

A Molecularly-defined Manganese Catalyst for Low Temperature Hydrogenation of Carbon Monoxide to Methanol.

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SUPPORTING INFORMATION

TABLE OF CONTENTS	PAGE
1. General Experimental	2
2. Literature preparations of metal complexes.....	5
3. Procedure for CO hydrogenation to methanol.	6
4. Preparation of <i>N</i> -formylazoles	7
5. Procedures for amide and CO hydrogenations.	13
6. Optimization of reaction parameters.....	16
7. GC analysis of the headspace	19
8. Mechanistic experiments	20
9. Crude NMR Spectra after CO hydrogenation.....	26
10. NMR Spectra of <i>N</i> -formylazoles	28
10. Computational methods	34
11. References	80

1. General Experimental

All reactions were performed in an oven (160 °C) and/or in flame-dried glassware under an atmosphere of dry argon unless otherwise noted. Chemicals used in this work were purchased from the following vendors: **Ru-1** (Strem); pyrrole, >98% (Alfa); diphenylamine (Alfa), ethylmagnesium bromide, 3M in ether (Alfa), 3-methylindole (Abcr), 99%, ethyl formate (Abcr), 9-methylcarbazole (Enamine), indole (TCI), *N*-methylformanilide (TCI), *N*-methylaniline (TCI), methyl formate (>98%, for spectrophotometry) (TCI), potassium phosphate tribasic (anhydrous, free-flowing, Redi-Dri™, reagent grade, ≥98%) (Sigma), *N*-methylpyrrole (Sigma), morpholine (Sigma).

Reaction solvents: dichloromethane, toluene, DMF and THF (Fisher, HPLC grade) were dried by percolation through neutral alumina in a solvent dispensing system. Cyclohexane was distilled over CaH₂ and dried over 3 Å molecular sieves. Carbon tetrachloride was dried over 3 Å molecular sieves. ACS reagent grade ethyl acetate, dichloromethane and heptane used for chromatography and recrystallization were purchased from Fisher.

Column chromatography was performed using Macherey-Nagel, 60 Å silica gel. Visualization was accomplished by UV light and/or potassium permanganate (KMnO₄), iodine vapor. Hydrogenation experiments were carried out in 300 mL autoclave (PARR Instrument Company) in 8-mL glass vials, which were placed inside the autoclave.

Deuteriochloroform, deuteromethylenechloride, deuterocyclohexane and deuterotetrahydrofuran were purchased from Eurisotop, were distilled and dried over 4Å molecular sieves before use.

NMR data were recorded on a Bruker ARX 300 and Bruker ARX 400 spectrometers (300 or 400 MHz, ^1H ; 75 MHz, ^{13}C). Spectra were referenced to residual CHCl_3 (7.26 ppm ^1H ; 77.00 ppm ^{13}C), CD_2Cl_2 (5.32 ppm ^1H ; 54.00 ppm ^{13}C), $\text{THF-}d_8$ (3.58 and 1.73 ppm ^1H ; 67.57 and 25.37 ppm ^{13}C), and cyclohexane-*d*12 (1.38 ppm ^1H ; 26.43 ppm ^{13}C). Chemical shifts are reported in ppm, multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), h (hextet), hep (heptet), m (multiplet) and br (broad). Coupling constants, *J*, are reported in Hertz. (+) and (-) represent positive and negative intensities of signals in ^{13}C DEPT-135 experiments.

GC Conversion and yields were determined by GC-FID, HP6890 with FID detector, column HP530 m x 250 mm x 0.25 μm . Analysis of the gas sample in the dehydrogenation process was performed using GC HP Plot Q (FID – hydrocarbons, Carboxen / TCD - permanent gases), Ar - carrier gas. The GC was externally calibrated using certified gas mixtures from commercial suppliers (Linde and Air Liquide) with the following gas vol%:

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

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

CO_2 : 1%, 50%

CH_4 : 1%

The systems allow for the determination of H₂, CH₄, CO and CO₂ within the ranges:

$$\text{H}_2 \geq 0.5 \text{ vol\%} - 100 \text{ vol\%}$$

$$\text{CO} \geq 10 \text{ ppm}$$

$$\text{CO}_2 \geq 100 \text{ ppm} - 100 \text{ vol\%}$$

$$\text{CH}_4 \geq 1 \text{ ppm}$$

Density functional theory (DFT) was used for the calculation of structures, total energy, and thermodynamic data. The hybrid PBE0 functional for exchange and correlation was used for optimizations and combined with a recent dispersion correction of Grimme (DFT-D version 3 with Becke-Johnson damping). The optimizations were performed using a triple zeta basis set def2-TZVP. The single point calculations were performed using DSD-PBE96-NL and a quadruple zeta valence basis set def2-QZVP.

2. Literature preparations of metal complexes

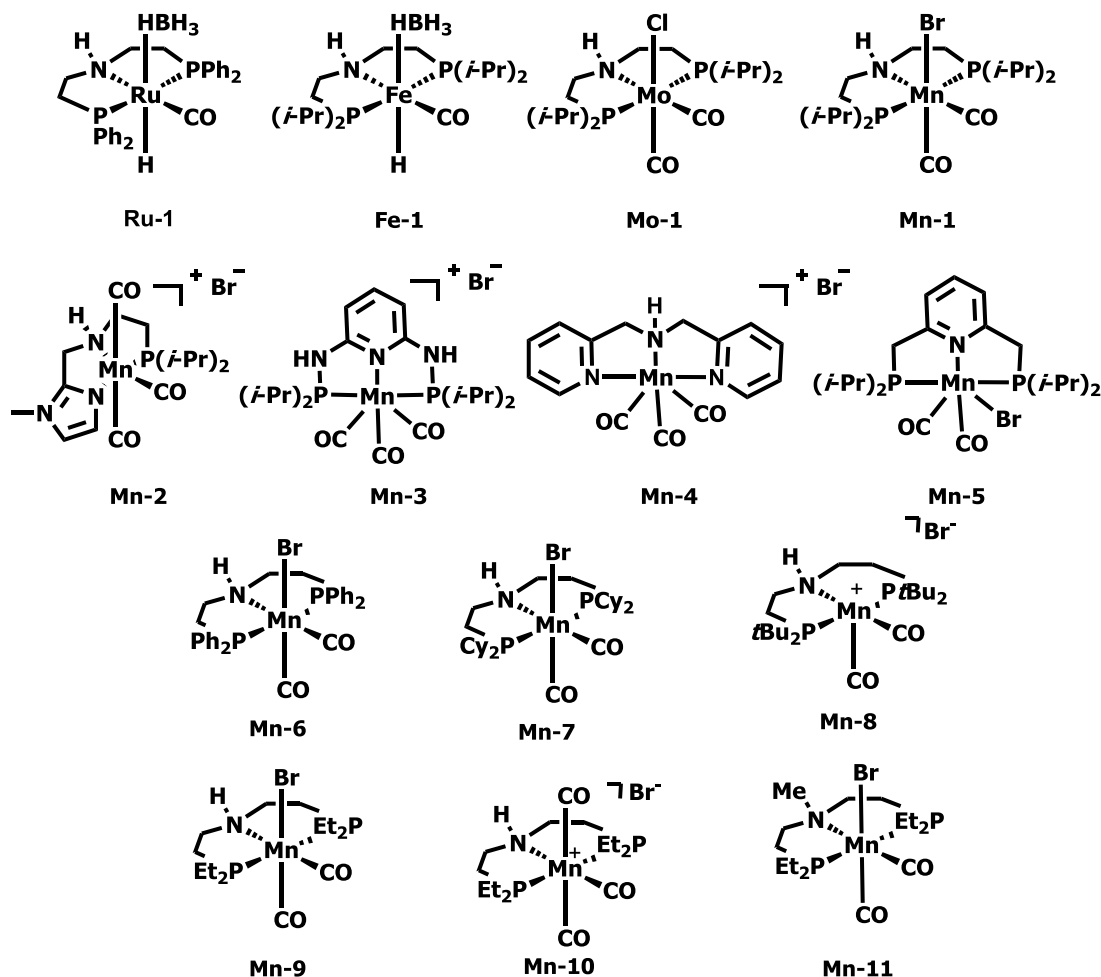
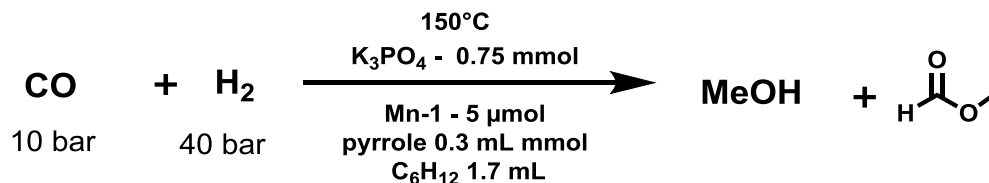


Figure S1. Metal complexes used in this work.

Metal catalysts were prepared following known literature procedures: **Fe-1**,¹ **Mo-1**,² **Mn-1**,³ **Mn-2**,⁴ **Mn-3**,⁵ **Mn-4**,⁶ **Mn-5**,⁷ **Mn-6**,⁸ **Mn-7**,³ **Mn-8**,⁴ **Mn-9**,⁹ **Mn-10**⁹ and **Mn-11**¹⁰.

3. Procedure for CO hydrogenation to methanol.



CO hydrogenation with Mn-1 and pyrrole (Table 3, entry 7). An 8 mL glass vial containing a stirring bar was charged under argon with **Mn-1** (2.5 mg, 5 μ mol) and freshly distilled pyrrole (0.3 mL, 4.43 mmol), followed by the addition of cyclohexane (1.7 mL) and anhydrous K₃PO₄ (159 mg, 0.75 mmol). The vial was capped with a septum equipped with a syringe needle and then placed into a 300 mL autoclave. Once sealed, the autoclave was purged three times with 5-10 bar of CO, then pressurized to 10 bar CO, followed by an additional 40 bar H₂ (total pressure 50 bar). The autoclave was placed into an aluminum block and heated at 150°C for 18 h. Afterwards, the autoclave was cooled in an ice bath, a drop in pressure to 42 bar was observed and the remaining gas was carefully released (Figure S2, B). To the reaction mixture *n*-hexadecane (50 μ L) was added as an internal standard, and then it was homogenized by the addition of CCl₄ (1 mL). GC analysis shows the formation of methanol (12.75 mmol, 408 mg, TON – 2550) and methyl formate (0.56 mmol, 33.5 mg, TON– 112). CO conversion - 27.6% (14.76 mmol) - based on the pressure change and composition of the gas phase. Mass balance (products/CO) - 94%.

Note: with scatole (4.32 mmol, 567 mg) as a promoter: methanol (15.85 mmol, 507 mg, TON – 3170) (Table 3, Entry 6)..

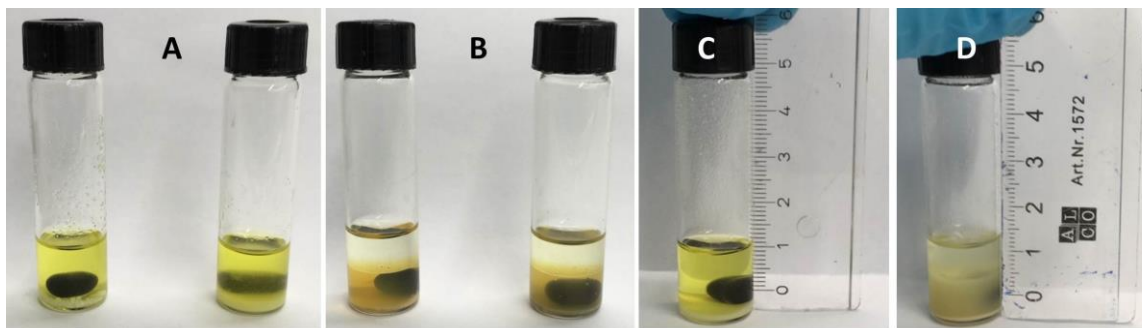
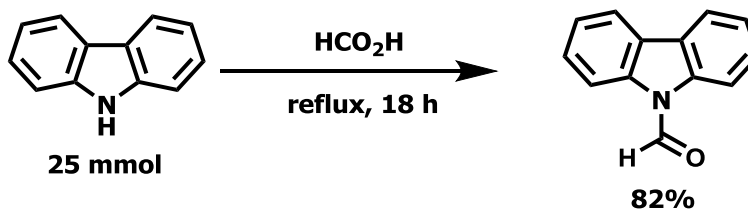


Figure S2. Photographs of the reaction mixtures.

Reaction mixtures before (A, C) and after (B, D) CO hydrogenation to methanol with **Mn-1** and pyrrole. Phase separation is visible after centrifugation and is caused by the formation of methanol (B). Photographs C and D clearly show the increase in the total volume of the reaction mixture.

4. Preparation of *N*-formylazoles



Preparation of N-formylcarbazole. A flame-dried 100-mL single-neck round-bottomed flask fitted with a magnetic stir bar, reflux condenser, and Ar inlet was charged with carbazole (4.18 g, 25 mmol, 1.0 equiv.) and dissolved in formic acid (30 mL). The reaction mixture was heated to reflux in an oil bath for 18 hours. Then the reaction mixture was cooled to room temperature, transferred to a 500 mL beaker and quenched with saturated aq. NaHCO_3 to a pH of 7. The mixture was transferred to a 250-mL separatory flask and the aqueous layer was extracted with dichloromethane (3×80 mL). The combined organic layers were washed with saturated brine solution (1×50 mL),

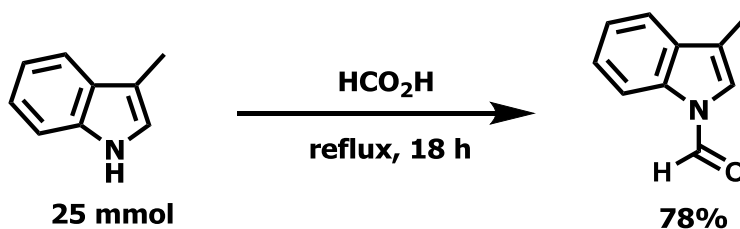
dried over MgSO_4 , and concentrated by rotary evaporation to give *N*-formylcarbazole (3.99 g 82%) as a light grey solid. The spectroscopic data is in agreement with previous reports.^{11,12}

^1H NMR (400 MHz, CDCl_3)

δ 9.66 (s, 1H), 8.56 (br. s, 1H), 7.96 (d, $J = 7.5$ Hz, 2H), 7.70 (br. s, 1H), 7.49 (br. s, 2H), 7.42 (t, $J = 7.4$ Hz, 2H).

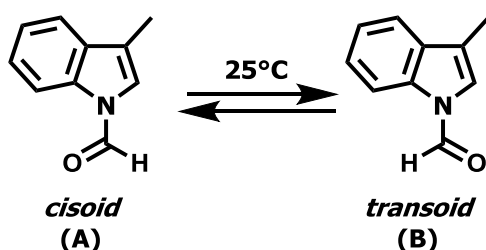
^{13}C NMR (101 MHz, CDCl_3)

δ 157.5 (+), 137.8, 137.3, 127.9 (+), 127.1 (+), 126.2, 124.8 (+), 124.4 (+), 120.9 (+), 119.9 (+), 116.9 (+), 110.0 (+).



Preparation of N-formyl-3-methylindole. A flame-dried, 100-mL, single-neck, round-bottomed flask fitted with a magnetic stir bar, reflux condenser, and Ar inlet was charged with scatole (3.28 g, 25 mmol, 1.0 equiv.) and dissolved in formic acid (30 mL). The reaction mixture was heated to reflux in an oil bath for 18 hours. Then the reaction mixture was cooled to room temperature, transferred to a 500 mL beaker and quenched with saturated aq. NaHCO_3 to a pH of 7. The mixture was transferred to a 250-mL separatory flask and the aqueous layer was extracted with dichloromethane (3×80 mL). Combined organic layer was washed with saturated brine solution (1×50 mL), dried over MgSO_4 , and concentrated by rotary evaporation to give crude product as a brown oil. Purification by flash chromatography (SiO_2 , 0-10% EtOAc/heptane) yielded *N*-

formyl-3-methylindole as a colorless oil (3.09 g, 78%) which slowly crystallized upon standing. The spectroscopic data is in agreement with previous reports.¹³ *N*-formyl-3-methylindole exhibits a conformational *cisoid* (A) and *transoid* (B) equilibrium through the rotation around the C-N bond. The ratio of A and B rotamers (59:41) is evaluated by comparing the integrated area of the characteristic CHO signals: 9.01 ppm, for A and 9.35 ppm for B respectively.

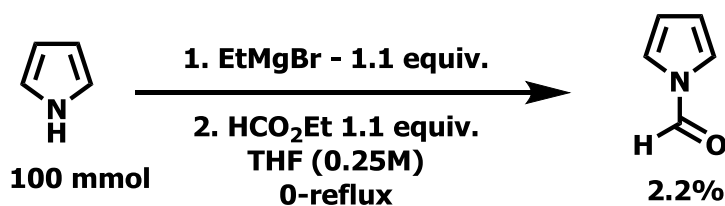


¹H NMR (300 MHz, CDCl₃)

δ 9.35 (s, 0.4H, B), 9.01 (s, 0.57H, A), 8.39 (d, J = 7.3 Hz, 0.55H, B), 7.61 (br. d, J = 4.2 Hz, 0.4H, A), 7.54 (s, 1H, A and B), 7.51 (s, 0.4H, A), 7.43 – 7.29 (m, 2H, A and B), 7.06 (s, 0.56 H), 2.29 (d, J = 1.4 Hz, 3H, A+B).

