800 -2.89360900 -0.91496700 H 6.40233100 -3.52758000 -1.26004500 C 4.33610800 -3.43280700 -0.69117700 H 4.15819700 -4.48727700 -0.86172400 C 3.29994300 -2.61926100 -0.25438800	 **10a**-singlet-M06L-SCRF C -2.45646500 -0.35757500 2.37116000 H -3.41806900 0.09303500 2.62108800 H -2.47964000 -1.41470200 2.64111600 C -1.27857000 0.34664500 3.00015000 H -1.37121900 1.43326500 2.79289300 H -1.33021500 0.26136500 4.09667700 C 1.02199400 0.73439200 2.88476100 H 1.08520800 0.80544800 3.98270600 H 0.79821800 1.76718900 2.54758900 C 2.36091800 0.30503400 2.33265400 H 2.68488500 -0.63771400 2.77790100 H 3.15021500 1.04161400 2.48891700 C -3.30809400 -1.21258000 -0.34842300 C -3.78558200 -0.77504400 -1.58428500 H -3.48230700 0.19146300 -1.97044500 C -4.64999100 -1.57033100 -2.32182700 H -5.01755700 -1.21903800 -3.27791700 C -5.04243400 -2.80996900 -1.83680700 H -5.72056700 -3.42815600 -2.41157300 C -4.55978600 -3.25789900 -0.61417600 H -4.85872900 -4.22665200 -0.23369600 C -3.68948900 -2.47002700 0.12340600 H -3.30616700 -2.83711700 1.06856000 C -2.45601600 1.51560400 0.16294400 C -1.43075800 2.36429100 -0.24704700 H -0.42188500 1.97314300 -0.34431600 C -1.69276300 3.70075000 -0.51735500 H -0.88780500 4.35264000 -0.83446600 C -2.98137100 4.19574900 -0.38166800 H -3.18752600 5.23744900 -0.59394500 C -4.00929800 3.35508300 0.02898100 H -5.01545600 3.74072300 0.13699800 C -3.75003200 2.02139400 0.30200500 H -4.55561900 1.36947500 0.62193500 C 3.46485700 -1.07525800 -0.03147300 C 4.78040700 -0.73387800 0.28716100 H 4.98274800 0.14935400 0.88304200 C 5.83065500 -1.52130400 -0.15739800 H 6.84867400 -1.25550000 0.09906900 C 5.57844900 -2.64620400 -0.93340600 H 6.40103000 -3.25815200 -1.28202200 C 4.27393000 -2.98397500 -1.26212600 H 4.07475700 -3.85789200 -1.86974400

H 2.31251100 -3.03545700 -0.08304500 C 2.40474400 1.39211400 -0.24635800 C 2.71806600 2.56274300 0.44277800 H 2.91311300 2.53696100 1.50749500 C 2.78667200 3.77625900 -0.23217500 H 3.02685400 4.67932800 0.31542300 C 2.55540300 3.83157000 -1.59770700 H 2.60863600 4.77835500 -2.12043600 C 2.25601500 2.66581300 -2.29529500 H 2.07871100 2.70170900 -3.36311600 C 2.17355700 1.45779500 -1.62471700 H 1.91940800 0.55449400 -2.17042000 C 0.09027500 -1.48687900 -0.98679800 Co 0.04406900 -0.73354400 0.54174300 N 0.01272800 -0.06385200 2.32790300 O 0.13610200 -1.98684100 -2.05026900 P -2.09233000 -0.32262800 0.57545900 P 2.14902300 -0.21924700 0.58759000	C 3.21854700 -2.20318500 -0.80959700 H 2.19756600 -2.46911400 -1.06166100 C 2.36994500 1.54440200 -0.33214600 C 2.36508700 2.77610700 0.32203800 H 2.27157100 2.82461100 1.39980600 C 2.48078000 3.95516900 -0.40198100 H 2.47605200 4.90443800 0.11951400 C 2.60031800 3.92001000 -1.78344000 H 2.68723700 4.84117300 -2.34581500 C 2.61602400 2.69650100 -2.44213300 H 2.71989100 2.66021000 -3.51952400 C 2.49888500 1.51774300 -1.72355200 H 2.51300000 0.56741100 -2.24671700 Co 0.01540900 -0.82876200 0.49636100 N -0.02238600 -0.20006400 2.51077200 P -2.08164100 -0.23136500 0.57997800 P 2.07371300 -0.03622000 0.55270500 C -0.01489500 -2.63473900 0.66586600 C -0.04609700 -0.63981400 -1.22160000 O -0.10350100 -3.77196200 0.44490900 O -0.12570400 -0.49825400 -2.37459600
 **3B**-triplet-M06L-SCRF C -1.83765100 -0.95482500 1.95048700 H -1.24067800 -0.26656700 2.54996200 H -2.85668800 -0.91716900 2.33847900 C -1.28605200 -2.36193700 2.05103600 H -1.23384900 -2.67328100 3.10100100 H -1.95497500 -3.05863200 1.53998800 C 1.16658400 -1.95837900 2.21815900 H 2.03676200 -2.58261900 2.00399500 H 0.94708800 -2.07261500 3.28557800 C 1.50919600 -0.51247700 1.90635700 H 2.42890500 -0.22682100 2.42220300 H 0.72197900 0.16305900 2.24666800 C -3.46731400 -0.82487600 -0.41058100 C -3.63000900 -1.93759200 -1.23308700 H -2.74860000 -2.49508400 -1.54064800 C -4.89382100 -2.31981200 -1.66305300 H -5.00833600 -3.18780800 -2.30093600 C -6.00628600 -1.58231600 -1.28338700 H -6.99250100 -1.87303700 -1.62375900 C -5.85332400 -0.46698100 -0.46803500 H -6.72082100 0.11059200 -0.17218200 C -4.59177700 -0.09189100 -0.03078400 H -4.47973800 0.77658000 0.61029600 C -1.78936800 1.41349000 0.24779000 C -1.48845200 2.10928400 -0.92711800	 ***mer*-3B**-triplet-M06L-SCRF P -2.21660700 -0.47726300 0.27146200 P 2.11826400 -0.45556500 0.29320800 C -2.50545600 -0.56058700 2.10737300 C 2.37088700 -0.43768800 2.13073600 H -2.61284300 -1.61153000 2.38467300 H 2.51720100 -1.47972200 2.42608500 H -3.42747400 -0.04628300 2.38482900 H 3.27137800 0.10660500 2.42115600 C -1.30828600 0.04793000 2.80386700 C 1.13492800 0.12907700 2.79753200 H -1.41792100 -0.02300800 3.89242500 H 1.23663900 0.09615900 3.88908500 H -1.23673700 1.11293500 2.56256800 H 1.00247900 1.18026000 2.52345700 N -0.06509100 -0.58671700 2.34166700 H -0.02649500 -2.78855700 0.18433700 H -0.03273900 -1.52952000 2.72127700 Co -0.03478600 -1.07302400 0.11296300 C -3.76207800 -1.19084900 -0.41633700 C -4.37156600 -0.63325000 -1.54215900 C -4.28632400 -2.37311800 0.11252600 C -5.48791900 -1.22923200 -2.10988800 H -3.97399900 0.27767400 -1.97521100 C -5.40482500 -2.96493500 -0.45525300 H -3.81994500 -2.83811700 0.97347300