¹³C NMR (75 MHz, CDCl₃)

δ 159.1(+, B), 155.7 (+, A), 135.4 (A), 134.5 (B), 132.3 (B), 132.0 (A), 125.2 (+, B), 124.6 (+, A), 124.4 (+, B), 123.9 (+, A), 121.9 (+, B), 120.5 (A), 120.0 (+, A), 119.6 (B), 119.1 (+, B), 119.0 (+, A), 116.1 (+, B), 109.5 (+, A), 9.9 (+, B), 9.7(+, A).



Preparation of N-formylpyrrole was done following Alessandri's protocol from 1914.¹⁴ A flame-dried 1 L three-necked round-bottomed flask fitted with a magnetic stir bar, reflux condenser, 100 mL addition funnel and a rubber septum was charged with freshly distilled pyrrole (6.92 mL, 100 mmol, 1.0 equiv.) and dissolved in THF (400 mL). The flask was cooled in an ice-bath and EtMgBr (3.0 M solution in ether; 36.7 mL, 110 mmol, 1.1 equiv.) was added dropwise to the solution of pyrrole over 30 minutes giving a dark green/brown solution. Over the course of the addition gas evolution was observed. The flask was warmed up at ambient temperature for 30 minutes under stirring. Then the reaction mixture was cooled again in an ice bath and ethyl formate (8.88 mL, 110 mmol, 1.1 equiv.) was added dropwise to the reaction mixture using syringe via a rubber septum. Then the ice bath was replaced with an oil bath set at 80°C and the reaction mixture refluxed for 45 minutes giving a dark brown mixture. The reaction was cooled to 0°C and quenched with 200 mL of sat. aq. NH₄Cl solution. The mixture was allowed to warm to room temperature and then was transferred to 1 L separatory funnel and was diluted with diethyl ether (100 mL). The aqueous layer was extracted with diethyl ether (3 × 200 mL); combined organic layers were washed with brine (1 × 250 mL), dried over MgSO₄, and concentrated by rotary evaporation to give the crude product as brown oil. NMR analysis of the crude mixture revealed the formation of *N*-formylpyrrole and pyrrole-2-carbaldehyde in 1:1 ratio along with significant quantities of unreacted pyrrole.

The pure product was obtained after 2 fractional distillations at atmospheric pressure,[†] giving *N*-formylpyrrole (212 mg, 2.2%) as a colorless oil. The spectroscopic data is in agreement with previous report.¹⁵

¹H NMR (300 MHz, CD₂Cl₂)

δ 8.90 (s, 1H), 7.27 (br. s, 2H), 6.58 – 6.28 (m, 2H).

¹³C NMR (75 MHz, CD₂Cl₂)

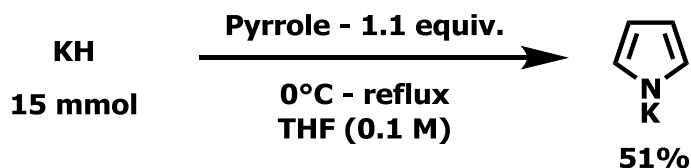
δ 159.5 (+), 114.7 (br. s, +).

HRMS (EI) calcd for C₅H₅ON (M⁺): 95.0366; found: 95.0362.

LRMS (ESI) (m/z, intensity %):

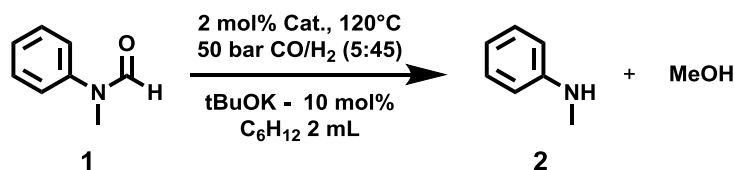
29 (43.7), 32 (1.3), 36 (2.6), 37 (19.5), 38 (38.4), 39 (100), 40 (65.6), 41 (84.4), 42 (2.9), 49 (2.0), 51 (6.0), 52 (4.4), 62 (1.9), 63 (2.1), 64 (3.8), 64 (4), 66 (11.9), 67 (56.2), 68 (2.5), 95 (71.8, M⁺), 96 (2.4).

[†] Separation of *N*-formylpyrrole from pyrrole by distillation was found to be challenging. To facilitate the isolation of *N*-formylpyrrole, before the second distillation, the remaining pyrrole was intentionally polymerized to polypyrrole with formic acid at rt for 24 h.



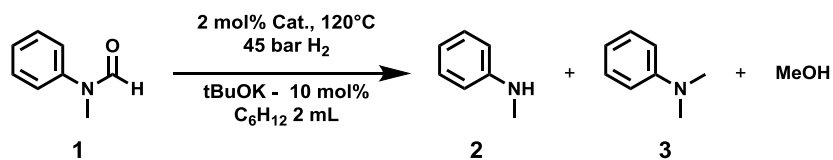
*Preparation of potassium pyrrole.*¹⁶ A flame-dried, 100-mL, Schlenck flask fitted with a magnetic stir bar and a rubber septum was charged with KH (600 mg, 15.0 mmol, 1.0 equiv.) followed by the addition of THF (15 mL). The resulting suspension was cooled in an ice-bath and pyrrole (1.145 mL, 16.5 mmol, 1.1 equiv.; freshly distilled) was added dropwise via syringe over the course of 5 minutes. During the addition of pyrrole gas evolution was observed. Under argon pressure the septum was replaced with a condenser and the flask was transfer into an oil bath and refluxed for 3 hours. The reaction mixture was cooled to room temperature and the the condenser was then replaced with a rubber septum. The suspension was allowed to settle and the liquid phase was carefully withdrawn with a syringe. The remaining white-yellow solid was washed with THF, diethyl ether and pentane (10 mL x 2 times each solvent) and dried under vacuum overnight giving potassium pyrrole (800 mg, 51%) as an off white solid. This material was stored under argon and used without further purification.

5. Procedures for amide and CO hydrogenations.



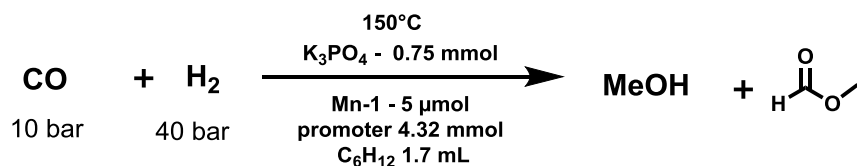
General procedure for hydrogenation of **1** in the presence of CO. (Table 1). An 8 mL glass vial containing a stirring bar was charged under argon with metal complex (5 μmol , 0.02 equiv.) and **1** (31 μL , 0.25 mmol, 1.0 equiv.). Then cyclohexane (2 mL) was added to the vial and followed by the addition *t*-BuOK (2.8 mg, 0.025 mmol, 0.1 equiv.). The vial was capped with a septum equipped with a syringe needle then placed into a 300 mL autoclave. Once sealed, the autoclave was purged three times with 5-10 bar of CO, then pressurized to 5 bar CO, followed by additional 45 bar H₂ (total pressure 50 bar). The autoclave was placed into an aluminum block and heated at 120°C for 18 h. Afterwards, the autoclave was cooled in an ice bath and the remaining gas was carefully released. To the reaction mixture *n*-hexadecane (50 μL) was added as an internal standard, and the reaction mixture was diluted with ethyl acetate and analyzed by gas chromatography.

Table S1. Hydrogenation of **1** with H₂.



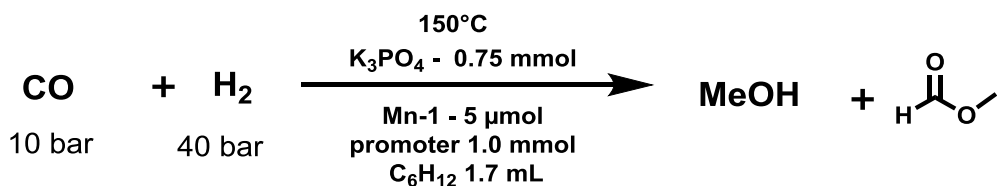
entry	Cat.	Conv., % ^b	2 ^b	3 ^b
1	Mn-1	99	94	0
2	Mn-2	99	90	10

^aReaction conditions: **1** (0.25 mmol), H₂ (45 bar at rt), **Cat.** (5 μmol), *t*-BuOK (0.025 mmol), C₆H₁₂ (2 mL), 120 °C, 18 h. ^bYields and conversions calculated from GC analysis using *n*-hexadecane as internal standard.



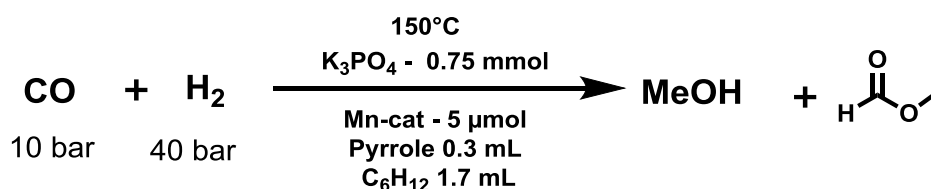
General procedure for hydrogenation of CO in the presence of N-promoter. (Table 2).

An 8 mL glass vial containing a stirring bar was charged under argon with **Mn-1** (2.5 mg, 5 μ mol) and *N*-promoter (4.32 mmol). Followed by the addition cyclohexane (1.7 mL) and anhydrous K_3PO_4 (159 mg, 0.75 mmol). The vial was capped with a septum equipped with a syringe needle then placed into a 300 mL autoclave. Once sealed, the autoclave was purged three times with 5-10 bar of CO, then pressurized to 10 bar CO, followed by additional 40 bar H_2 (total pressure 50 bar). The autoclave was placed into an aluminum block and heated at 150°C for 18 h. Then the autoclave was cooled in an ice bath and the remaining gas was carefully released. To the reaction mixture *n*-hexadecane (50 μ L) was added as an internal standard, and it was diluted with CCl_4 (1 mL) and analyzed by gas chromatography.



General procedure for CO hydrogenation with azole derivatives (Table 3). An 8 mL glass vial containing a stirring bar was charged under argon with **Mn-1** (2.5 mg, 5 μ mol) and tested promoter (1.0 mmol). Followed by the addition cyclohexane (1.7 mL) and anhydrous K_3PO_4 (159 mg, 0.75 mmol). The vial was capped with a septum equipped with a syringe needle then placed into a 300 mL autoclave. Once sealed, the autoclave

was purged three times with 5-10 bar of CO, then pressurized to 10 bar CO, followed by additional 40 bar H₂ (total pressure 50 bar). The autoclave was placed into an aluminum block and heated at 150°C for 18 h. Then the autoclave was cooled in an ice bath and the remaining gas was carefully released. To the reaction mixture *n*-hexadecane (50 µL) was added as an internal standard, and it was diluted with CCl₄ (1 mL) and analyzed by gas chromatography.



General procedure for hydrogenation of CO with various Mn-PNP complexes (Table 4).

General procedure for CO hydrogenation withazole derivatives (Table 3). An 8 mL glass vial containing a stirring bar was charged under argon with **Mn-cat** (5µmol) and pyrrole (0.3 mL, 4.32 mmol). Followed by the addition cyclohexane (1.7 mL) and anhydrous K₃PO₄ (159 mg, 0.75 mmol). The vial was capped with a septum equipped with a syringe needle then placed into a 300 mL autoclave. Once sealed, the autoclave was purged three times with 5-10 bar of CO, then pressurized to 10 bar CO, followed by additional 40 bar H₂ (total pressure 50 bar). The autoclave was placed into an aluminum block and heated at 150°C for 18 h. Then the autoclave was cooled in an ice bath and the remaining gas was carefully released. To the reaction mixture *n*-hexadecane (50 µL) was added as an internal standard, and the it was diluted with CCl₄ (1 mL) and analyzed by gas chromatography.

6. Optimization of reaction parameters.

Table S2. *N*-promoter optimization

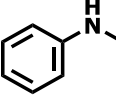
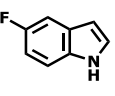
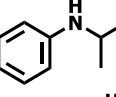
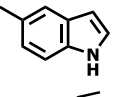
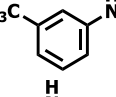
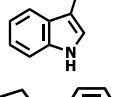
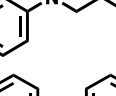
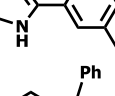
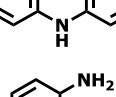
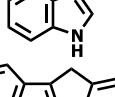
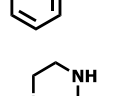
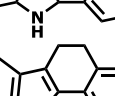
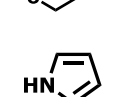
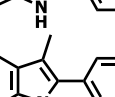
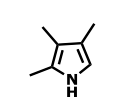
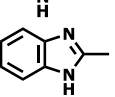
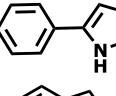
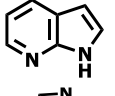
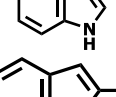
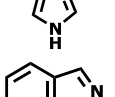
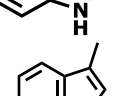
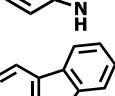
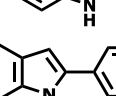
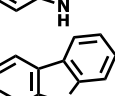
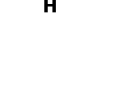



$ \begin{array}{c} \text{CO} + \text{H}_2 \xrightarrow[\text{C}_6\text{H}_{12} \text{ 2.0mL, 18 h}]{\begin{array}{c} 150^\circ\text{C} \\ \text{Mn-1- 5 } \mu\text{mol} \\ \text{promoter - 0.25 mmol} \\ t\text{-BuOK - 0.125 mmol} \end{array}} \text{MeOH} \end{array} $					
entry	Promoter	TON _{MeOH}	entry	Promoter	TON _{MeOH}
1		19	15		17
2		6	16		74
3		44	17		116
4		49	18		135
5		71	19		60
6		0	20		152
7		0	21		110
8		114	22		30
9		3	23		3
10		134	24		3
11		83	25		4
12		8	26		4
13		144	27		163
14		150	28		1

Table S3. Amount of pyrrole promoter.

CO + H ₂		150°C Mn-1- 5 µmol promoter - x, mmol t-BuOK - 0.125 mmol C ₆ H ₁₂ 2.0mL, 18 h	MeOH
20 bar	30 bar		
entry	Promoter	X, mmol	TON _{MeOH}
1	Pyrrole	0.25	118
2	Pyrrole	0.5	132
3	Pyrrole	1.0	169
4	Pyrrole	2.0	270
5	Pyrrole	4.0	413
6	Pyrrole	6.0	379
7	3-methylindole	4.0	550

Table S4. Solvent optimization

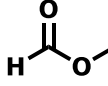
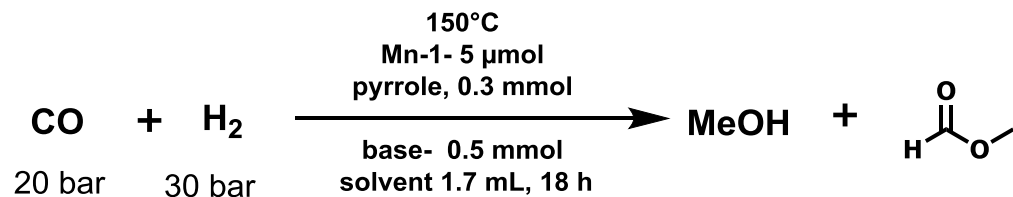
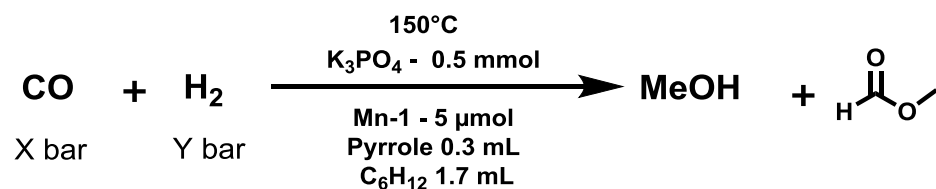
CO + H ₂		150°C Mn-1- 5 µmol pyrrole, 0.3 mmol t-BuOK - 0.125 mmol solvent 1.7 mL, 18 h	MeOH + 
20 bar	30 bar		
entry	Solvent	TON _{MeOH}	TON _{MF}
1	cyclohexane	305	35
2	heptane	307	37
3	CH ₃ CN	45	6
4	Et ₂ O	68	4
5	DCM	26	3
6	<i>i</i> -PrOH	165	32
7	toluene	259	33
8	THF	192	12
9	EtOH	46	5

Table S5. Base optimization

entry	Solvent	Base	TON _{MeOH}	TON _{MF}
1	THF	KOH	7	0
2	THF	<i>t</i> -BuOK	191	30
3	cyclohexane	<i>t</i> -BuOK	305	35
4	THF	<i>t</i> -BuONa	190	30
5	cyclohexane	<i>t</i> -BuONa	303	36
6	THF	<i>t</i> -BuOLi	75	14
7	THF	K ₂ CO ₃	8	0
8	THF	CS ₂ CO ₃	45	9
9	THF	K ₃ PO ₄	505	82
10	cyclohexane	K ₃ PO ₄	731	144

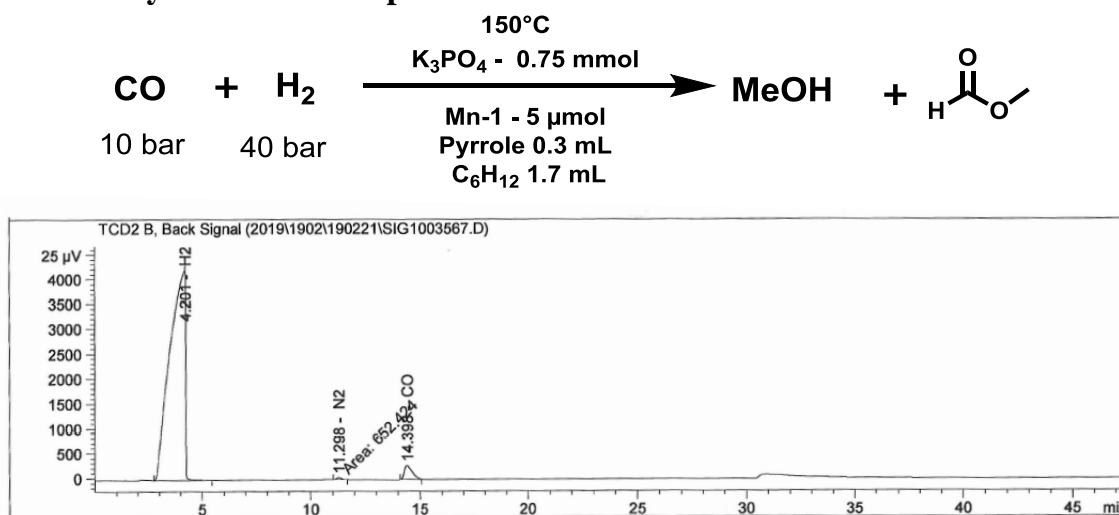
Table S6. Effect of CO to H₂ ratio

entry	P _{CO} , bar	P _{H₂} , bar	TON _{MeOH}	TON _{MF}
1	0	50	0	0
2	5	45	47	0
3	10	40	2094	27
4	20	30	700	128
5*	10	40	2550	112

* 0.75 mmol of K₃PO₄.