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C -1.45681000 3.49453600 -0.94233400	H -5.95171900 -0.77910200 -2.97917000
H -1.21719200 4.01840400 -1.85990500	H -5.80375500 -3.87630300 -0.02676300
C -1.71559400 4.20878500 0.22171900	H -6.88414600 -2.85828500 -2.00877400
H -1.67893600 5.29123400 0.21458500	C -2.39207300 1.33022300 -0.04079300
C -2.01006900 3.52957000 1.39501200	C -1.28457900 2.00305700 -0.55560800
H -2.21357300 4.08090200 2.30506800	C -3.53496800 2.05968100 0.28873500
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H -2.29813600 1.62840400 2.33108900	H -0.39452600 1.43183000 -0.80998900
C 3.34879600 -0.95972100 -0.24921200	C -3.56506700 3.43394700 0.10278600
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C 2.30971800 3.31235400 -1.70160800	C 3.39991100 -2.65561000 -0.86210300
H 2.53331300 3.65011400 -2.70623800	C 4.88441700 -0.89650400 -0.16527800
C 2.16974400 1.95810900 -1.44604500	C 4.48788600 -3.40512400 -1.28950800
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Co -0.03226000 -1.64098300 -0.62974500	C 5.97055500 -1.64490300 -0.59278300
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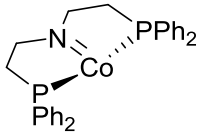	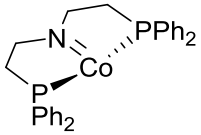
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H -2.53960800 -1.76031600 2.39254000	H -2.57239500 -1.85300800 2.25703400
C -1.19783700 -0.13403600 2.84188600	C -1.23423600 -0.24254100 2.75864000
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H -1.21681000 -0.34542300 3.92054000	H -1.26989500 -0.52183700 3.82733900
C 1.13960900 0.10455200 2.82387600	C 1.12605800 -0.15416600 2.77362000
H 1.18587700 -0.05950100 3.91037500	H 1.16906100 -0.43286100 3.84245100
H 0.95986400 1.18961900 2.70296100	H 1.08910600 0.95546600 2.77655400
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C	-3.42157300	-1.38354700	-0.50625900	C	-3.76164800	-1.25822500	-0.47940900
C	-3.88487900	-0.90742300	-1.73541800	C	-4.33349200	-0.67899900	-1.61494500
H	-3.47673600	0.00979100	-2.14578900	H	-3.90218400	0.22360600	-2.03418300
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H	-5.22131700	-1.20209200	-3.38247000	H	-5.88872400	-0.77200000	-3.08320100
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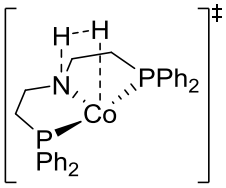
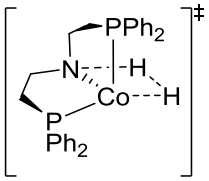
H	-6.17945600	-3.29231700	-2.46213700	H	-6.89627200	-2.83151900	-2.14559900
C	-4.94732400	-3.25004200	-0.70286500	C	-5.45349900	-2.98539800	-0.56184000
H	-5.36041800	-4.16402900	-0.29366200	H	-5.88729300	-3.88633300	-0.14511100
C	-3.95831900	-2.57201600	-0.00570400	C	-4.33234300	-2.42562900	0.03338100
H	-3.60509200	-2.97304100	0.93711300	H	-3.90355000	-2.90360700	0.90615400
C	-2.42164800	1.24385500	0.07191500	C	-2.41693100	1.24096300	0.01943500
C	-1.40267700	2.10947500	-0.31618300	C	-1.37338500	1.94791500	-0.57681200
H	-0.41062000	1.70051900	-0.49157000	H	-0.50601500	1.40059800	-0.94038800
C	-1.64723600	3.46801500	-0.47248900	C	-1.43722800	3.32828400	-0.70820800
H	-0.84281200	4.12848600	-0.77452800	H	-0.61871200	3.86510700	-1.17297100
C	-2.91892300	3.97309100	-0.24295200	C	-2.55020200	4.01501200	-0.24107500
H	-3.11437900	5.03144800	-0.36482100	H	-2.60356900	5.09227000	-0.33932900
C	-3.94395300	3.11738600	0.14476700	C	-3.59688700	3.31956500	0.35181100
H	-4.93753800	3.50955900	0.32557200	H	-4.46541200	3.85503900	0.71556800
C	-3.69702600	1.76207300	0.30348900	C	-3.53123800	1.93951800	0.48383500
H	-4.50201100	1.10135700	0.60868100	H	-4.35102000	1.40226800	0.94899700
C	3.59782900	-1.21607200	-0.30581200	C	3.71925000	-1.32447500	-0.34531400
C	4.65691600	-0.57004600	-0.94217300	C	4.77873500	-0.64298500	-0.94282500
H	4.63446100	0.50514200	-1.07655700	H	4.73667900	0.43421500	-1.05541600
C	5.74884700	-1.29444100	-1.40169000	C	5.89662500	-1.33435900	-1.39161400
H	6.56483800	-0.77967700	-1.89443800	H	6.71233400	-0.79123100	-1.85342300
C	5.79932900	-2.67045200	-1.22875500	C	5.97369000	-2.71186300	-1.24602400
H	6.65161400	-3.23296600	-1.58920400	H	6.84680400	-3.24843400	-1.59580100
C	4.74997800	-3.32365100	-0.59447000	C	4.92286000	-3.40015900	-0.65150200
H	4.78111500	-4.39771000	-0.45763300	H	4.97424500	-4.47589300	-0.53532000
C	3.65551900	-2.60235000	-0.14426300	C	3.80277500	-2.71329300	-0.21192000
H	2.82884300	-3.11543100	0.33791800	H	2.97965900	-3.25854900	0.23916700
C	2.31064800	1.36483000	-0.26951500	C	2.45129700	1.26977900	-0.16039700
C	2.53333200	2.46599000	0.55812500	C	2.83086900	2.23960100	0.76680200
H	2.70941500	2.32771400	1.61766900	H	3.04268800	1.96272900	1.79216200
C	2.52932800	3.75503100	0.03565300	C	2.94330500	3.57163400	0.38657200
H	2.69413000	4.59890000	0.69483100	H	3.23375500	4.31459400	1.11934600
C	2.32426600	3.96223500	-1.31940400	C	2.69278300	3.94964000	-0.92419900
H	2.32284500	4.96690600	-1.72345400	H	2.78343400	4.98808200	-1.21770000
C	2.11694600	2.87031300	-2.15770100	C	2.32066000	2.99021700	-1.85882200
H	1.96058100	3.02191100	-3.21888200	H	2.12219300	3.27744300	-2.88419000
C	2.09847700	1.58886500	-1.63546200	C	2.19182200	1.66486800	-1.47708400
H	1.90675900	0.74469000	-2.29085200	H	1.88283400	0.92139000	-2.20537900
Co	0.06755300	-1.06333000	0.42036900	Co	0.00200300	-0.92667300	0.13343200
N	0.03413400	-0.66738100	2.25521300	N	-0.03041200	-0.72161900	2.11774400
P	-2.03095100	-0.54599200	0.35623100	P	-2.21364100	-0.57328600	0.24354700
P	2.11148400	-0.35115900	0.36288500	P	2.19097700	-0.49600400	0.26829700



***mer*-TS(3B/3A1)**-triplet-M06L-SCRF

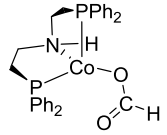
P	-2.16204900	-0.45417300	0.24846300
P	2.21499000	-0.53472600	0.21433400
C	-2.37376000	-0.53319100	2.08975100
C	2.48079300	-0.72957800	2.04385200
H	-2.52498400	-1.59266500	2.31316700
H	2.55260100	-1.80000400	2.24846000
H	-3.27090100	-0.00514500	2.41860700
H	3.41958800	-0.26567000	2.35353000
C	-1.11869700	-0.02513300	2.77646400
C	1.28604800	-0.13594500	2.76706000
H	-1.21024000	-0.21193300	3.86125000
H	1.37912300	-0.35044400	3.84647300
H	-1.06857300	1.07752900	2.67848900
H	1.33065800	0.96896000	2.69050300
N	0.05567200	-0.64017500	2.21369200
H	-0.02911400	-2.61593600	0.92301300
H	0.00048300	-1.92309400	1.60708100
Co	0.00920200	-1.00484900	0.05494700
C	-3.66980400	-1.33628900	-0.33427000
C	-4.76078000	-0.69859400	-0.92236100
C	-3.70121300	-2.72525900	-0.18264000
C	-5.86001100	-1.43432000	-1.34605900
H	-4.75769500	0.37782500	-1.04906200
C	-4.80310300	-3.45595300	-0.59685300
H	-2.84999200	-3.23432900	0.25949900
C	-5.88596600	-2.81173500	-1.18307200
H	-6.70092600	-0.92599900	-1.80215100
H	-4.81491000	-4.53135600	-0.46810700
H	-6.74458800	-3.38278300	-1.51361700
C	-2.48310500	1.29763200	-0.20175600
C	-2.23603400	1.68240300	-1.52324700
C	-2.90425300	2.26466700	0.70940900
C	-2.41967100	2.99516900	-1.92619000
H	-1.89172300	0.94178400	-2.23845100
C	-3.07327900	3.58418500	0.30837400
H	-3.10311100	1.99670200	1.73985900
C	-2.83538100	3.95188800	-1.00780500
H	-2.22928700	3.27474400	-2.95513900
H	-3.39697700	4.32539500	1.02884300
H	-2.96833000	4.98103300	-1.31745200
C	3.76889700	-1.21181900	-0.49658800
C	4.37571500	-0.60942800	-1.60080800
C	4.30516000	-2.40511200	-0.00631000
C	5.50018000	-1.17359600	-2.18470500
H	3.97009400	0.31256400	-2.00249400



TS(3B/3A1)-triplet-M06L-SCRF

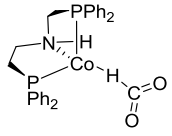
N	0.11131500	-2.54029300	1.38705400
Co	-0.03760500	-1.57068400	-0.59062900
P	-1.74176300	-0.35424100	0.21127900
P	1.75460000	-0.33890800	-0.01302800
H	0.48336100	-3.26347900	-0.86152600
H	0.33144400	-3.13570200	0.07922700
C	-1.70491000	-0.89630300	1.99017100
H	-1.05181200	-0.22883500	2.55322100
H	-2.70400700	-0.82069700	2.42802500
C	-1.16438200	-2.33151200	2.03232600
H	-1.13436600	-2.64993200	3.08717300
H	-1.90294100	-2.98259600	1.54576500
C	1.27515400	-2.05299200	2.10191200
H	2.13435300	-2.68602600	1.83976600
H	1.14072000	-2.17707300	3.18727200
C	1.68880500	-0.60241700	1.82843600
H	2.64813500	-0.36872000	2.29897900
H	0.95118800	0.10626600	2.21355600
C	-3.40759600	-0.93709600	-0.31829700
C	-3.46879400	-2.03167600	-1.17878100
H	-2.54063200	-2.47203700	-1.53595100
C	-4.69362800	-2.55556400	-1.57097500
H	-4.72868800	-3.40723200	-2.23919900
C	-5.86993300	-1.98179300	-1.11087400
H	-6.82694500	-2.38328900	-1.42044700
C	-5.81990100	-0.88998600	-0.25168000
H	-6.73775800	-0.44298100	0.11048000
C	-4.59664600	-0.37295900	0.14633300
H	-4.56395700	0.47609800	0.82084000
C	-1.92805700	1.47060600	0.26480400
C	-2.59155400	2.13089700	-0.77354500
H	-3.08165400	1.55441900	-1.55073600
C	-2.63593200	3.51580800	-0.81938900
H	-3.16061800	4.00891900	-1.62872200
C	-2.00966300	4.26873400	0.16590600
H	-2.04288700	5.35054100	0.12955000
C	-1.33545800	3.62436700	1.19417200
H	-0.83629600	4.20233300	1.96278600
C	-1.28885900	2.23803200	1.24160800
H	-0.74560600	1.75582800	2.04630000
C	3.49024900	-0.86301900	-0.39069100
C	4.58100700	0.00551800	-0.42045900
H	4.43811500	1.06490200	-0.24168400
C	5.85776500	-0.47481900	-0.67941800
H	6.69477200	0.21268800	-0.70343200
C	6.06467300	-1.82885400	-0.90505900

C 5.43045300 -2.96651500 -0.59145800	H 7.06188300 -2.20089200 -1.10504800
H 3.84440700 -2.90262300 0.83920900	C 4.98547800 -2.70204500 -0.88155800
C 6.03304400 -2.35289900 -1.68132900	H 5.13675300 -3.75909900 -1.06423700
H 5.96265000 -0.68844200 -3.03570100	C 3.70797100 -2.22032700 -0.63675600
H 5.83793900 -3.88776400 -0.19317400	H 2.85986600 -2.89888700 -0.64353500
H 6.91215400 -2.79158100 -2.13648300	C 1.81438800 1.49004900 -0.17870200
C 2.39990100 1.28367600 0.01145000	C 2.36098700 2.32660400 0.79650500
C 3.53280300 1.97776800 0.43769500	H 2.80757000 1.89979900 1.68741200
C 1.32173900 1.99914000 -0.50666700	C 2.33996600 3.70495400 0.63452400
C 3.58294300 3.36054700 0.34187600	H 2.76484900 4.34326400 1.39972900
H 4.37865900 1.43413400 0.84521100	C 1.77444600 4.26512000 -0.50339200
C 1.36858400 3.38377000 -0.59748300	H 1.75433500 5.34108600 -0.62614800
H 0.44112400 1.45664900 -0.84263600	C 1.22399200 3.44306800 -1.47808700
C 2.50040800 4.06514600 -0.17189600	H 0.77074600 3.87553500 -2.36192500
H 4.46673600 3.89205500 0.67314300	C 1.24005200 2.06577200 -1.31266900
H 0.52143900 3.92707100 -0.99931900	H 0.78591400 1.42453300 -2.06183700
H 2.54175300 5.14519800 -0.24051400	