Table S7. Temperature effect on CO hydrogenation

		$\text{CO} + \text{H}_2 \xrightarrow[\text{Mn-cat - 5 } \mu\text{mol}]{\text{X } ^\circ\text{C}, \text{K}_3\text{PO}_4 - 0.75 \text{ mmol}} \text{MeOH} + \text{H}-\text{C}(=\text{O})-\text{O}-\text{CH}_3$	
		10 bar 40 bar Pyrrole 0.3 mL C ₆ H ₁₂ 1.7 mL	
entry	T, °C	TON _{MeOH}	TON _{MF}
1	80	24	32
2	100	157	88
3	120	948	224
4	140	2080	3
5	150	2550	112
6	160	1940	24
7	180	20	6

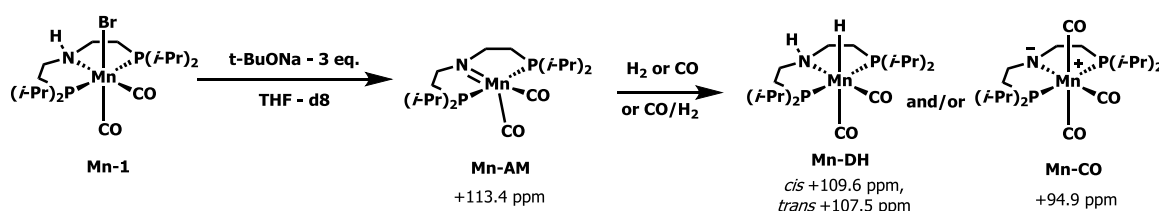
7. GC analysis of the headspace

RetTime [min]	Type	Area [25 µV*s]	Amt/Area	Amount [% Vol.]	Grp	Name
4.201	BB	2.10848e5	2.62629e-4	55.37477	H2	
10.800		-	-	-	O2	
11.298	MM	652.42438	0.00000	0.00000	N2	
14.398	BB	6644.58105	3.74022e-3	24.85223	CO	
26.900		-	-	-	CH4	
33.110		-	-	-	CO2	
54.300		-	-	-	Ethen	
Totals :				80.22700		

Figure. S3. Gas composition analysis by GC of the gas mixture after 18 h using pyrrole and Mn-1. (H₂ : CO : CO₂ – 69 : 31 : 0).

8. Mechanistic experiments

Treatment of in situ generated amido complex and with H₂/CO mixtures.



General procedure. An 8 mL glass vial containing a stirring bar was charged under argon with **Mn-1** (20.0 mg, 0.04 mmol, 1.0 equiv.), THF-*d*₈ (1 mL). Upon addition of *t*-BuONa (11.5 mg, 0.12 mmol, 3.0 equiv.) a deep red-orange solution was formed immediately. The vial was capped with a septum equipped with a syringe needle connected to an argon line and stirred at room temperature for 1 h. Under argon the reaction mixture was filtered through a Teflon filter using syringe and transferred into a new capped 8 mL vial with a stir bar. Then it was placed into a 300 mL autoclave and sealed. The autoclave was purged 3 times with H₂ or CO depending on the experiment and pressurized to desired pressure. The autoclave was placed into an aluminum block set at 25°C and stirred for 1 h. Finally the reaction mixture was transferred to J. Young valve NMR tube and analyzed by ³¹P NMR.

Table S8. Ratio of the observed complexes under CO and/or H₂ pressure.

entry	P _{CO} , bar	P _{H₂} , bar	Mn-AM	<i>cis</i> -Mn-DH	<i>trans</i> -Mn-AM	Mn-CO	Mn-(<i>t</i> -BuO) ¹⁷
³¹ P, ppm	NA	NA	+113.4	+109.6	+107.5	+94.9	+93.3
1	0	5	22	73	5	0	0
2	2	8	4	56	5	35	0
3	5	5	16	18	8	52	6
4	5	0	12	0	0	47	30

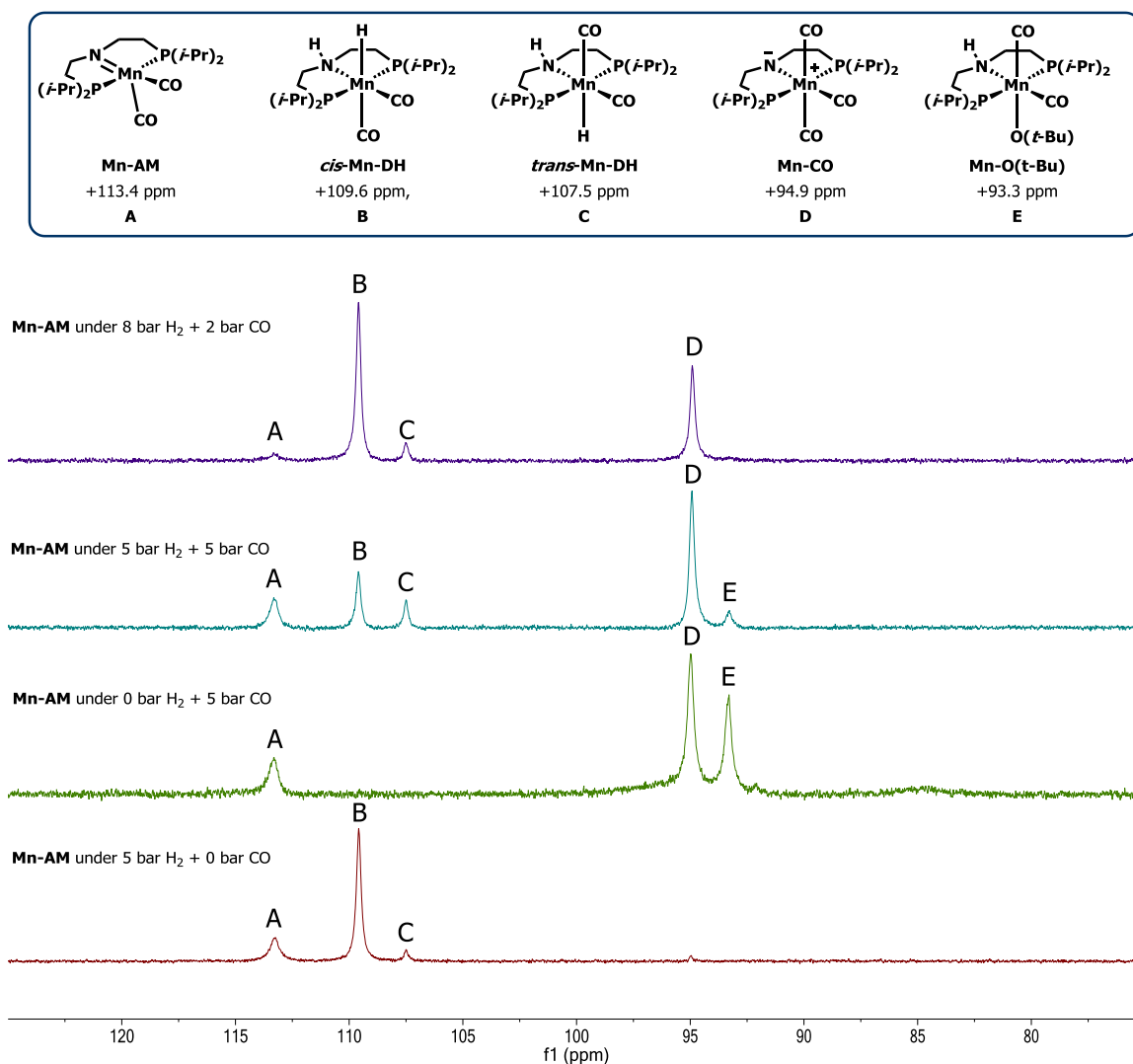
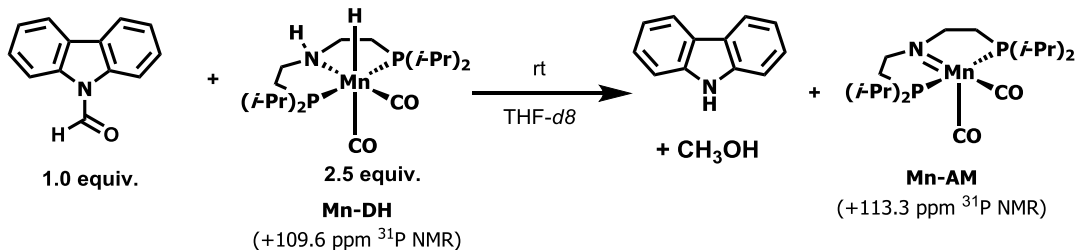


Figure S4. ³¹P NMR spectra of **Mn-AM** exposed to CO and/or H₂. Manganese dihydride complexes required for hydrogenation are formed even in the presence of CO gas.

Stoichiometric hydrogenation of formamides to methanol.

Complex **Mn-DH** was generated from corresponding **Mn-1** precursor via hydrodebromination and used for hydrogenation *N*-formylcarbazole.

Reaction procedure. An 8 mL glass vial containing a stirring bar was charged under argon with **Mn-1** (100.0 mg, 0.2 mmol, 2.5 equiv.), THF-*d*8 (2 mL). Upon addition of *t*-BuONa (38.33 mg, 0.4 mmol, 5.0 equiv.) a deep red-orange solution was formed immediately. The vial was capped with a septum equipped with a syringe needle connected to an argon line and stirred at room temperature for 1 h. Under argon the reaction mixture was filtered through a Teflon filter using syringe and transferred into a new capped 8 mL vial with a stir bar. Then it was placed into a 300 mL autoclave and sealed. The autoclave was purged 3 times with 5 bar H_2 pressurized to 10 bar H_2 . The autoclave was placed into an aluminum block set at 25°C and stirred for 1 h. The resulting reaction mixture was transferred to J. Young valve NMR tube containing *N*-formylcarbazole (15.6 mg, 0.08 mmol, 1.0 equiv) and analyzed by ^1H NMR, ^{13}C NMR and ^{31}P NMR.

Formation of carbazole and methanol was observed by ^1H and ^{13}C NMR. ^{31}P NMR shows the consumption of dihydride complex **Mn-DH** and regeneration of the amido **Mn-AM** complex.

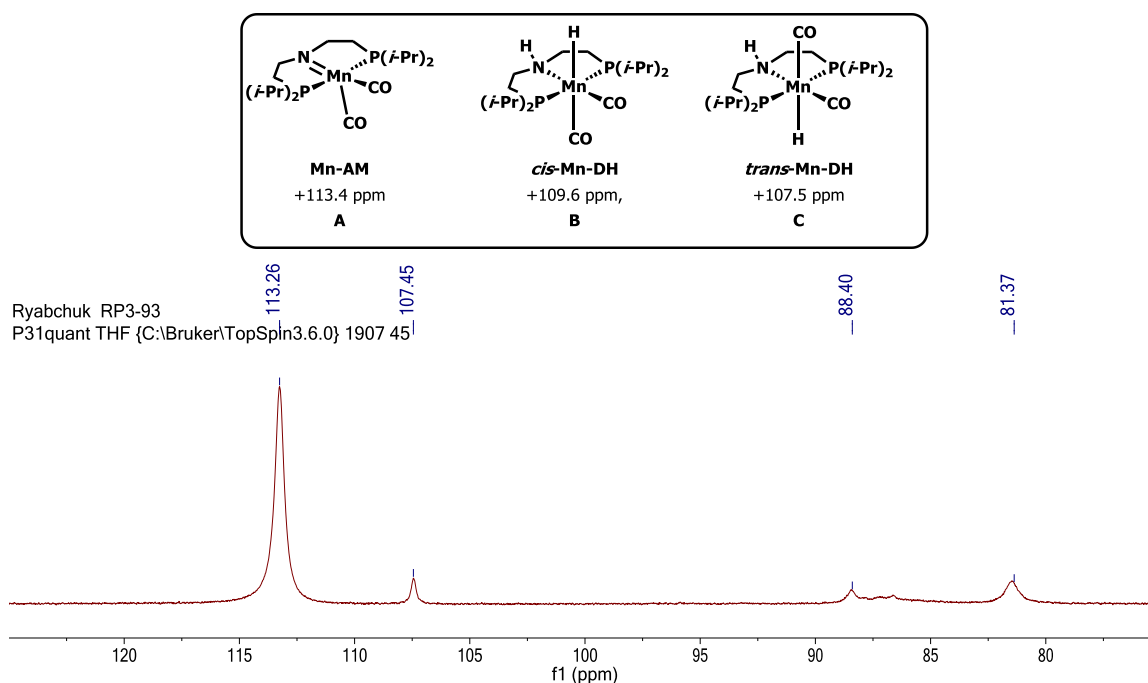


Figure S5. Crude ^{31}P NMR spectrum of N-formylcarbazole hydrogenation with **Mn-DH**. Comment: *cis*- isomer of **Mn-DH** is completely consumed (no signal at $+109.6 \text{ ppm}$), while the amido complex **Mn-AM** ($+113.4 \text{ ppm}$) is formed.

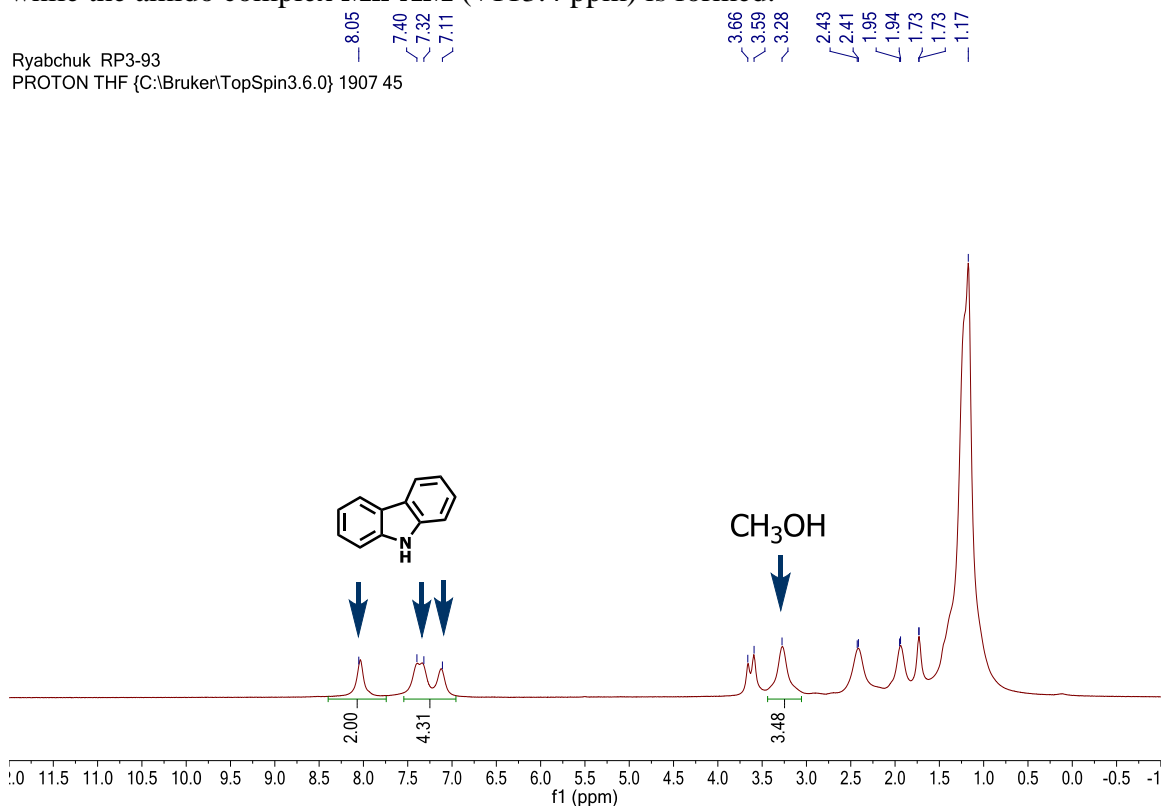


Figure S6. Crude ^1H NMR spectrum of N-formylcarbazole hydrogenation with **Mn-DH**. Upon addition of excess Mn-DH to formamide, methanol and free carbazole are formed.