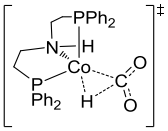
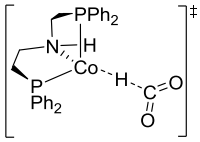
3A1-triplet-M06L-SCRF

N 0.11871700 -1.95851500 1.98960100	
Co -0.00940900 -1.44302800 -0.16471700	
P -1.74457900 -0.14139300 0.43231600	
P 1.68687100 -0.04099700 0.25474700	
O -0.12161400 -2.62460100 -2.81599400	
C -1.79594400 -0.39963400 2.27545300	
H -1.20652600 0.38160800 2.75672600	
H -2.81151200 -0.31669500 2.66509800	
C -1.21754600 -1.76477400 2.59065800	
H -1.17972300 -1.91396200 3.67677200	
H -1.86209700 -2.54537500 2.17817900	
C 1.21994000 -1.25349000 2.69071000	
H 2.10393600 -1.89022200 2.61657200	
H 0.98937700 -1.15283800 3.75734800	
C 1.54246300 0.10836700 2.09803600	
H 2.45740000 0.50500600 2.54424300	
H 0.74521100 0.82713900 2.29965800	
C -3.47119900 -0.55725500 -0.08200900	
C -3.65537700 -1.51005700 -1.08113800	
H -2.78685900 -1.97920600 -1.53305500	
C -4.93447800 -1.85942700 -1.49607200	
H -5.06603700 -2.60207400 -2.27351600	
C -6.03991500 -1.25639700 -0.91467800	
H -7.03799600 -1.52738800 -1.23615500	
C -5.86608200 -0.30132700 0.08081600	
H -6.72859800 0.17222000 0.53392600	
C -4.58963700 0.04723100 0.49377200	
H -4.46008800 0.79674700 1.26799800	
C -1.74041500 1.68995500 0.23934600	
C -1.46207400 2.19447100 -1.03435200	

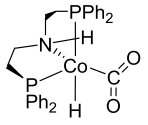


3A2-triplet-M06L-SCRF

N 0.11076300 -1.95126800 1.57999100	
Co 0.11524000 -1.12503600 -0.45674800	
P -1.81945000 -0.12858300 0.07034000	
P 1.69775700 0.29731400 0.27116400	
O 1.85893100 -4.57143800 -1.43836700	
C -1.73125900 -0.27417500 1.92303600	
H -1.11056500 0.55291400 2.27526900	
H -2.71615300 -0.15905200 2.38009300	
C -1.13934100 -1.62284200 2.30040900	
H -0.97699400 -1.66703500 3.38367500	
H -1.86060300 -2.40691300 2.05707500	
C 1.35301800 -1.55708200 2.27173600	
H 2.15401700 -2.16926900 1.84627000	
H 1.29594200 -1.79848100 3.34005500	
C 1.68620100 -0.08684100 2.09279000	
H 2.65468100 0.14654500 2.53825600	
H 0.94439800 0.53946900 2.58802100	
C -3.42106100 -0.96534900 -0.29808600	
C -3.37620800 -2.33091300 -0.58443600	
H -2.41498800 -2.83765600 -0.61696500	
C -4.54286100 -3.04003600 -0.83098900	
H -4.49417000 -4.10022900 -1.04708200	
C -5.76786000 -2.38692900 -0.81421500	
H -6.67883500 -2.93628400 -1.01686500	
C -5.82143300 -1.02602800 -0.54369400	
H -6.77494900 -0.51206700 -0.53466000	
C -4.65613100 -0.31864000 -0.28356900	
H -4.71104000 0.74282500 -0.06991600	
C -2.14881300 1.65457400 -0.20656800	
C -1.67557000 2.22625200 -1.38876700	

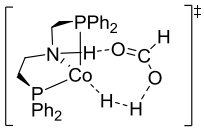
H -1.26813600 1.50444100 -1.85040300 C -1.41649300 3.56056700 -1.26201200 H -1.19693100 3.93469100 -2.25479400 C -1.63329400 4.44739300 -0.21375400 H -1.58489900 5.51543400 -0.38685700 C -1.90283100 3.95864000 1.05627400 H -2.07273100 4.64491600 1.87706700 C -1.96194500 2.58868200 1.28257600 H -2.18697600 2.22714500 2.27862400 C 3.37088700 -0.76652900 0.05329800 C 4.53653800 -0.07422200 0.38224200 H 4.47353300 0.94589900 0.74730600 C 5.77467400 -0.68275900 0.24257600 H 6.67574400 -0.13834400 0.49787900 C 5.86055600 -1.98952900 -0.22357100 H 6.82883300 -2.46216500 -0.33292000 C 4.70628400 -2.68640400 -0.55168200 H 4.77082900 -3.70369500 -0.91780900 C 3.46687800 -2.07489700 -0.41671300 H 2.55645200 -2.60962500 -0.67873700 C 1.93861400 1.69010000 -0.30693200 C 1.84349400 2.79784300 0.53550300 H 1.66243500 2.66885600 1.59541600 C 1.98466500 4.08316400 0.02626900 H 1.90491100 4.93353400 0.69290300 C 2.22433400 4.27932200 -1.32576400 H 2.33196500 5.28223800 -1.71982000 C 2.32148600 3.18164200 -2.17326400 H 2.50666900 3.32626400 -3.23065000 C 2.17337900 1.89988700 -1.66930800 H 2.23746400 1.04788400 -2.33909300 H 0.31650000 -2.95094600 2.05047800 C -0.42781300 -3.51399100 -1.99974500 H -0.62930900 -4.53551100 -2.38277500 O -0.53951900 -3.37517600 -0.74208100	H -1.14801400 1.60547100 -2.10606000 C -1.85458400 3.57801300 -1.64167200 H -1.47897700 4.00933500 -2.56156900 C -2.49875500 4.37861600 -0.70748600 H -2.62915600 5.43682900 -0.89785600 C -2.96525000 3.82253200 0.47634000 H -3.46343000 4.44554000 1.20907400 C -2.79353800 2.46803300 0.72673500 H -3.16297000 2.04519600 1.65378300 C 3.41492900 -0.17608800 -0.18306200 C 4.54805900 0.53422500 0.21442600 H 4.44008700 1.45824500 0.77227600 C 5.81287800 0.06084300 -0.09988700 H 6.68884100 0.61889900 0.20766500 C 5.95972500 -1.13092000 -0.80094500 H 6.94998300 -1.49850500 -1.03994400 C 4.83853400 -1.84829800 -1.19262100 H 4.94620500 -2.77941500 -1.73591200 C 3.57240700 -1.36690600 -0.88988800 H 2.68700400 -1.91856900 -1.19635800 C 1.66993600 2.12636100 0.17326700 C 0.88793000 2.88212500 1.05019600 H 0.36494900 2.40274700 1.86986100 C 0.76102300 4.25319200 0.87904300 H 0.15228300 4.82394200 1.57003300 C 1.39998700 4.88967800 -0.17638700 H 1.29597900 5.95913600 -0.31085800 C 2.16953900 4.14564600 -1.06118300 H 2.66990900 4.63308700 -1.88898800 C 2.30043700 2.77572800 -0.89130200 H 2.90053100 2.20476400 -1.59130400 H 0.14668000 -2.96173500 1.44949600 C 0.91925800 -4.20126000 -0.70229700 H 0.27591700 -3.35914100 -1.10335100 O 0.58917400 -4.65328200 0.42098300
 **TS(3A2/3B)**-triplet-M06L-SCRF Co -0.18638200 -1.42705400 0.28306900 P -1.80579300 0.16718800 0.44403100 P 1.87532800 -0.39742500 0.52395900 N -0.26633800 -1.40579200 2.48980400 C -2.02118700 0.33723100 2.26797500 H -1.38448300 1.16647400 2.58345600 H -3.04202600 0.60336700 2.54326000 C -1.60563500 -0.96402200 2.93977800 H -1.63306700 -0.84558500 4.02838400 H -2.30790000 -1.75910000 2.68271300 C 0.81291200 -0.59975600 3.10344000 H 0.96109900 -0.89741900 4.14594100	 **TS(3A2/3B)'**-triplet-M06L-SCRF N -0.06033500 -2.04024500 1.62893100 Co 0.01587700 -1.26156600 -0.50261600 P -1.77425700 -0.04002700 0.12642800 P 1.69521300 0.05289600 0.26689800 O 1.92286000 -4.11685800 -0.38347500 C -1.73929300 -0.19553100 1.97543800 H -1.05610500 0.56858200 2.35133700 H -2.71956000 -0.00065300 2.41513200 C -1.28250500 -1.59491500 2.34529800 H -1.13452000 -1.66776800 3.42894700 H -2.07207800 -2.30350200 2.08398200 C 1.20698300 -1.71843600 2.32209200