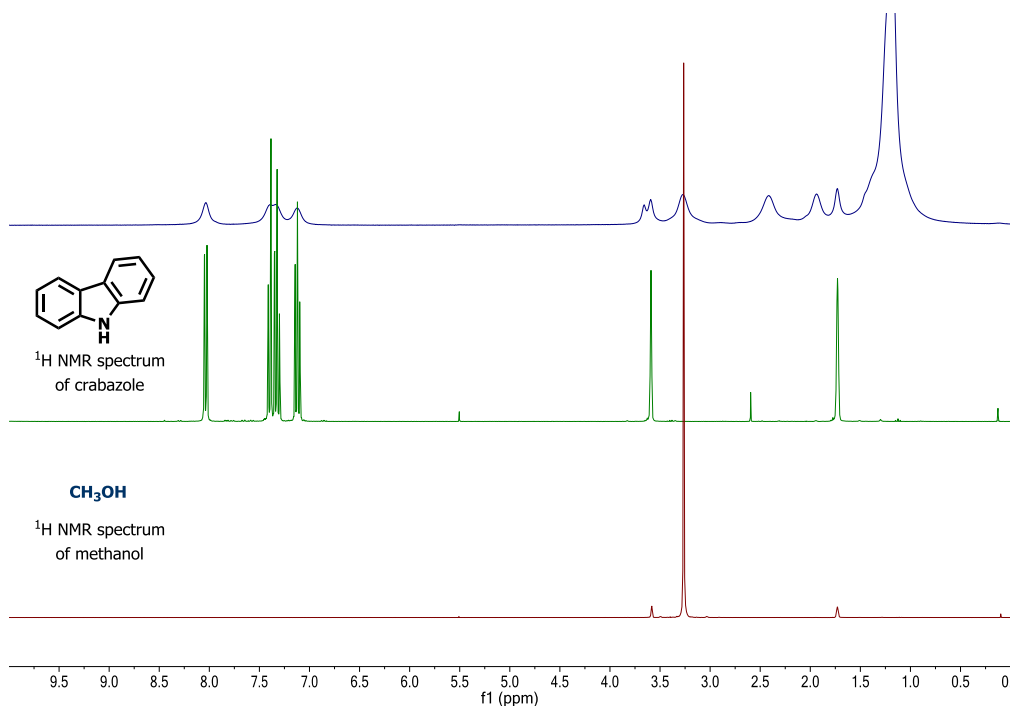


Figure S7. Crude ¹H NMR spectrum of N-formylcarbazole hydrogenation with **Mn-DH**. ¹H NMR spectra of free carbazole and methanol in THF-*d*₈ are presented for comparison

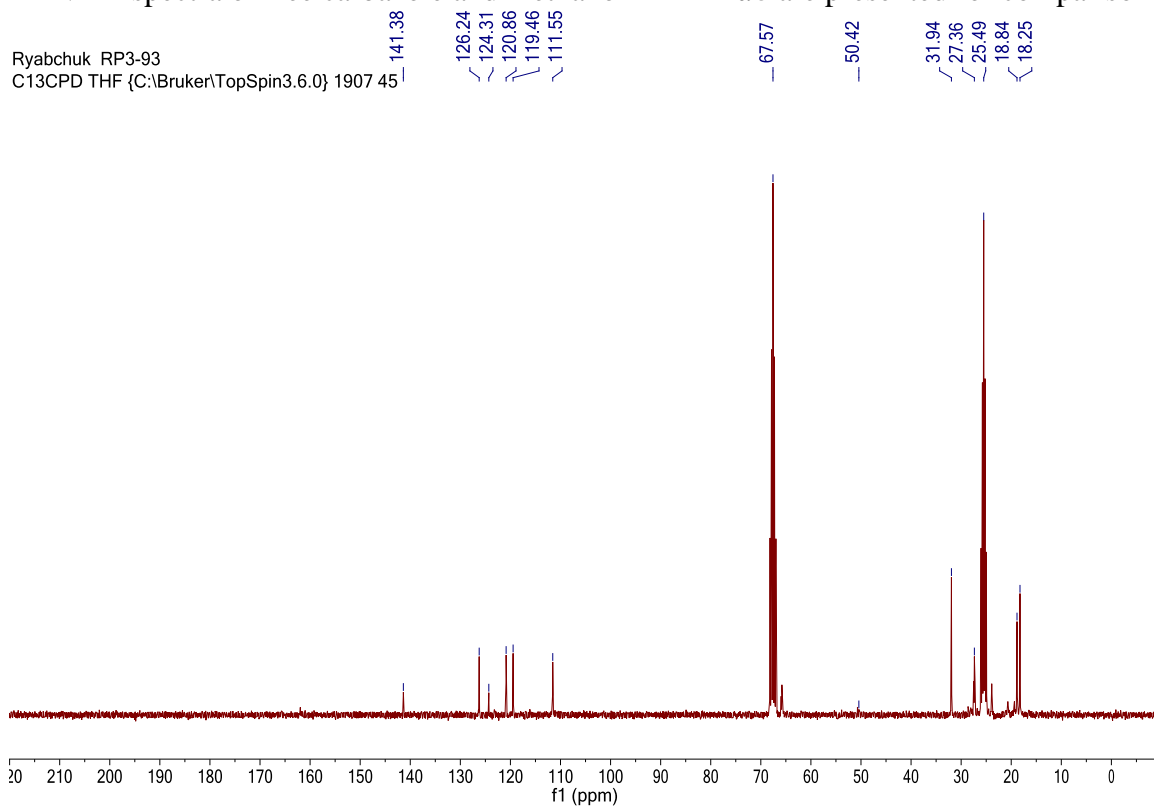


Figure S8. Crude ¹³C NMR spectrum of N-formylcarbazole hydrogenation with **Mn-DH**. Methanol and carbazole are observed.

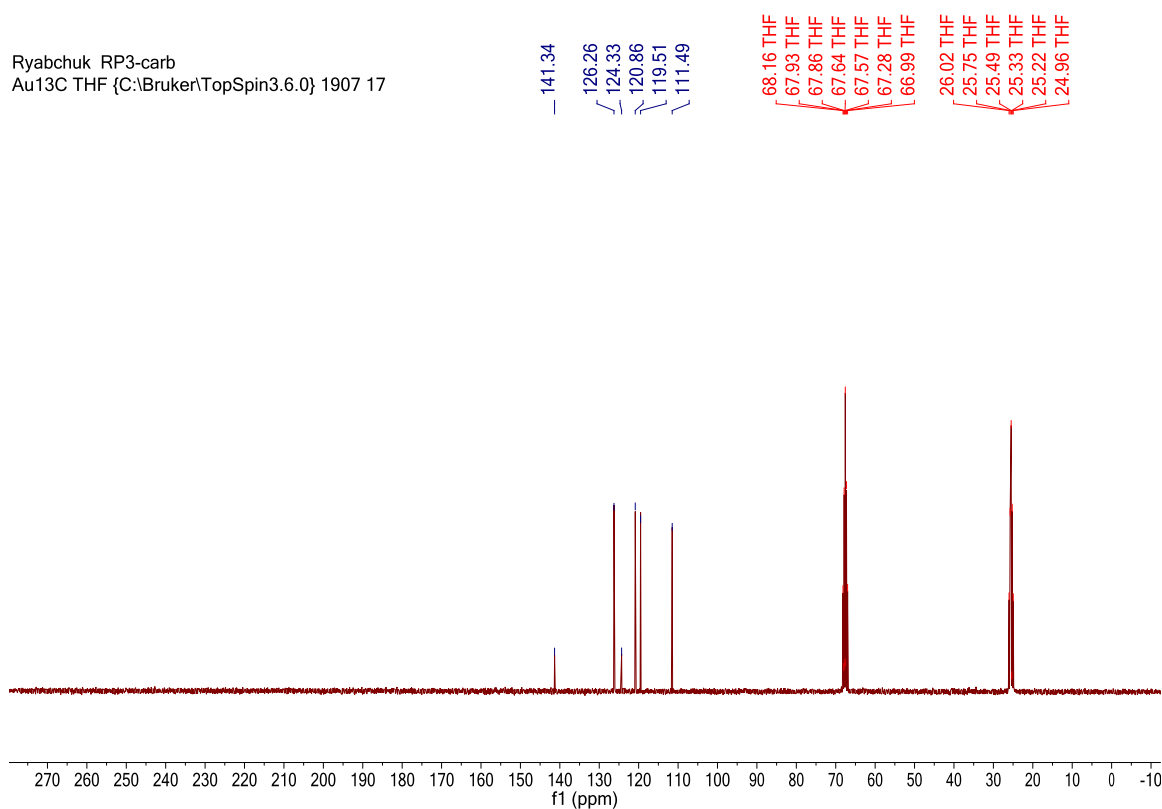


Figure S9. ^{13}C NMR spectrum of carbazole in $\text{THF-}d_8$ as reference.

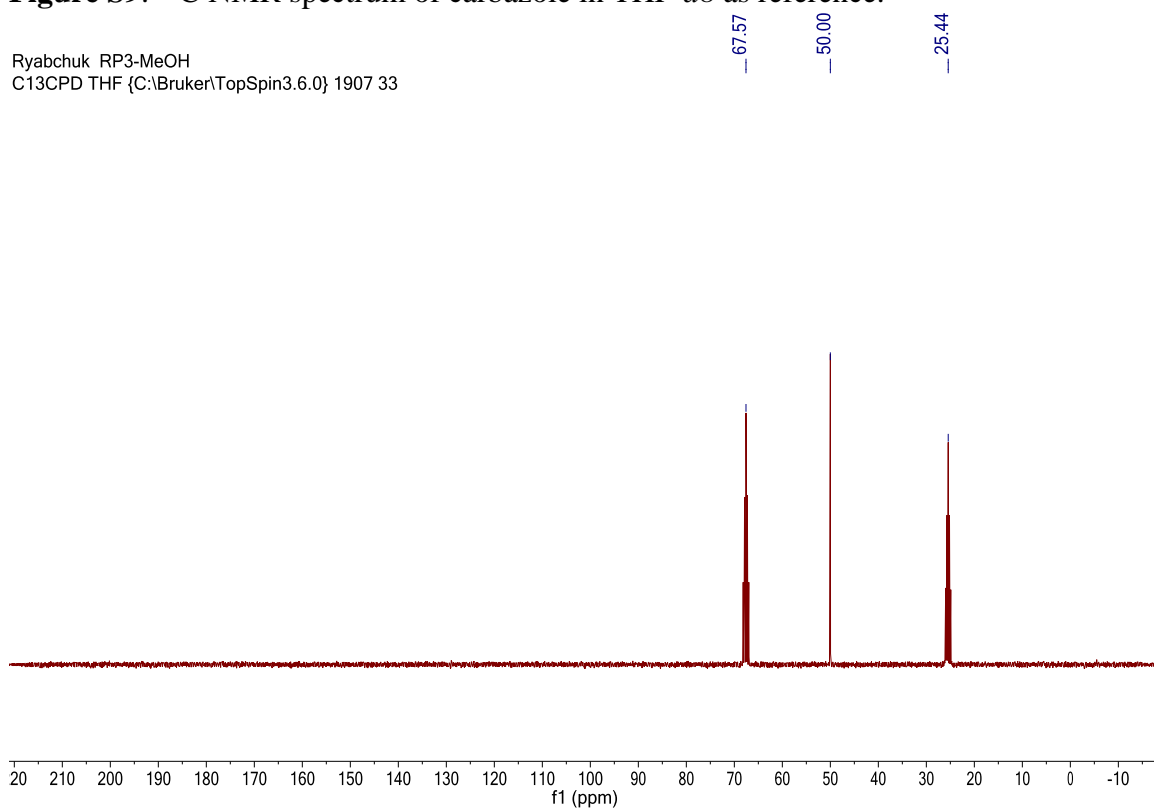
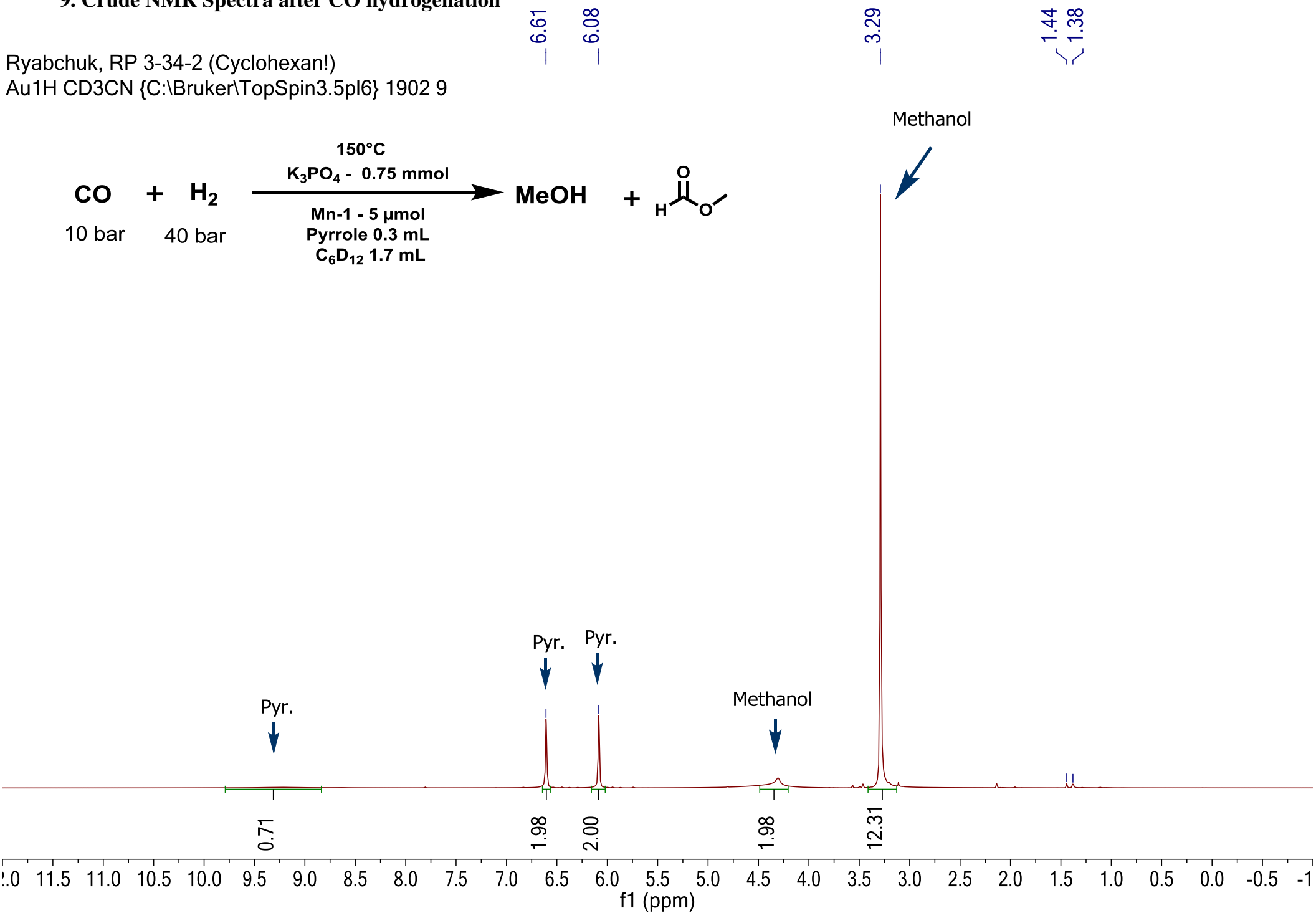
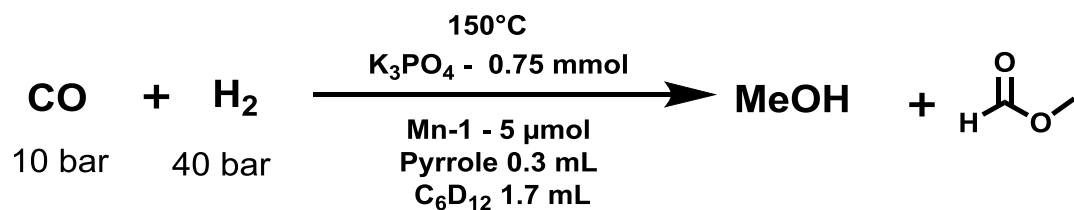


Figure S10. ^{13}C NMR spectrum of methanol in $\text{THF-}d_8$ as reference.

9. Crude NMR Spectra after CO hydrogenation

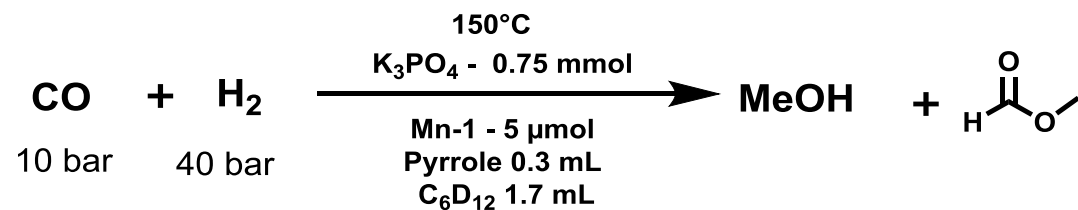
Ryabchuk, RP 3-34-2 (Cyclohexan!)