H	0.48006500	0.43694100	3.12551400	H	1.96126500	-2.40522300	1.93052400
C	2.11593300	-0.71042000	2.33990700	H	1.11604900	-1.91631800	3.39704600
H	2.50894300	-1.72764400	2.40634000	C	1.65646600	-0.28953600	2.09542300
H	2.86584400	-0.03970700	2.76195000	H	2.63874800	-0.12634700	2.54178500
H	0.51968700	-2.81890500	0.06379300	H	0.97165800	0.40960400	2.57340300
H	-0.14169200	-2.36524900	2.79526600	C	-3.41116200	-0.79691900	-0.27411800
C	-0.83781800	-2.68411400	-1.10166700	C	-3.40829100	-2.09092200	-0.79376600
O	-0.40834700	-2.30298900	-2.20129500	H	-2.45608400	-2.58174100	-0.98107500
C	-3.42821300	-0.38885400	-0.20984500	C	-4.60132500	-2.74284200	-1.07366800
C	-4.42310600	-0.92264100	0.60679300	H	-4.58613900	-3.74929100	-1.47375600
C	-3.61023400	-0.39784600	-1.59530100	C	-5.81033800	-2.09921300	-0.84984900
C	-5.58328300	-1.44312200	0.04804000	H	-6.74274800	-2.60202600	-1.07500800
H	-4.30251500	-0.93866200	1.68302700	C	-5.82313500	-0.80666600	-0.34013000
C	-4.77178000	-0.91120400	-2.14812200	H	-6.76585000	-0.30166800	-0.16751100
H	-2.83522900	-0.00368300	-2.24467100	C	-4.63082300	-0.15918700	-0.05048400
C	-5.76119000	-1.43877900	-1.32722800	H	-4.65082600	0.84863400	0.35020300
H	-6.34966600	-1.85314500	0.69425600	C	-2.03417400	1.75219100	-0.16307200
H	-4.90280800	-0.90632800	-3.22312200	C	-1.58756300	2.28421600	-1.37418600
H	-6.66629000	-1.84623300	-1.75976000	H	-1.11332400	1.63169900	-2.10054000
C	-1.59789500	1.85140500	-0.23454300	C	-1.72899200	3.63637800	-1.64694500
C	-2.16869000	2.97550600	0.36070100	H	-1.37403700	4.03647600	-2.58891700
C	-0.81929400	2.00274700	-1.38282400	C	-2.30824400	4.47749400	-0.70554800
C	-1.95757300	4.23341800	-0.18588600	H	-2.41002500	5.53561700	-0.91294600
H	-2.77743400	2.87126800	1.25143400	C	-2.74665300	3.96074200	0.50621100
C	-0.62464300	3.25955600	-1.93598100	H	-3.19326000	4.61479100	1.24517000
H	-0.35753100	1.12970900	-1.83480700	C	-2.61166200	2.60599100	0.77780500
C	-1.18900000	4.37638900	-1.33384100	H	-2.95551300	2.21654800	1.72889300
H	-2.39706600	5.10424500	0.28460300	C	3.45110700	-0.34849900	-0.15418600
H	-0.01827300	3.36834900	-2.82677500	C	4.52289200	0.25565200	0.50657300
H	-1.02624800	5.35995500	-1.75694800	H	4.33395200	0.99500700	1.27811300
C	3.35578000	-1.17045100	-0.23039700	C	5.82784600	-0.07757900	0.18005500
C	4.64101000	-0.88234600	0.23263700	H	6.65216200	0.39666100	0.69880500
C	3.19544700	-2.05992700	-1.28978000	C	6.07902100	-1.01810400	-0.81303300
C	5.74460800	-1.48369500	-0.35165100	H	7.09938000	-1.27791300	-1.06680900
H	4.77820800	-0.18306100	1.05010200	C	5.02153800	-1.62073500	-1.47753300
C	4.30330000	-2.65563900	-1.87867000	H	5.21267700	-2.35150200	-2.25399400
H	2.19707400	-2.28498600	-1.65074600	C	3.71360100	-1.28514900	-1.14941400
C	5.57664500	-2.37033700	-1.40876000	H	2.88028400	-1.75370400	-1.66417100
H	6.73819300	-1.25963300	0.01650200	C	1.71823300	1.89092800	0.15952400
H	4.16987500	-3.34390900	-2.70404300	C	1.01509300	2.69864100	1.05587100
H	6.44047400	-2.83740300	-1.86532800	H	0.50702800	2.26189600	1.90784300
C	2.19051000	1.39660700	0.27651600	C	0.94650700	4.07230100	0.86821000
C	1.60574000	2.34500700	1.12052300	H	0.39889800	4.68117700	1.57783200
C	2.89557500	1.84392900	-0.84280400	C	1.56599100	4.66338200	-0.22430700
C	1.75003300	3.70092900	0.86797800	H	1.50696600	5.73464900	-0.37145300
H	1.02537100	2.03118300	1.98048300	C	2.25881200	3.86940600	-1.12932500
C	3.03271600	3.20128400	-1.09711300	H	2.74437600	4.31940000	-1.98679000
H	3.34438900	1.12699200	-1.52085600	C	2.33236900	2.49779000	-0.94024600
C	2.46468000	4.13446200	-0.24137400	H	2.87695600	1.88916300	-1.65459900
H	1.29506700	4.42109100	1.53733900	H	-0.11241700	-3.05234700	1.60463200
H	3.58621200	3.52859800	-1.96879100	C	0.77249200	-4.12718200	-0.64951900
H	2.57084200	5.19346500	-0.44120300	H	0.56371600	-2.44943000	-1.58091600
O	-1.74134800	-3.45430100	-0.75366100	O	-0.31424100	-4.58460600	-0.72477000