Au1H CD3CN {C:\Bruker\TopSpin3.5pl6} 1902 9

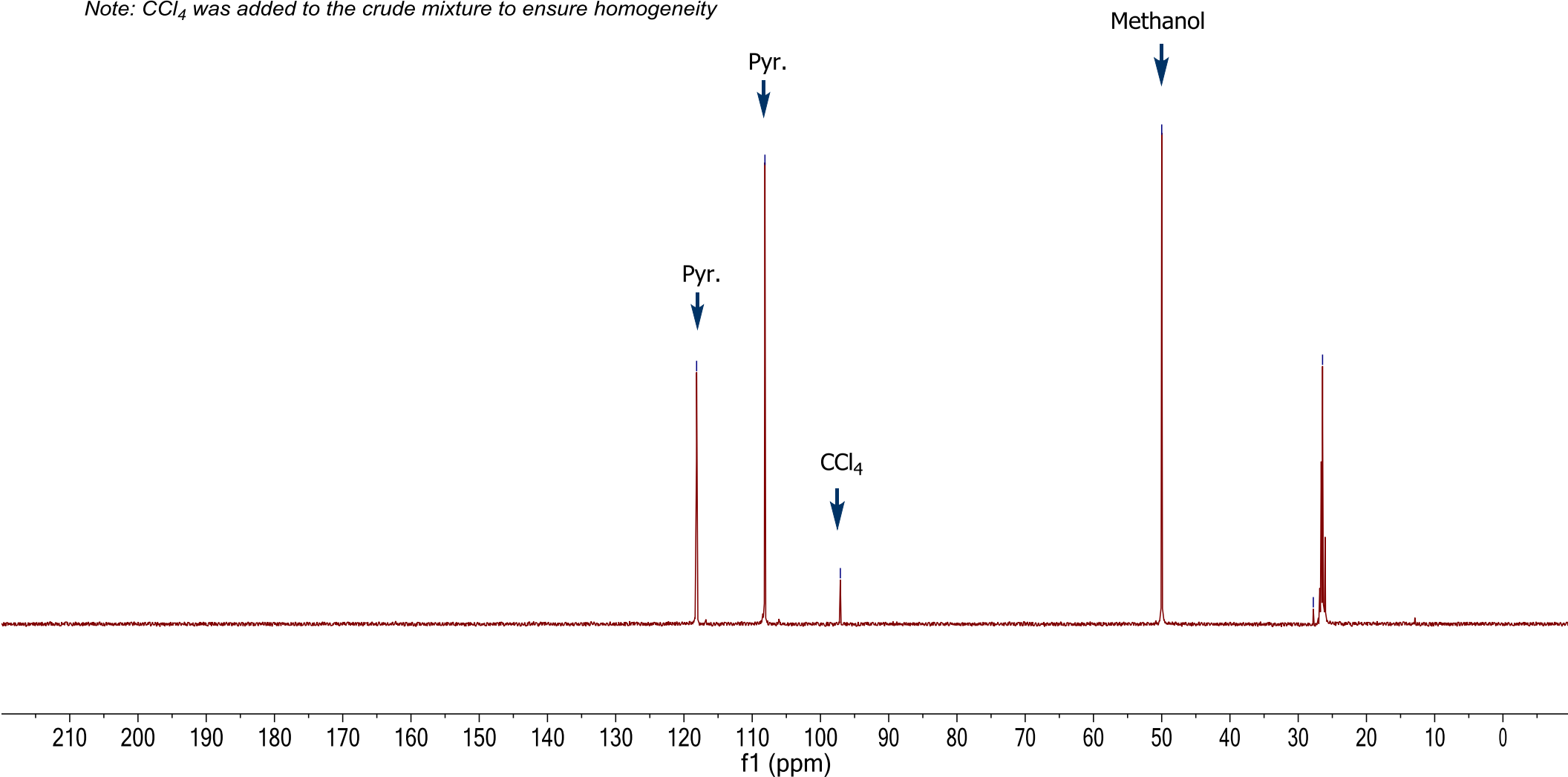


Ryabchuk, RP 3-34-2 (Cyclohexan!)

Au13C CD3CN {C:\Bruker\TopSpin3.5pl6} 1902 9



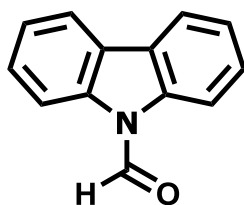
Note: CCl₄ was added to the crude mixture to ensure homogeneity



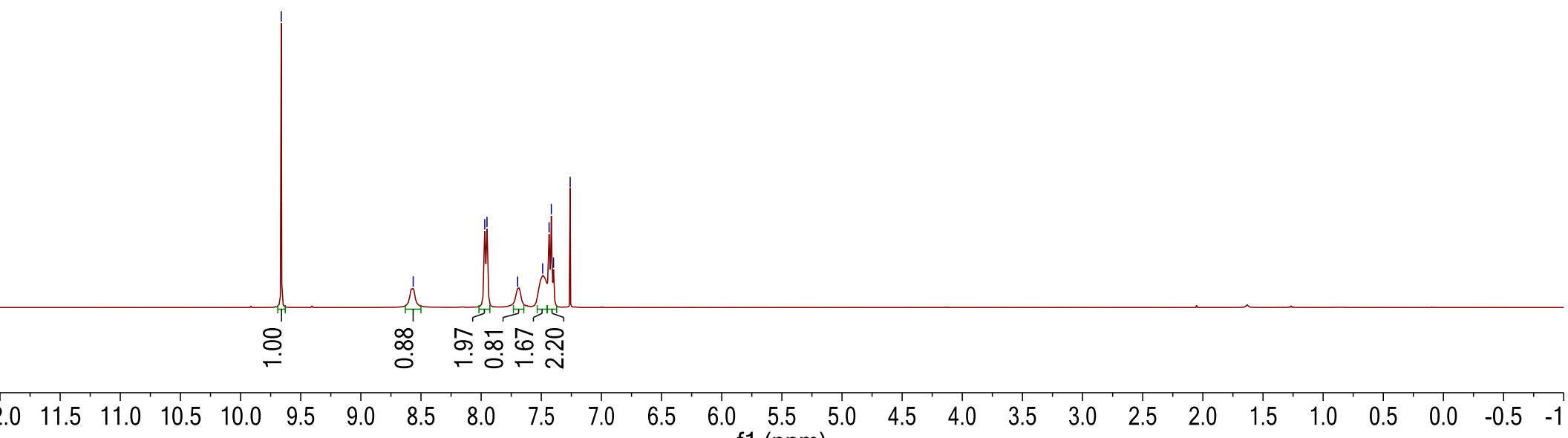
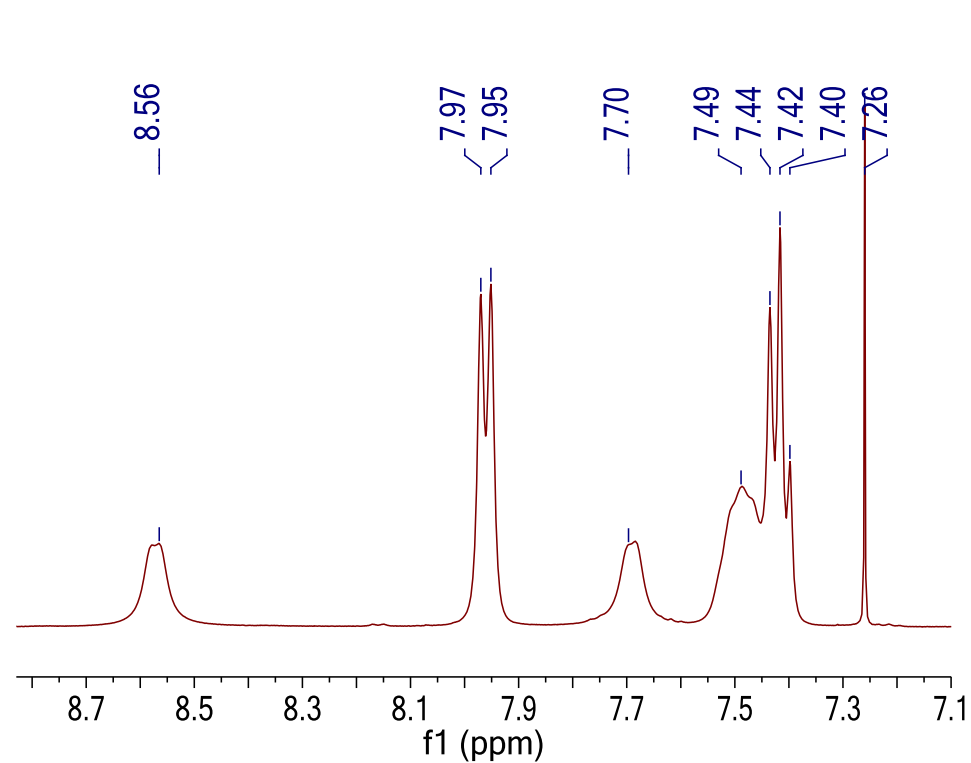
10. NMR Spectra of N-formylazoles.