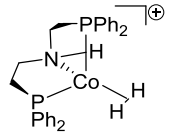
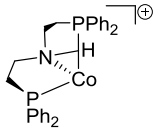
3B-CO_2-triplet-M06L-SCRF

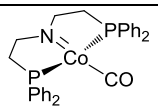
Co	-0.20606400	-1.52394800	0.30463800
P	-1.77642500	0.12387100	0.44927400
P	1.86321900	-0.43902600	0.52400200
N	-0.27869300	-1.46329600	2.49852100
C	-1.97649600	0.32298400	2.27436400
H	-1.31312800	1.13603900	2.57716800
H	-2.98889500	0.62386200	2.54453000
C	-1.59816900	-0.97946200	2.96099500
H	-1.60637800	-0.84655400	4.04805100
H	-2.32599800	-1.75720300	2.72394700
C	0.83222200	-0.69787800	3.10908300
H	0.98836600	-1.02161500	4.14228700
H	0.52684600	0.34656100	3.15747600
C	2.11962600	-0.82653400	2.32258100
H	2.48033000	-1.85725600	2.34889000
H	2.89603100	-0.19356400	2.75440500
H	0.60915300	-2.86785800	0.21120000
H	-0.18146100	-2.42924900	2.79368300
C	-1.12552600	-2.46879200	-1.17058200
O	-0.65180100	-2.04338100	-2.23143600
C	-3.44505000	-0.28769200	-0.19512300
C	-4.42540700	-0.86820900	0.60757200
C	-3.68972000	-0.13472900	-1.56166300
C	-5.63199000	-1.27622400	0.05485800
H	-4.25789500	-1.00655600	1.66875100
C	-4.89635000	-0.54030700	-2.10886600
H	-2.93101000	0.30417100	-2.20136200
C	-5.87027700	-1.11518300	-1.30203800
H	-6.38712400	-1.72195900	0.69054100
H	-5.07571100	-0.41011700	-3.16892600
H	-6.81178000	-1.43527500	-1.73033800
C	-1.46362300	1.78883300	-0.23671500
C	-2.01591800	2.93846600	0.32680900
C	-0.64982600	1.89862400	-1.36409000
C	-1.74851300	4.18135900	-0.22849700
H	-2.65485900	2.86500900	1.19948400
C	-0.39608700	3.14157800	-1.92521100
H	-0.20534600	1.00505100	-1.79244100
C	-0.94150100	4.28372900	-1.35449200
H	-2.17344300	5.07207500	0.21746500
H	0.23850000	3.21875200	-2.79950000
H	-0.73394300	5.25573500	-1.78471000
C	3.30046000	-1.23050900	-0.28920500
C	4.59745400	-1.04970800	0.19386700
C	3.09623200	-2.01787200	-1.41967800
C	5.66931500	-1.65756700	-0.44103100
H	4.76955500	-0.42935700	1.06645600



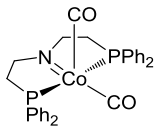
TS(3B/3A1)-triplet-M06L-SCRF

C	-1.82435200	-0.38285100	1.96121200
H	-1.16822700	0.24261200	2.56769900
H	-2.83573400	-0.25611900	2.35000000
C	-1.39189300	-1.83242800	2.04828600
H	-1.38708000	-2.15923700	3.09592700
H	-2.10482800	-2.46731200	1.51469300
C	1.07665200	-1.60006000	2.24222800
H	1.89363700	-2.30259100	2.06111700
H	0.83579800	-1.66278400	3.30972600
C	1.55045000	-0.19708600	1.89890000
H	2.49168300	0.02078300	2.40897500
H	0.82639600	0.55758300	2.21359900
C	-3.47042900	0.02444600	-0.36320600
C	-3.80603200	-0.97010100	-1.27816500
H	-3.02181100	-1.60917400	-1.67232300
C	-5.12346900	-1.14140400	-1.68425600
H	-5.37193600	-1.91982900	-2.39547100
C	-6.11637900	-0.31188600	-1.18402800
H	-7.14351900	-0.44026800	-1.50256000
C	-5.79029000	0.68779100	-0.27466300
H	-6.56352600	1.33818600	0.11613700
C	-4.47616300	0.85423300	0.13454000
H	-4.22963000	1.63574200	0.84603300
C	-1.49889000	1.99133900	0.29127800
C	-1.14926300	2.66005300	-0.88589400
H	-1.02536600	2.09409600	-1.80428900
C	-0.94472000	4.03046100	-0.89104300
H	-0.67154100	4.53155300	-1.81197500
C	-1.07217400	4.75657800	0.28736600
H	-0.89935600	5.82576500	0.28838000
C	-1.41056300	4.10400800	1.46375600
H	-1.51149300	4.66409300	2.38552000
C	-1.62808300	2.73119900	1.46676500
H	-1.90566400	2.24317200	2.39318900
C	3.32916200	-0.92497800	-0.22684800
C	4.56132700	-0.36773600	0.11532700
H	4.60338600	0.62957000	0.54097500
C	5.73297100	-1.08177500	-0.08725400
H	6.68614300	-0.64020100	0.17724200
C	5.68561200	-2.36148200	-0.62721500
H	6.60209500	-2.91645200	-0.78520400
C	4.46384300	-2.92610800	-0.96532500
H	4.42324900	-3.92289800	-1.38706100
C	3.29181300	-2.20763900	-0.77140100
H	2.33067400	-2.63880500	-1.04259700
C	2.16701700	1.70041100	-0.22088000
C	2.15901000	2.66677500	0.78496500