Ryabchuk RP3-44

Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1903 12

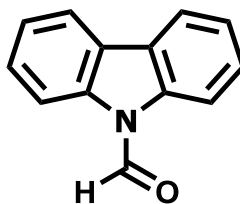


¹H NMR spectrum of
N-formylcarbazole

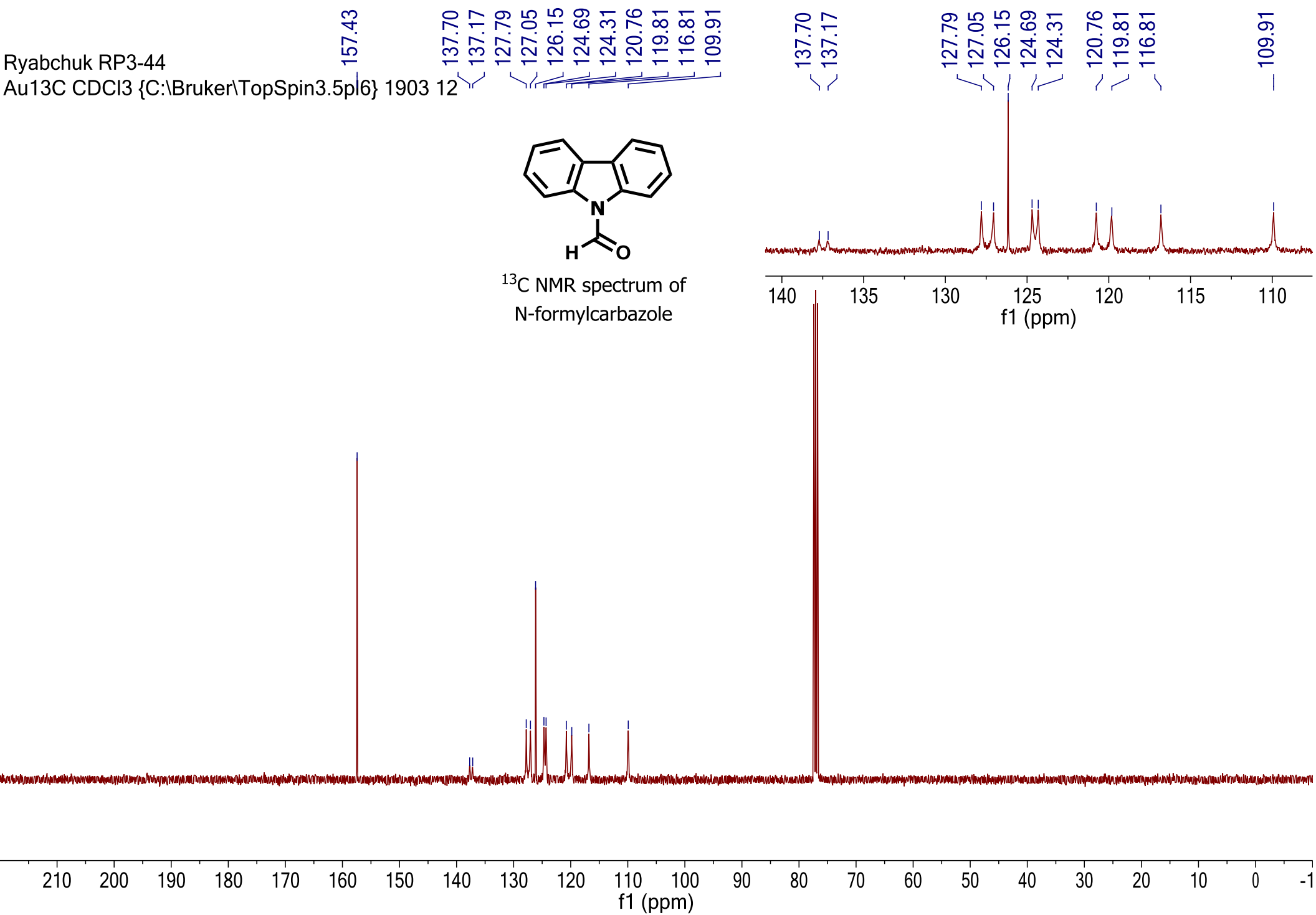


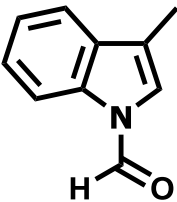
Ryabchuk RP3-44

Au13C CDCl₃ {C:\Bruker\TopSpin3.5pl6} 1903 12

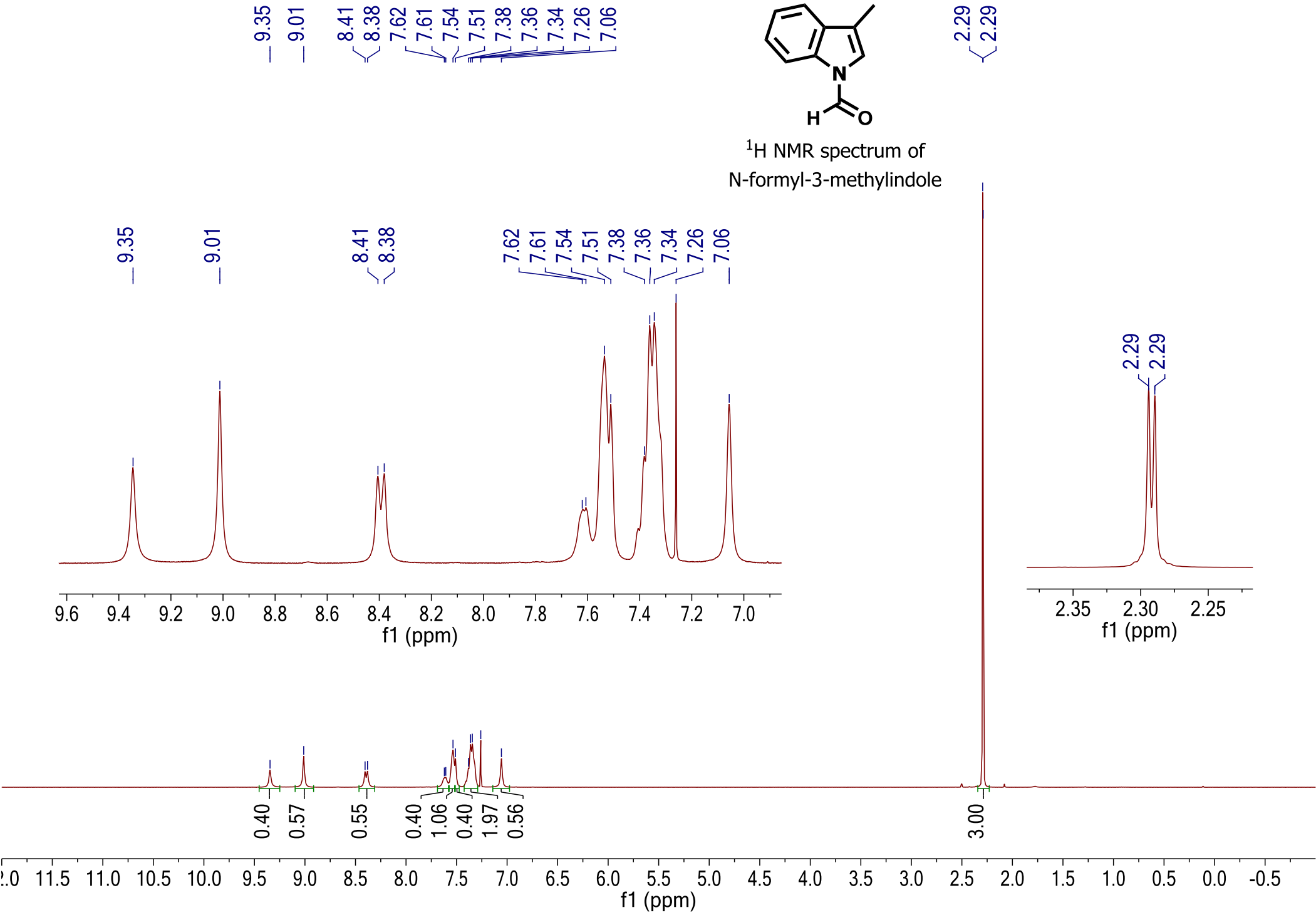


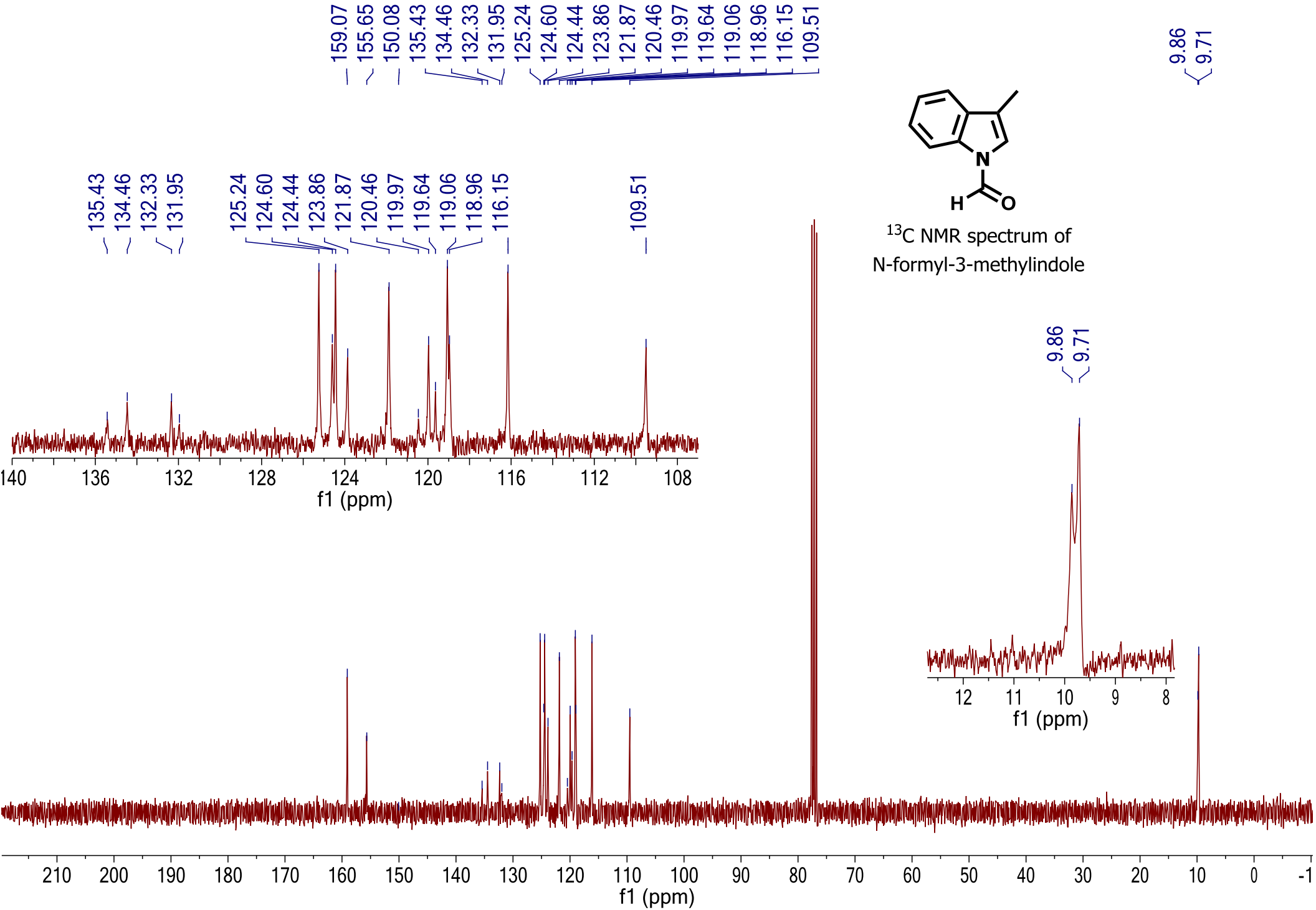
¹³C NMR spectrum of
N-formylcarbazole



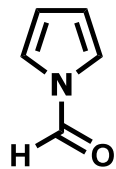


¹H NMR spectrum of
N-formyl-3-methylindole



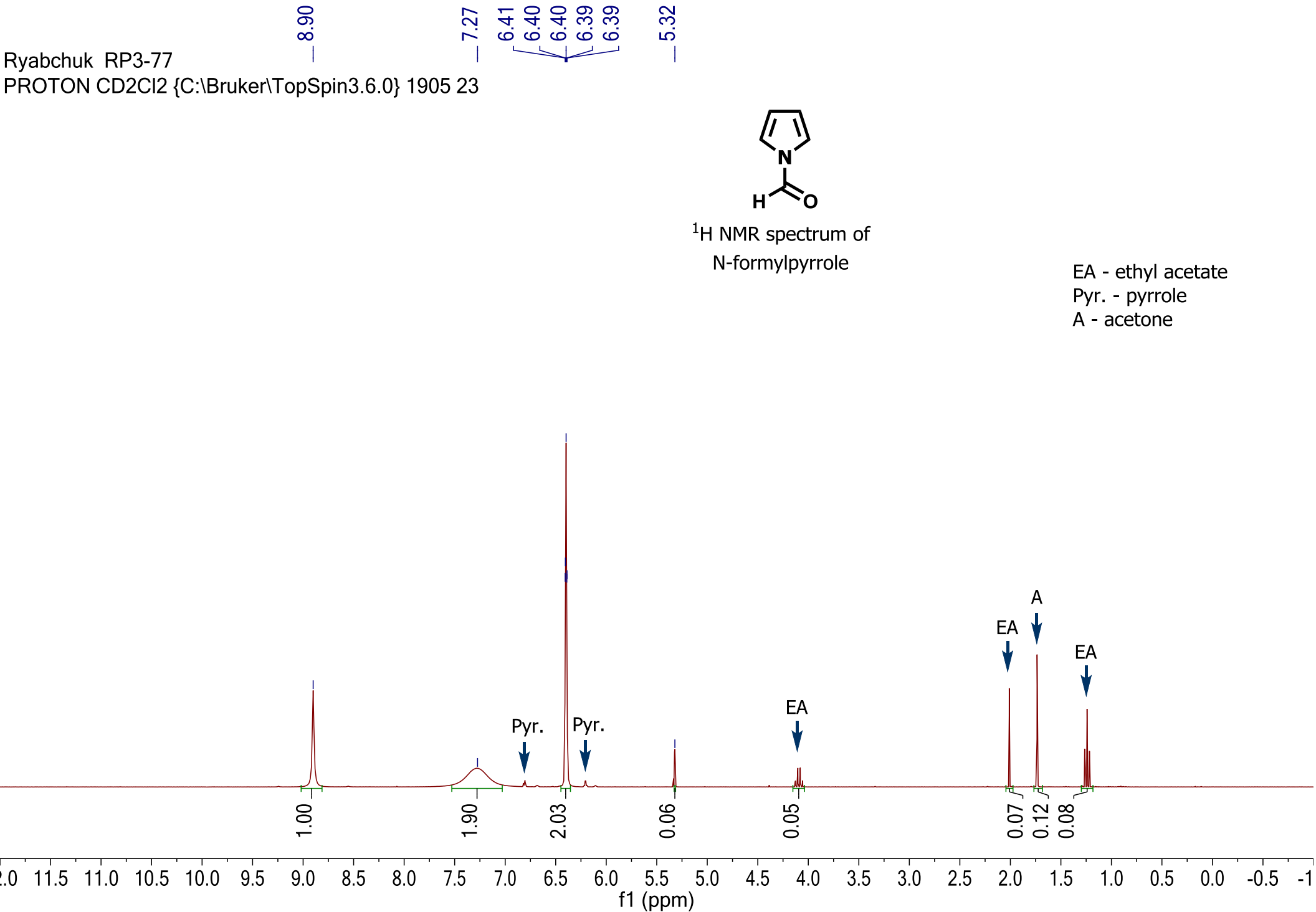


Ryabchuk RP3-77
PROTON CD2Cl2 {C:\Bruker\TopSpin3.6.0} 1905 23

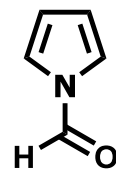


¹H NMR spectrum of
N-formylpyrrole

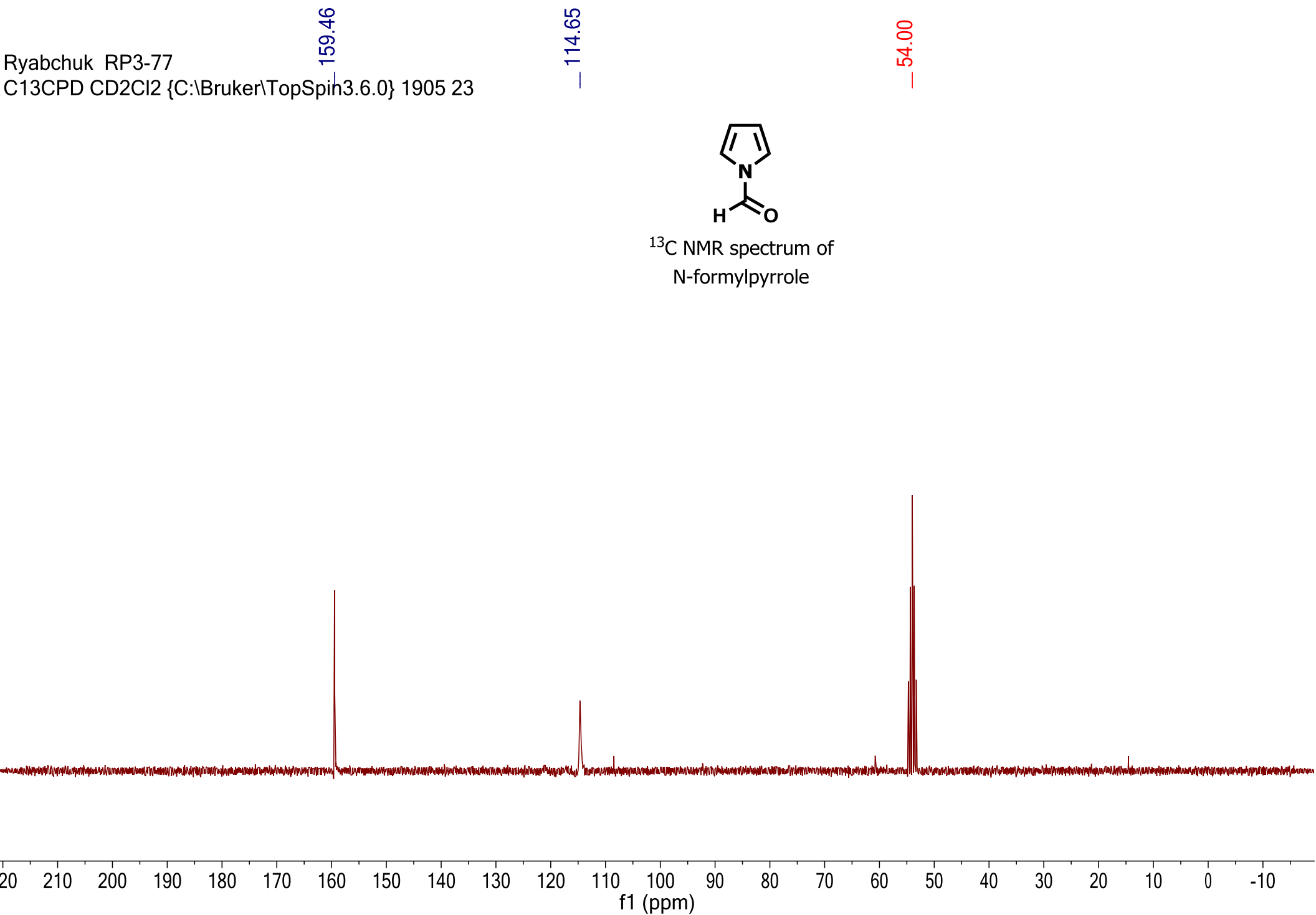
EA - ethyl acetate
Pyr. - pyrrole
A - acetone



Ryabchuk RP3-77
C13CPD CD2Cl2 {C:\Bruker\TopSpin3.6.0} 1905 23



^{13}C NMR spectrum of
N-formylpyrrole



10. Computational methods

Density functional theory (DFT) was used for the calculation of structures, total energy, and thermodynamic data. The hybrid PBE0 functional for exchange and correlation was used for optimizations and combined with a recent dispersion correction of Grimme (DFT-D version 3 with Becke-Johnson damping). The optimizations were performed using a triple zeta basis set def2-TZVP. The single point calculations were performed using DSD-PBE96-NL and a quadruple zeta valence basis set def2-QZVP. To check the integrity of the DSD-PBE96-NL//def2-QZVP total energies a comparison with DSD-PBE96-NL//def2-TZVP, B3LYP5-NL//def2-QZVP, and B3LYP5-NL//def2-TZVP total energies were performed.

Setup:

Density convergence	2.0E-5
Cutoff	1.0E-10
Optimization convergence	1.0E-4
Optimizer	BFGS

Structures and Energies:

C	-0.3781	-0.2589	-5.7995
O	0.7452	-0.2589	-5.7995

Promoters:

CO

TE [hartree]: -113.16854

ZPE [kJ/mol]: 13.41

G° [hartree]: -113.16343

Coordinates [Å]:

H2

TE [hartree]: -1.16707

ZPE [kJ/mol]: 26.39

G° [hartree]: -1.15702

Coordinates [Å]:

H 0.3051 -0.4104 0.2621

H -0.3040 -0.6260 0.6352

H₂O

TE [hartree]: -76.34193

ZPE [kJ/mol]: 56.36

G° [hartree]: -76.32046

Coordinates [Å]:

O -0.3466 -0.2727 -0.0239

H 0.6122 -0.2913 -0.0561

H -0.6317 -0.7308 -0.8174

CH₂O

TE [hartree]: -114.34792

ZPE [kJ/mol]: 70.07

G° [hartree]: -114.32123

Coordinates [Å]:

C 0.1054 0.9756 -0.2232

O -1.0647 1.2194 -0.2182

H 0.7137 0.9937 0.7034

H 0.6482 0.7179 -1.1550

NH₂Me

TE [hartree]: -95.70341

ZPE [kJ/mol]: 168.42

G° [hartree]: -95.63926

Coordinates [Å]:

N -0.7290 0.0012 -2.0395

C 0.7235 -0.0326 3.3261

H -1.0967 -0.4771 0.8122

H -1.0967 -0.4774 -0.8120

H 1.0979 0.4987 -0.8777

H 1.0979 0.4991 0.8776

H 1.1717 -1.0371 0.0002

HCONHMe

TE [hartree]: -208.90036

ZPE [kJ/mol]: 195.56

G° [hartree]: -208.82588

Coordinates [Å]:

C -0.6907 0.1802 0.2206

N 0.5871 -0.0353 -0.1577

O -1.2501 1.2508 0.2026

H -1.1877 -0.7508 0.5587

H 1.0941 0.7757 -0.4765

C 1.2431 -1.3140 -0.1326

H 0.5405 -2.0622 0.2375

H 2.1117 -1.3100 0.5314

H 1.5675 -1.6216 -1.1305

H₂COHNHMe

TE [hartree]: -210.08057

ZPE [kJ/mol]: 257.67

G° [hartree]: -209.98243

Coordinates [Å]:

C 0.0961 0.6622 -0.2286

N -0.1096 -0.7456 -0.0130

O -1.1180 1.3531 -0.1607

H 0.8105 1.0053 0.5349

H -0.6669 -1.1221 -0.7706

C 1.1168 -1.4981 0.1405

H 0.8823 -2.5542 0.2817

H 1.6454 -1.1549 1.0034

H 1.8110 -1.4134 -0.7106

H 0.5179 0.9083 -1.2148

H -1.5561 1.0526 0.6425

NH₂Et

TE [hartree]: -134.94925

ZPE [kJ/mol]: 243.55

G° [hartree]: -134.85649

Coordinates [Å]:

N -0.7974 0.1278 -0.1686

C 0.6271 0.1117 0.1210

H -1.2937 -0.4754 0.4766

H -0.9714 -0.2380 -1.0974

H 1.1164 0.8036 -0.5717

H 0.7687 0.5382 1.1191

C 1.3017 -1.2493 0.0458

H 0.8493 -1.9490 0.7548

H 2.3687 -1.1810 0.2772

H 1.2032 -1.6791 -0.9553

HCONHEt

TE [hartree]: -248.14632

ZPE [kJ/mol]: 270.59

G° [hartree]: -248.04325

Coordinates [Å]:

C -0.6529 0.3499 0.2318

N 0.6428 0.0088 0.0674

O -1.0827 1.4792 0.2290

H -1.3006 -0.5372 0.3803

H 1.2822 0.7721 -0.0956

C 1.1351 -1.3453 0.0168

H 0.3219 -1.9956 0.3503

H 1.9454 -1.4659 0.7433

C 1.6051 -1.7597 -1.3657

H 0.7885 -1.6958 -2.0876

H 1.9777 -2.7864 -1.3537

H 2.4153 -1.1145 -1.7144

H₂COHNHEt

TE [hartree]: -249.32598

ZPE [kJ/mol]: 331.96

G° [hartree]: -249.19954

Coordinates [Å]:

C 0.9982 -0.7050 -0.2444

N -0.2368 -0.6546 0.4847

O 0.7740 -1.0420 -1.5903

H 1.5380 0.2511 -0.2841

H -0.0934 -0.8664 1.4625

C -1.0241 0.5542 0.3068

H -1.0727 0.7465 -0.7682

H -2.0491 0.3460 0.6284

H 1.6462 -1.4400 0.2513

H 0.1531 -1.7782 -1.5795

C -0.4975 1.7809 1.0365

H -0.4894 1.6191 2.1184

H -1.1239 2.6537 0.8354

H 0.5205 2.0263 0.7251

NHMe₂

TE [hartree]: -134.93658

ZPE [kJ/mol]: 243.30

G° [hartree]: -134.84391

Coordinates [Å]:

N -0.1111 -0.5271 0.5231
 C -0.6319 0.4340 -0.4210
 C 1.3322 -0.5859 0.5211
 H -0.4923 -1.4431 0.3263
 H -0.3262 1.4404 -0.1205
 H -1.7233 0.4064 -0.4180
 H -0.2839 0.2801 -1.4571
 H 1.7349 0.3704 0.8677
 H 1.7725 -0.7882 -0.4705
 H 1.6752 -1.3579 1.2128

HCONMe2

TE [hartree]: -248.13908

ZPE [kJ/mol]: 268.38

G° [hartree]: -248.03686

Coordinates [Å]:

C 0.6662 -1.1185 -0.9103
 N -0.0393 -0.1243 -0.3245
 O 1.8731 -1.1965 -0.9560
 C 0.6410 0.9679 0.3196
 C -1.4750 -0.1195 -0.3213
 H 0.0039 -1.8822 -1.3607
 H 1.7129 0.8052 0.2238
 H 0.3744 1.0186 1.3802
 H 0.3745 1.9206 -0.1491
 H -1.8447 -1.0035 -0.8429
 H -1.8679 0.7693 -0.8264
 H -1.8675 -0.1320 0.7010

H2COHNMe2

TE [hartree]: -249.31752

ZPE [kJ/mol]: 331.05

G° [hartree]: -249.19142

Coordinates [Å]:

C 0.3447 -0.5256 -0.8027
 N 0.6117 0.1858 0.4045
 O -1.0211 -0.6178 -1.1863
 C 0.1277 -0.4732 1.5932
 C 0.2325 1.5800 0.3551
 H 0.8326 -0.0037 -1.6280
 H 0.7798 -1.5280 -0.7112
 H -1.4581 -1.2541 -0.6155
 H -0.9714 -0.4566 1.6921
 H 0.5390 0.0158 2.4794
 H 0.4599 -1.5147 1.6003
 H -0.8566 1.7307 0.3194
 H 0.6682 2.0470 -0.5306
 H 0.6211 2.0944 1.2372

Piperidin

TE [hartree]: -251.47909

ZPE [kJ/mol]: 418.68

G° [hartree]: -251.31962

Coordinates [Å]:

C 0.6690 1.2243 -0.2368
 C 1.4310 -0.0009 0.2381
 C 0.7194 -1.2739 -0.1999
 C -0.7392 -1.2507 0.2373
 C -1.4171 0.0228 -0.2369
 N -0.6934 1.1780 0.2591
 H 0.7090 1.2575 -1.3425
 H 1.1456 2.1361 0.1328
 H 1.4940 0.0280 1.3310

H 2.4530 0.0246 -0.1508
 H 1.2275 -2.1566 0.1984
 H 0.7650 -1.3519 -1.2936
 H -0.7959 -1.2907 1.3302
 H -1.2738 -2.1221 -0.1517
 H -2.4446 0.0676 0.1335
 H -1.4670 0.0053 -1.3426
 H -1.1835 2.0288 0.0182

HCO Piperidin

TE [hartree]: -364.68178

ZPE [kJ/mol]: 445.06

G° [hartree]: -364.51227

Coordinates [Å]:

C 0.7264 0.7720 -0.1489
 C 1.4771 -0.4774 0.2868
 C 0.7501 -1.7300 -0.1842
 C -0.6995 -1.7227 0.2831
 C -1.4056 -0.4479 -0.1507
 N -0.6540 0.7150 0.2662
 C -1.2137 1.6648 1.0464
 O -2.3557 1.6687 1.4498
 H 0.7730 0.8634 -1.2433
 H 1.1773 1.6733 0.2727
 H 1.5523 -0.4833 1.3797
 H 2.4960 -0.4473 -0.1089
 H 1.2638 -2.6256 0.1744
 H 0.7767 -1.7705 -1.2805
 H -0.7357 -1.7910 1.3756
 H -1.2378 -2.5883 -0.1121
 H -2.4011 -0.3621 0.2835

H -1.5082 -0.4322 -1.2444
 H -0.4953 2.4714 1.2897

H₂COHPiperidin

TE [hartree]: -365.85699

ZPE [kJ/mol]: 505.94

G° [hartree]: -365.66429

Coordinates [Å]:

C 1.0966 0.9543 0.1873
 C 1.8439 -0.1085 -0.6119
 C 1.6405 -1.4782 0.0216
 C 0.1559 -1.7713 0.1900
 C -0.5324 -0.6450 0.9548
 N -0.3146 0.6699 0.3680
 C -1.1467 0.9425 -0.7713
 O -2.4734 1.1824 -0.3788
 H 1.1961 1.9376 -0.2807
 H 1.5493 1.0281 1.1846
 H 2.9079 0.1431 -0.6596
 H 1.4752 -0.1202 -1.6445
 H 2.1241 -1.4904 1.0069
 H 2.1246 -2.2574 -0.5736
 H 0.0026 -2.7190 0.7146
 H -0.3078 -1.8835 -0.7965
 H -0.1501 -0.6205 1.9826
 H -1.6095 -0.8117 1.0174
 H -1.2164 0.1159 -1.4931
 H -0.7147 1.8087 -1.2910
 H -2.4242 1.7901 0.3668

NH₂Ph

TE [hartree]: -287.12486

ZPE [kJ/mol]: 308.39

G° [hartree]: -287.00740

Coordinates [Å]:

C -0.6604 1.1249 0.0790

C 0.7227 1.1710 0.0684

C 1.4722 0.0061 -0.0117

C 0.8109 -1.2117 -0.0788

C -0.5718 -1.2687 -0.0688

C -1.3293 -0.0985 0.0098

H -1.2343 2.0443 0.1379

H 1.2204 2.1327 0.1256

H 2.5543 0.0467 -0.0196

H 1.3780 -2.1340 -0.1382

H -1.0765 -2.2280 -0.1262

N -2.7138 -0.1468 -0.0385

H -3.1867 0.6496 0.3553

H -3.1247 -1.0185 0.2522

HCONHPh

TE [hartree]: -400.31723

ZPE [kJ/mol]: 336.32

G° [hartree]: -400.18913

Coordinates [Å]:

C -1.0460 -2.5609 -0.0834

N -1.4566 -1.2722 0.0577

O 0.0922 -2.9522 -0.1639

H -1.9131 -3.2473 -0.1181

H -2.4541 -1.1422 0.1057

C -0.6919 -0.1024 0.1408

C 0.7010 -0.1030 0.1001

C 1.3809 1.1018 0.1884

C 0.7026 2.3037 0.3161

C -0.6840 2.2978 0.3565

C -1.3774 1.1049 0.2697

H 1.2308 -1.0380 7.4928

H 2.4643 1.0937 0.1559

H -1.2323 3.2274 0.4560

H -2.4627 1.1059 0.3014

H 1.2480 3.2371 0.3837

H₂COHNHPh

TE [hartree]: -401.50218

ZPE [kJ/mol]: 397.79

G° [hartree]: -401.35067

Coordinates [Å]:

C 1.4982 1.7603 -0.9472

N 0.1272 1.3629 -0.9324

O 2.0333 2.1036 0.3120

H 2.0880 0.9674 -1.4197

H -0.5184 2.1243 -0.7935

H 1.5889 2.6566 -1.5603

H 1.9646 1.3335 0.8852

C -0.2674 0.1853 -0.3123

C 0.6251 -0.8578 -0.0507

C 0.1782 -2.0350 0.5305

C -1.1532 -2.2030 0.8723

C -2.0423 -1.1661 0.6203

C -1.6093 0.0101 0.0393

H 1.6723 -0.7666 -0.3138

H 0.8912 -2.8300 0.7185

H -3.0894 -1.2727 0.8807
H -2.3157 0.8109 -0.1552
H -1.4938 -3.1237 1.3292

NHPhPh

TE [hartree]: -517.77372

ZPE [kJ/mol]: 521.35

G° [hartree]: -517.57515

Coordinates [Å]:

C -0.5367 0.3788 -0.1876
C 0.8465 0.2821 -0.0235
C 1.4111 -0.8939 0.4414
C 0.6255 -1.9973 0.7388
C -0.7478 -1.9094 0.5603
C -1.3248 -0.7360 0.1112
N -1.1596 1.5139 -0.6825
H -2.0482 1.3593 -1.1260
H -2.4018 -0.6709 -0.0072
H -1.3812 -2.7607 0.7829
H 1.0764 -2.9139 1.0982
H 2.4876 -0.9485 0.5592
H 1.4809 1.1183 -0.2858
C -0.7053 2.8236 -0.6996
C -1.2091 3.6931 -1.6706
C -0.8253 5.0214 -1.6971
C 0.0809 5.5124 -0.7683
C 0.5810 4.6533 0.1988
C 0.1925 3.3248 0.2451
H -1.9028 3.0313 -2.4138
H -1.2310 5.6756 -2.4605
H 1.2778 5.0230 0.9427

H 0.5649 2.6801 1.0301
H 0.3879 6.5506 -0.7945

HCONHPhPh

TE [hartree]: -630.96460

ZPE [kJ/mol]: 548.10

G° [hartree]: -630.75584

Coordinates [Å]:

C -0.6608 0.4530 -0.2763
C 0.6722 0.2607 -0.6257
C 1.3709 -0.8167 -0.1120
C 0.7461 -1.7172 0.7418
C -0.5813 -1.5252 1.0879
C -1.2828 -0.4357 0.5916
N -1.3806 1.5503 -0.8154
H -2.8270 0.2329 -1.4165
H -2.3086 -0.2595 0.8930
H -1.0741 -2.2143 1.7637
H 1.2962 -2.5615 1.1395
H 2.0409 -0.9610 -0.3882
H 1.1519 0.9626 -1.2974
C -0.8304 2.8543 -0.7114
C -0.9692 3.7777 -1.7416
C -0.4118 5.0392 -1.6093
C 0.2885 5.3890 -0.4647
C 0.4246 4.4644 0.5599
C -0.1351 3.2039 0.4418
H -1.5203 3.5127 -2.6321
H -0.5258 5.7540 -2.4159
H 0.9640 4.7253 1.4629
H -0.0306 2.4822 1.2429

H 0.7244 6.3766 -0.3710
 C -2.6063 1.3137 -1.3887
 O -3.3597 2.1483 -1.8215

H₂COHNHPhPh

TE [hartree]: -632.14505

ZPE [kJ/mol]: 609.24

G° [hartree]: -631.91300

Coordinates [Å]:

C -0.6894 0.4198 -0.2762
 C 0.6942 0.3718 -0.4899
 C 1.4399 -0.7042 -0.0529
 C 0.8355 -1.7703 0.6028
 C -0.5299 -1.7292 0.8206
 C -1.2895 -0.6458 0.4002
 N -1.4175 1.5032 -0.7675
 H -3.2008 0.4697 -0.8991
 H -2.3481 -0.6354 0.6223
 H -1.0215 -2.5442 1.3401
 H 1.4231 -2.6156 0.9392
 H 2.5083 -0.7158 -0.2375
 H 1.1754 1.1890 -1.0133
 C -0.8285 2.7931 -0.6983
 C -0.8177 3.6105 -1.8247
 C -0.2772 4.8871 -1.7542
 C 0.2714 5.3493 -0.5682
 C 0.2718 4.5317 0.5545
 C -0.2800 3.2638 0.4934
 H -1.2252 3.2254 -2.7511
 H -0.2705 5.5152 -2.6376
 H 0.7002 4.8868 1.4848

H -0.2773 2.0619 1.3650
 H 0.7036 6.3418 -0.5184
 C -2.8669 1.4777 -0.6546
 O -3.4919 2.3302 -1.5611
 H -3.3056 3.2395 -1.3080
 H -3.1806 1.7153 0.3766

Pyrrol

TE [hartree]: -209.82546

ZPE [kJ/mol]: 217.89

G° [hartree]: -209.74246

Coordinates [Å]:

C -0.9756 -0.0441 0.0000
 N -0.1556 -1.1337 0.0000
 C 1.1485 -0.7357 0.0000
 C -0.1819 1.0742 0.0000
 C 1.1655 0.6354 0.0000
 H -2.0482 -0.1502 0.0000
 H -0.4661 -2.0873 0.0000
 H 1.9530 -1.4530 0.0000
 H -0.5310 2.0947 0.0000
 H 2.0485 1.2548 0.0000

HCOPyrrol

TE [hartree]: -323.01135

ZPE [kJ/mol]: 243.40

G° [hartree]: -322.91864

Coordinates [Å]:

C -0.9761 0.5918 -0.0178
 N -0.1343 -0.5057 0.0052
 C 1.1763 -0.0746 0.0176

C -0.2030 1.7087 -0.0201
 C 1.1625 1.2848 0.0023
 C -0.5556 -1.8228 0.0143
 O 0.1807 -2.7670 0.0345
 H -2.0464 0.4631 -0.0304
 H 1.9784 -0.7926 0.0361
 H -0.5627 2.7255 -0.0361
 H 2.0327 1.9224 0.0066
 H -1.6563 -1.9014 0.0007

H2COHPyrrol

TE [hartree]: -324.20400

ZPE [kJ/mol]: 305.27

G° [hartree]: -324.08772

Coordinates [Å]:

C -0.9591 0.4728 0.7125
 N -0.1431 -0.6256 0.6501
 C 1.1568 -0.2125 0.5527
 C -0.1738 1.5934 0.6630
 C 1.1717 1.1568 0.5603
 C -0.5929 -1.9870 0.5871
 O -0.4842 -2.5529 -0.6879
 H -2.0282 0.3598 0.8047
 H 1.9571 -0.9304 0.4703
 H -0.5233 2.6128 0.7087
 H 2.0515 1.7788 0.5080
 H -1.6244 -2.0009 0.9564
 H 0.0236 -2.6073 1.2390
 H -0.9825 -2.0087 -1.3053

NH2Indol

TE [hartree]: -363.21408

ZPE [kJ/mol]: 341.77

G° [hartree]: -363.08390

Coordinates [Å]:

C 2.3026 -0.7163 -0.0740
 C 1.1133 -1.4166 -0.0407
 C -0.0643 -0.6780 0.0012
 C -0.0704 0.7364 0.0105
 C 1.1513 1.4149 -0.0238
 C 2.3213 0.6856 -0.0656
 C -1.4396 1.1442 0.0570
 N -1.3702 -1.0889 0.0404
 C -2.1926 0.0081 0.0738
 H 3.2393 -1.2604 -0.1072
 H 1.1015 -2.5009 -0.0473
 H 1.1774 2.4989 -0.0177
 H 3.2741 1.2011 -0.0926
 H -1.8187 2.1535 0.0755
 H -1.6785 -2.0430 0.0443
 H -3.2644 -0.1108 0.1073

HCONH2Indol

TE [hartree]: -476.40058

ZPE [kJ/mol]: 368.16

G° [hartree]: -476.26035

Coordinates [Å]:

C 2.3788 -0.6246 -0.0602
 C 1.1980 -1.3474 -0.0918
 C 0.0174 -0.6205 -0.0640
 C -0.0053 0.7857 -0.0056
 C 1.1977 1.4863 0.0245

C 2.3806 0.7714 -0.0033
 C -1.3866 1.1900 0.0093
 N -1.3085 -1.0516 -0.0845
 C -2.1362 0.0685 -0.0388
 H 3.3224 -1.1566 -0.0805
 H 1.1873 -2.4266 -0.1361
 H 1.2045 2.5691 0.0688
 H 3.3265 1.2998 0.0193
 H -1.7627 2.2001 0.0511
 H -3.2077 -0.0584 -0.0457
 C -1.7755 -2.3435 -0.1421
 O -1.0859 -3.3256 -0.1833
 H -2.8795 -2.3746 -0.1463

H2COHNH2Indol

TE [hartree]: -477.59180

ZPE [kJ/mol]: 429.36

G° [hartree]: -477.42826

Coordinates [Å]:

C 0.3904 -1.3049 -2.1641
 C 0.0837 -1.3699 -0.8180
 C -0.1536 -0.1706 -0.1539
 C -0.0781 1.0786 -0.8106
 C 0.2274 1.1106 -2.1728
 C 0.4591 -0.0777 -2.8355
 C -0.3607 2.0787 0.1717
 N -0.4850 0.0684 1.1618
 C -0.5895 1.4288 1.3446
 H 0.5796 -2.2216 -2.7100
 H 0.0286 -2.3267 -0.3109
 H 0.2839 2.0562 -2.7000

H 0.6987 -0.0657 -3.8923
 H -0.3962 3.1459 0.0204
 H -0.8228 1.8223 2.3224
 C -0.5155 -0.9147 2.2001
 O 0.7144 -1.0939 2.8486
 H -1.2163 -0.5920 2.9702
 H -0.8816 -1.8501 1.7641
 H 1.3625 -1.3834 2.1996

NH2Indol3Me

TE [hartree]: -402.46099

ZPE [kJ/mol]: 414.70

G° [hartree]: -402.30304

Coordinates [Å]:

C 2.2891 -0.6887 -0.0734
 C 1.1127 -1.4119 -0.0411
 C -0.0791 -0.6971 0.0013
 C -0.1097 0.7162 0.0119
 C 1.0973 1.4190 -0.0218
 C 2.2825 0.7129 -0.0640
 C -1.4866 1.1144 0.0591
 N -1.3764 -1.1289 0.0401
 C -2.2145 -0.0397 0.0747
 H 3.2356 -1.2155 -0.1068
 H 1.1221 -2.4962 -0.0485
 H 1.1026 2.5035 -0.0147
 H 3.2257 1.2461 -0.0904
 H -1.6711 -2.0087 0.0433
 H -3.2855 -0.1717 0.1083
 C -2.0050 2.5076 0.0860
 H -1.6367 3.0550 0.9589