C 4.17244700 -2.61801400 -2.05964300 H 2.08856900 -2.16105900 -1.79547500 C 5.45785700 -2.44087700 -1.56921200 H 6.67225200 -1.51843100 -0.05680600 H 4.00485000 -3.22581100 -2.94006400 H 6.29704200 -2.91284900 -2.06497600 C 2.23465100 1.35145100 0.33826800 C 1.65400100 2.28965200 1.19661700 C 2.98956500 1.81247500 -0.74211900 C 1.85101100 3.64749400 0.99681800 H 1.03374700 1.96590100 2.02466300 C 3.17911300 3.17253700 -0.94388500 H 3.43588600 1.10579000 -1.43205600 C 2.61493300 4.09438700 -0.07400300 H 1.39781900 4.35915400 1.67630100 H 3.77049800 3.51027900 -1.78616700 H 2.76248600 5.15537400 -0.23260800 O -2.03306300 -3.24363300 -0.86213500	H 1.92842200 2.39345100 1.80728800 C 2.45146800 3.99251800 0.48813500 H 2.43825100 4.73246300 1.27941500 C 2.75643500 4.36934500 -0.81142300 H 2.98227100 5.40358600 -1.03949200 C 2.76693200 3.41336000 -1.82050500 H 3.00266700 3.69963400 -2.83818700 C 2.46899000 2.09247700 -1.52849900 H 2.46966600 1.35275000 -2.32274700 Co -0.09305600 -1.19039600 -0.63410600 N -0.07313800 -2.05259100 1.42561600 H 0.02245800 -3.05444300 1.28439300 P -1.70691700 0.16525700 0.18332200 P 1.72475400 -0.05881800 0.05878800 H -0.66378400 -2.43123300 -1.65313300 H -1.26394000 -3.23828700 -1.12187200 O -1.95456600 -4.08916900 -0.79371900 C -1.36484900 -4.95370500 -0.02805600 H -2.02237600 -5.80240800 0.22969700 O -0.21479200 -4.89649400 0.39524700
 **3BH**$^{+}$-M06L-SCRF-Cation C -1.84924700 -0.92235000 1.97057700 H -1.24768800 -0.22901800 2.55905900 H -2.86403700 -0.88159000 2.36802600 C -1.30086400 -2.33119900 2.07451600 H -1.24450500 -2.63672800 3.12490600 H -1.97283900 -3.02833000 1.56902600 C 1.15912100 -1.93606700 2.22958500 H 2.02691700 -2.56068900 2.00909200 H 0.94532500 -2.04969200 3.29733900 C 1.50000000 -0.48861400 1.91897700 H 2.41195500 -0.20020700 2.44580200 H 0.70814300 0.18704800 2.24744200 C -3.49091600 -0.81670500 -0.40128200 C -3.62893100 -1.91620000 -1.24643600 H -2.74058100 -2.45889900 -1.55804200 C -4.88438700 -2.30893200 -1.69052700 H -4.98238900 -3.16583300 -2.34553200 C -6.00942800 -1.59595900 -1.30205500 H -6.98909800 -1.89603800 -1.65272900 C -5.87938300 -0.49408000 -0.46466600 H -6.75759500 0.06333600 -0.16256000 C -4.62701700 -0.10652100 -0.01369600 H -4.53048700 0.75137400 0.64358000 C -1.79722600 1.43713900 0.24454300 C -1.45349000 2.11104800 -0.93065800 H -1.21180300 1.54071000 -1.82270000 C -1.40225000 3.49540600 -0.96108500	 **3B-H$_2$**$^{+}$-M06L-SCRF-Cation C -1.86531300 -1.01468700 1.90488900 H -1.26891100 -0.32968900 2.50819900 H -2.88088000 -0.98979900 2.30205600 C -1.30339300 -2.41970300 1.98046900 H -1.24908200 -2.74482800 3.02590300 H -1.96837400 -3.11311700 1.46055000 C 1.14511100 -1.99622100 2.14810600 H 2.01966300 -2.61335800 1.93204900 H 0.92607300 -2.11520400 3.21492800 C 1.47905800 -0.54529800 1.84822300 H 2.38565200 -0.25371900 2.38337900 H 0.67956300 0.12228000 2.17492500 C -3.54511400 -0.78880600 -0.42745800 C -3.76697700 -1.95012100 -1.16627400 H -2.92483400 -2.58794700 -1.41850400 C -5.04772300 -2.28934900 -1.58011500 H -5.20856300 -3.19501500 -2.15191900 C -6.11759700 -1.46135800 -1.27049000 H -7.11640100 -1.71914500 -1.60013800 C -5.90499100 -0.29874700 -0.54016600 H -6.73849500 0.34951300 -0.29845800 C -4.62684200 0.03530500 -0.11782300 H -4.46963800 0.94242500 0.45581800 C -1.77658900 1.39002300 0.24679400 C -1.41614900 2.09500200 -0.90444700 H -1.17843700 1.54896200 -1.81220000 C -1.33909500 3.47854900 -0.89197500

H -1.13135000 4.00520700 -1.87769700 C -1.67814100 4.22603500 0.18849600 H -1.62434800 5.30757500 0.16976900 C -2.01230900 3.56649700 1.36246600 H -2.22808700 4.13201400 2.26068300 C -2.07674200 2.17911600 1.39182500 H -2.35087700 1.67951800 2.31312100 C 3.34695000 -0.97882000 -0.23785200 C 4.52969100 -0.33044300 0.11699300 H 4.48997500 0.64812100 0.58389500 C 5.75456400 -0.93243900 -0.12766600 H 6.67016600 -0.42269600 0.14630000 C 5.80898800 -2.18794700 -0.72169200 H 6.76746300 -2.65477000 -0.91199100 C 4.63658400 -2.84182900 -1.07348600 H 4.67703100 -3.81903800 -1.53850700 C 3.41036000 -2.23597500 -0.83675100 H 2.48444000 -2.73229400 -1.11937700 C 1.92311900 1.52286200 -0.14565000 C 1.76653600 2.45914900 0.87622900 H 1.53948700 2.13938900 1.88556600 C 1.90605200 3.81609000 0.61180000 H 1.77935000 4.53216500 1.41479100 C 2.20431000 4.25373800 -0.67006500 H 2.31116700 5.31211300 -0.87266700 C 2.36122500 3.32752100 -1.69462700 H 2.59180700 3.66141100 -2.69881400 C 2.21513400 1.97465100 -1.43626200 H 2.32864700 1.25753200 -2.24309300 H -0.05914100 -1.96442100 -2.28590600 Co -0.03391400 -1.63403700 -0.57076300 H -0.05696000 -1.15581600 -2.22859200 N 0.02751100 -2.47984000 1.42898700 P -1.80044700 -0.39425300 0.18775800 P 1.68036400 -0.27748500 0.08819600 H 0.19045700 -3.47856300 1.35890000	H -1.05568600 4.01137200 -1.79161100 C -1.60628000 4.17817900 0.27870200 H -1.53158000 5.25855300 0.29441100 C -1.95785900 3.48826800 1.42991400 H -2.16755800 4.02921100 2.34461200 C -2.04928400 2.10205800 1.41483000 H -2.34026100 1.58010400 2.31840000 C 3.35630100 -1.00405400 -0.27925100 C 4.52576800 -0.34243200 0.09523900 H 4.46741600 0.63797700 0.55634000 C 5.76214700 -0.93234800 -0.12036600 H 6.66615300 -0.41098700 0.16992700 C 5.84270900 -2.19022700 -0.70587400 H 6.80970000 -2.64797900 -0.87378800 C 4.68421400 -2.85819900 -1.07676100 H 4.74392700 -3.83788900 -1.53453100 C 3.44711700 -2.26391500 -0.86887000 H 2.53494600 -2.77680900 -1.16362600 C 1.93921900 1.49206600 -0.16883200 C 1.80307200 2.40024400 0.88103600 H 1.57072600 2.05524500 1.88068000 C 1.97044100 3.76171500 0.65884500 H 1.85897400 4.45488200 1.48396300 C 2.27691000 4.23269300 -0.60907900 H 2.40633800 5.29431000 -0.77897300 C 2.41407600 3.33507500 -1.66165000 H 2.65202300 3.69480800 -2.65517700 C 2.24022200 1.97803500 -1.44455700 H 2.34025200 1.28397100 -2.27288500 Co -0.05541400 -1.59099500 -0.64078300 N 0.02490000 -2.53829700 1.33434400 P -1.82253500 -0.44115100 0.13141000 P 1.67452600 -0.31489300 0.01816000 H 0.20035200 -3.53297700 1.24447100
Gas phase	
CO-M06L C 0.00000000 0.00000000 -0.64564200 O 0.00000000 0.00000000 0.48423200	 **10**-singlet-M06L C -2.42063900 -0.21790000 2.35970200 H -3.35929000 0.28734900 2.59601700 H -2.45797100 -1.24046300 2.74091500 C -1.20832100 0.50512000 2.90816200 H -1.33088900 1.59249500 2.74156400 H -1.15046000 0.38312500 4.00095100 C 1.14933200 0.67441800 2.87691600 H 1.11912400 0.57620300 3.97368200 H 1.11939500 1.76459400 2.68369600 C 2.44234400 0.10026500 2.33475200

	H 2.63620000 -0.88335400 2.76666600 H 3.31520000 0.72724400 2.52722000 C -3.41559200 -1.33757000 -0.18040700 C -3.42340400 -1.52376700 -1.56443300 H -2.65498700 -1.05985600 -2.17301600 C -4.40200100 -2.29823300 -2.16340400 H -4.39600000 -2.43520500 -3.23752500 C -5.38366300 -2.90260700 -1.38899400 H -6.14682500 -3.51132300 -1.85762400 C -5.38217900 -2.72654400 -0.01407900 H -6.14608800 -3.19476800 0.59444600 C -4.40466100 -1.94712400 0.58877800 H -4.41886500 -1.81321400 1.66357900 C -2.48728000 1.38155400 -0.03636000 C -1.44850300 2.30177200 -0.16856800 H -0.43017400 1.97324500 0.02523000 C -1.71413500 3.60771500 -0.55230200 H -0.89874200 4.31391500 -0.65251500 C -3.01777600 4.00263200 -0.81613700 H -3.22532000 5.01993300 -1.12487100 C -4.05725100 3.09111600 -0.68895100 H -5.07543200 3.39675300 -0.89723100 C -3.79537000 1.78703900 -0.29745800 H -4.61048100 1.07746300 -0.20253200 C 3.50619600 -1.26621300 -0.02901200 C 4.75712000 -0.74113800 -0.35133600 H 4.91941100 0.33047300 -0.30741200 C 5.78875100 -1.58269300 -0.73631800 H 6.75753100 -1.16819000 -0.98698900 C 5.58001800 -2.95357300 -0.80416700 H 6.38625200 -3.60904100 -1.10961100 C 4.33722400 -3.48242900 -0.48814300 H 4.16941700 -4.55050100 -0.54904700 C 3.30273400 -2.64244200 -0.10456800 H 2.32336200 -3.04598100 0.13080200 C 2.42085200 1.38948800 -0.30665600 C 2.76812000 2.56402300 0.35947600 H 2.95015700 2.55358300 1.42686600 C 2.88389100 3.76071400 -0.33754000 H 3.14980000 4.66627600 0.19409900 C 2.66802000 3.79549500 -1.70555000 H 2.76177500 4.72832900 -2.24746400 C 2.32927600 2.62756200 -2.38006200 H 2.15882900 2.64782900 -3.44931600 C 2.19626900 1.43849000 -1.68624300 H 1.90741300 0.53473500 -2.21272900 C 0.08283400 -1.58688900 -0.96478000 Co 0.03893700 -0.73793700 0.53094100 N 0.00543100 0.00143700 2.28603600 O 0.12734800 -2.14627700 -1.98607300 P -2.08698600 -0.31988500 0.55234600 P 2.12740600 -0.20590600 0.54893400



10a-singlet-M06L

C	-2.46873200	-0.44967000	2.21974100
H	-3.41903100	0.01840400	2.48296900
H	-2.53990900	-1.52137500	2.41315300
C	-1.28820600	0.15853300	2.94049900
H	-1.35047800	1.26347400	2.83183100
H	-1.36725600	-0.02962100	4.02348200
C	1.02648700	0.50144400	2.86802400
H	1.10854500	0.47061600	3.96737600
H	0.82172900	1.56871600	2.62574300
C	2.34409700	0.09541900	2.24842200
H	2.63520800	-0.90221400	2.58317700
H	3.16489000	0.78064400	2.47046200
C	-3.32199900	-1.09209200	-0.52214700
C	-3.91301500	-0.52519700	-1.65035500
H	-3.66207800	0.48881700	-1.93867300
C	-4.82356900	-1.24960300	-2.40562600
H	-5.27550300	-0.79637400	-3.27931700
C	-5.15267200	-2.54775700	-2.04673700
H	-5.86480100	-3.11125200	-2.63648000
C	-4.55887800	-3.12557700	-0.93277400
H	-4.80439600	-4.14216100	-0.65157900
C	-3.64322800	-2.40781300	-0.18163200
H	-3.16700900	-2.87722800	0.67228600
C	-2.38452900	1.56138000	0.16263900
C	-1.34017000	2.40753700	-0.19431500
H	-0.35058400	1.98731700	-0.34052500
C	-1.55918000	3.76970800	-0.34883400
H	-0.73547000	4.41650500	-0.62514700
C	-2.82662400	4.29358100	-0.14757300
H	-3.00056600	5.35601100	-0.26665500
C	-3.87678500	3.45563900	0.20817600
H	-4.86752500	3.86427100	0.36547500
C	-3.65822400	2.09671000	0.36375800
H	-4.48235800	1.44540200	0.63566000
C	3.44936100	-0.98511400	-0.23315200
C	4.69253500	-0.37242900	-0.39602000
H	4.80753400	0.68222600	-0.17008700
C	5.77841700	-1.10266300	-0.85101700
H	6.73973600	-0.61882700	-0.97321700
C	5.63410200	-2.45040100	-1.15283200
H	6.48297800	-3.01857100	-1.51266100
C	4.40170100	-3.06586800	-0.99666200
H	4.28358100	-4.11546600	-1.23553700
C	3.31375200	-2.33652800	-0.53954100
H	2.34660200	-2.81163900	-0.41681000
C	2.27388700	1.61005300	-0.27321000
C	2.42463200	2.75765300	0.50307700

H 2.45961300 2.68465800 1.58314900 C 2.52159000 4.00654200 -0.09629000 H 2.63871800 4.88863000 0.52152000 C 2.47013200 4.12586200 -1.47629500 H 2.54540600 5.10066100 -1.94184600 C 2.32227200 2.98756100 -2.25985900 H 2.28293100 3.07185100 -3.33883400 C 2.22011800 1.74255400 -1.66427300 H 2.09636800 0.86008400 -2.28354600 Co 0.01819600 -0.98420500 0.45914400 N -0.03886500 -0.36857200 2.43122800 P -2.03219100 -0.22057600 0.44141300 P 2.01109800 -0.06118300 0.44460600 C 0.03082400 -1.26699300 -1.27270300 O 0.03463900 -1.42175800 -2.41760300 C 0.01186400 -2.68184900 1.12721000 O -0.03832700 -3.71416200 1.63393800	

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