H -3.0957 2.5212 0.1207

H -1.6925 3.0683 -0.8001

HCONHIndol3Me

TE [hartree]: -515.65069

ZPE [kJ/mol]: 441.32

G° [hartree]: -515.48260

Coordinates [Å]:

C 2.3640 -0.6036 -0.0601

C 1.1921 -1.3421 -0.0931

C 0.0024 -0.6311 -0.0653

C -0.0375 0.7732 -0.0058

C 1.1545 1.4906 0.0260

C 2.3482 0.7917 -0.0016

C -1.4256 1.1759 0.0094

N -1.3178 -1.0768 -0.0864

C -2.1558 0.0393 -0.0401

H 3.3145 -1.1234 -0.0803

H 1.1954 -2.4214 -0.1385

H 1.1477 2.5736 0.0715

H 3.2871 1.3324 0.0224

H -3.2269 -0.0955 -0.0473

C -1.7691 -2.3716 -0.1425

O -1.0691 -3.3479 -0.1829

H -2.8727 -2.4156 -0.1463

C -1.9266 2.5723 0.0686

H -1.5737 3.0789 0.9716

H -3.0168 2.0603 0.0687

H -1.5719 3.1543 -0.7868

H2COHNH2Indol3Me

TE [hartree]: -516.83976

ZPE [kJ/mol]: 501.70

G° [hartree]: -516.64868

Coordinates [Å]:

C 0.3800 -1.2857 -2.1721

C 0.0717 -1.3685 -0.8266

C -0.1631 -0.1787 -0.1455

C -0.0861 1.0771 -0.7876

C 0.2212 1.1289 -2.1480

C 0.4530 -0.0508 -2.8278

C -0.3682 2.0800 0.1996

N -0.4951 0.0477 1.1712

C -0.5968 1.4104 1.3629

H 0.5671 -2.0196 -2.7298

H 0.0138 -2.3320 -0.3330

H 0.2804 2.0819 -2.6621

H 0.6957 -0.0255 -3.8836

H -0.8294 1.7979 2.3439

C -0.5125 -0.9353 2.2077

O 0.7102 -1.0760 2.8819

H -1.2371 -0.6375 2.9662

H -0.8395 -1.8818 1.7651

H 1.3793 -1.3470 2.2462

C -0.4061 3.5495 -0.0207

H 0.5570 3.9227 -0.3813

H -0.6451 4.0799 0.9022

H -1.1570 3.8228 -0.7682

NH2Carbazol

TE [hartree]: -516.60355

ZPE [kJ/mol]: 465.26

G° [hartree]: -516.42633

Coordinates [Å]:

C 2.3135 -0.6387 -0.0437

C 1.1595 -1.4018 -0.0699

C -0.0560 -0.7313 -0.0451

C -0.1280 0.6778 0.0057

C 1.0488 1.4196 0.0316

C 2.2626 0.7570 0.0065

C -1.5291 1.0189 0.0168

N -1.3362 -1.2343 -0.0643

C -2.2415 -0.1992 -0.0284

H 3.2766 -1.1355 -0.0631

H 1.2064 -2.4841 -0.1093

H 1.0150 2.5027 0.0705

H 3.1861 1.3230 0.0255

H -1.5734 -2.2081 -0.0974

C -3.6159 2.1876 0.0536

C -4.3033 0.9716 0.0071

C -3.6295 -0.2361 -0.0341

C -2.2330 2.2183 0.0586

H -5.3872 0.9732 0.0030

H -1.7049 3.1645 0.0946

H -4.1756 3.1146 0.0855

H -4.1690 -1.1757 -0.0705

HCONHCarbazol

TE [hartree]: -629.79365

ZPE [kJ/mol]: 492.14

G° [hartree]: -629.60620

Coordinates [Å]:

C 2.4839 -0.6269 -0.1661

C 1.3214 -1.3801 -0.2341

C 0.1216 -0.7052 -0.0721

C 0.0703 0.6802 0.1515

C 1.2484 1.4122 0.2158

C 2.4528 0.7491 0.0554

C -1.3235 1.0465 0.2709

N -1.1914 -1.2012 -0.0931

C -2.0751 -0.1285 0.1160

H 3.4388 -1.1241 -0.2892

H 1.3405 -2.4457 -0.4059

H 1.2250 2.4820 0.3881

H 3.3825 1.3035 0.1021

C -1.5691 -2.5049 -0.2826

O -0.8123 -3.4234 -0.4622

H -2.6628 -2.6292 -0.2531

H -3.8737 3.2081 0.7209

C -4.0851 1.0980 0.3948

C -1.9704 2.2558 0.4904

C -3.3529 2.2735 0.5510

H -5.1669 1.1317 0.4448

H -1.4012 3.1701 0.6115

C -3.4594 -0.1196 0.1754

H -4.0503 -1.0185 0.0567

H2COHNHCarbazol

TE [hartree]: -630.98476

ZPE [kJ/mol]: 552.89

G° [hartree]: -630.77418

Coordinates [Å]:

C 0.3481 -1.2578 -2.1915

C 0.0806 -1.3533 -0.8357

C -0.1061 -0.1721 -0.1286
 C -0.0223 1.0861 -0.7615
 C 0.2459 1.1535 -2.1239
 C 0.4297 -0.0203 -2.8326
 C -0.2556 2.0783 0.2578
 N -0.3901 0.0184 1.2132
 C -0.4649 1.3777 1.4624
 H 0.4968 -2.1653 -2.7650
 H 0.0215 -2.3232 -0.3559
 H 0.3117 2.1134 -2.6237
 H 0.6399 0.0174 -3.8946
 C -0.5226 -1.0076 2.1964
 O 0.6222 -1.1977 2.9851
 H -1.3173 -0.7358 2.8928
 H -0.8168 -1.9266 1.6798
 H 1.3545 -1.4371 2.4097
 H -0.9238 3.9634 3.5517
 C -0.5516 4.1317 1.4436
 C -0.6996 2.0374 2.6609
 C -0.7432 3.4209 2.6310
 H -0.5910 5.2143 1.4583
 H -0.8231 1.4964 3.0591
 C -0.3045 3.4683 0.2554
 H -0.1505 4.0229 -0.6632

Catalysts:

MnHImi2_H_H

TE [hartree]: -1961.68237

ZPE [kJ/mol]: 605.83

G° [hartree]: -1961.45162

Coordinates [Å]:

N -0.0880 2.1203 0.5718
 C 1.2226 2.2314 0.5400
 C 2.0941 1.0848 0.1555
 N 1.3110 0.2418 -0.7257
 C 1.6960 -1.1471 -0.8773
 C 0.4941 -1.8730 -1.3779
 N -0.7240 -1.4564 -1.1061
 Mn -0.8363 0.3144 -0.0662
 C -2.5643 0.5524 0.0859
 H 2.3345 0.4937 1.0479
 H 3.0431 1.4299 -0.2801
 H 1.2389 -3.5248 -2.4509
 H 2.5633 -1.3039 -1.0535
 H 1.9600 -1.5240 0.1185
 O -3.7070 0.7286 0.1493
 C -1.5848 -2.3490 -1.6793
 H -2.6517 -2.2228 -1.6064
 C -0.5776 3.3258 0.9881
 H -1.6364 3.4951 1.0881
 C -0.8712 -3.3262 -2.3080
 H -1.1748 -4.1931 -2.8691
 N 0.4489 -3.0062 -2.1117
 C 0.4593 4.1817 1.2146
 H 0.4899 5.2065 1.5424
 N 1.5969 3.4725 0.9200
 H 2.5385 3.8157 0.9795
 C -0.6963 -0.4654 1.5360
 H -1.1021 1.0592 -1.5557
 H 1.1094 0.6887 -1.6134
 O -0.6995 -0.9613 2.5847

MnHImi2

TE [hartree]: -1960.52548

ZPE [kJ/mol]: 541.49

G° [hartree]: -1960.31924

Coordinates [Å]:

N	-0.0599	2.0212	0.7249
C	1.2409	2.1915	0.6071
C	2.0647	1.1402	-0.0394
N	1.1303	0.1265	-0.4067
C	1.6718	-1.0214	-1.0581
C	0.4987	-1.8928	-1.3162
N	-0.7001	-1.5037	-0.9342
Mn	-0.7251	0.2858	-0.0291
C	-2.1533	0.9238	-0.8351
H	2.8412	0.7851	0.6645
H	2.6097	1.5669	-0.9027
H	1.1923	-3.6164	-2.2946
H	2.1816	-0.7847	-2.0112
H	2.4146	-1.5640	-0.4428
O	-3.0732	1.3514	-1.3906
C	-1.5797	-2.4897	-1.2959
H	-2.6340	-2.4085	-1.0921
C	-0.5584	3.1335	1.3501
H	-1.6087	3.2379	1.5639
C	-0.8958	-3.4937	-1.9088
H	-1.2168	-4.4296	-2.3323
N	0.4215	-3.0983	-1.9131
C	0.4639	3.9917	1.6144
H	0.4886	4.9585	2.0865
N	1.5982	3.3779	1.1362

H 2.5306 3.7484 1.1738

C -1.7708 -0.1564 1.3133

O -2.4299 -0.4609 2.2136

MnHImi2_CO

TE [hartree]: -2073.71875

ZPE [kJ/mol]: 561.79

G° [hartree]: -2073.50477

Coordinates [Å]:

N	-0.1111	2.1765	0.4838
C	1.2038	2.2363	0.5204
C	2.0254	1.0689	0.1141
N	1.2023	0.2820	-0.7418
C	1.6453	-1.0664	-0.8634
C	0.4761	-1.8457	-1.3424
N	-0.7493	-1.4043	-1.1485
Mn	-0.8101	0.4235	-0.2660
C	-2.5492	0.5828	0.0684
H	2.3308	0.5312	1.0447
H	2.9712	1.4123	-0.3482
H	1.2307	-3.5874	-2.2294
H	2.5026	-1.2069	-1.5501
H	1.9710	-1.5106	0.1086
O	-3.6754	0.6819	0.2965
C	-1.6087	-2.3437	-1.6506
H	-2.6772	-2.2131	-1.6139
C	-0.5898	3.3701	0.9521
H	-1.6458	3.5713	1.0192
C	-0.8855	-3.3779	-2.1615
H	-1.1801	-4.2933	-2.6443
N	0.4320	-3.0425	-1.9582

C 0.4610 4.1716 1.2787
 H 0.5086 5.1734 1.6688
 N 1.5876 3.4362 0.9964
 H 2.5378 3.7395 1.1126
 C -0.6371 -0.3637 1.3904
 C -1.0569 1.2205 -1.9205
 O -1.2209 1.7108 -2.9346
 O -0.6185 -0.8418 2.4279

MnHImi2_H_Pyr

TE [hartree]: -2170.37606

ZPE [kJ/mol]: 768.18

G° [hartree]: -2170.08347

Coordinates [Å]:

N 0.5743 2.1876 0.3110
 C 1.8707 1.9808 0.3787
 C 2.4597 0.6440 0.0902
 N 1.5108 -0.0470 -0.7671
 C 1.5685 -1.5006 -0.7959
 C 0.2564 -1.9514 -1.3375
 N -0.8198 -1.2036 -1.2246
 Mn -0.4820 0.5980 -0.3679
 C -2.1338 1.2207 -0.2377
 H 2.5529 0.0786 1.0249
 H 3.4624 0.7283 -0.3483
 H 0.6047 -3.8309 -2.2160
 H 2.4051 -1.8944 -1.3882
 H 1.6882 -1.8592 0.2327
 O -3.2075 1.6287 -0.1544
 C -1.8452 -1.8834 -1.8177
 H -2.8379 -1.4699 -1.8719

C 0.3553 3.4808 0.6953
 H -0.6355 3.9016 0.7191
 C -1.3774 -3.0707 -2.2959
 H -1.8598 -3.8762 -2.8218
 N -0.0399 -3.0964 -1.9846
 C 1.5473 4.0669 0.9976
 H 1.7991 5.0611 1.3235
 N 2.4995 3.1004 0.7890
 C 0.1359 0.7058 -3.3987
 C 0.3942 1.5915 -4.4333
 C 0.1362 2.8773 -3.9221
 C -0.2599 2.6973 -2.6068
 N -0.2626 1.3810 -2.2759
 H 0.1375 -0.3749 -3.4383
 H 0.7021 1.3332 -5.4366
 H 0.2174 3.8191 -4.4452
 H -0.5395 3.4501 -1.8848
 H 1.5347 0.3302 -1.7205
 H 3.4904 3.2142 0.9064
 C -0.6102 -0.0791 1.2660
 O -0.7166 -0.5104 2.3337

MnHImi2_H_OMe

TE [hartree]: -2076.10559

ZPE [kJ/mol]: 684.51

G° [hartree]: -2075.84487

Coordinates [Å]:

N 0.4014 2.1593 0.4170
 C 1.7084 2.0028 0.3386
 C 2.3404 0.7459 -0.0837
 N 1.3201 0.0287 -0.8112

C 1.4950 -1.3855 -1.0464
 C 0.1458 -1.9047 -1.4100
 N -0.9517 -1.2643 -1.0731
 Mn -0.6335 0.5209 -0.1746
 C -2.2982 1.0645 0.0625
 H 2.6281 0.1665 0.8032
 H 3.2556 0.9288 -0.6667
 H 0.4901 -3.6980 -2.4538
 H 2.2320 -1.6165 -1.8297
 H 1.8390 -1.8655 -0.1207
 O -3.3881 1.4106 0.2194
 C -2.0046 -2.0018 -1.5344
 H -3.0222 -1.6793 -1.3933
 C 0.1525 3.4259 0.8678
 H -0.8528 3.7840 1.0113
 C -1.5321 -3.1155 -2.1608
 H -2.0308 -3.9321 -2.6535
 N -0.1634 -3.0366 -2.0750
 C 1.3348 4.0725 1.0666
 H 1.5639 5.0686 1.4039
 N 2.3126 3.1712 0.7225
 C -0.8547 2.4154 -2.5209
 O -0.4205 1.1841 -2.0828
 H -1.9534 2.5107 -2.4838
 H -0.5573 2.5889 -3.5681
 H -0.4504 3.2626 -1.9349
 H 0.9754 0.5602 -1.6637
 H 3.3025 3.3378 0.7460
 C -0.6328 -0.1789 1.4479
 O -0.6439 -0.6275 2.5147

FeOMeImi2_H_H
 TE [hartree]: -2076.14340
 ZPE [kJ/mol]: 683.80
 G° [hartree]: -2075.88295
 Coordinates [Å]:
 N -0.1833 2.1212 0.4357
 C 1.1189 2.1953 0.5799
 C 1.9925 1.0506 0.2123
 N 1.2727 0.2825 -0.8035
 C 1.6243 -1.1351 -0.8770
 C 0.4136 -1.8603 -1.3447
 N -0.7868 -1.3542 -1.1833
 Fe -0.7682 0.4120 -0.3347
 C -2.4668 0.6225 -0.1303
 H 2.0747 0.4023 1.0882
 H 2.9911 1.3744 -0.1083
 H 1.1004 -3.6789 -2.1477
 H 2.4957 -1.3324 -1.5151
 H 1.8393 -1.4604 0.1430
 O -3.6029 0.8069 -0.0741
 C -1.6793 -2.2672 -1.6673
 H -2.7401 -2.0824 -1.6513
 C -0.7086 3.2916 0.9016
 H -1.7689 3.4801 0.8882
 C -1.0002 -3.3541 -2.1298
 H -1.3326 -4.2740 -2.5783
 N 0.3298 -3.0762 -1.9222
 C 0.3028 4.0916 1.3422
 H 0.3062 5.0776 1.7735
 N 1.4591 3.3811 1.1244
 H 2.3899 3.6861 1.3444

H -1.0580 1.0914 -1.6881
H 1.3308 0.7245 -1.7120
O -0.0574 -0.4682 1.3088
C -0.9017 -1.2391 2.0638
H -0.3655 -1.7296 2.8982
H -1.7289 -0.6637 2.5242
H -1.3879 -2.0576 1.4919

FeOMeImi2

TE [hartree]: -2074.95777

ZPE [kJ/mol]: 627.27

G° [hartree]: -2074.71886

Coordinates [Å]:

N 0.0472 1.9362 0.9029
C 1.2815 2.2328 0.5574
C 2.0003 1.3035 -0.3314
N 1.2713 0.0919 -0.3000
C 1.6302 -0.8974 -1.2608
C 0.5181 -1.8829 -1.2220
N -0.6159 -1.5875 -0.6149
Fe -0.5736 0.2395 0.1579
C -1.0422 0.9395 -1.1461
H 3.0687 1.1850 0.0261
H 2.1047 1.7509 -1.3448
H 1.1671 -3.5759 -2.2712
H 1.7147 -0.5010 -2.2951
H 2.5930 -1.3980 -1.0494
O -1.9901 1.4146 -2.0261
C -1.4578 -2.6557 -0.7823
H -2.4545 -2.6589 -0.3773
C -0.4098 2.9196 1.7322

H -1.3981 2.8682 2.1564
C -0.8145 -3.6184 -1.4963
H -1.1221 -4.5958 -1.8253
N 0.4361 -3.1110 -1.7635
C 0.5776 3.8433 1.8908
H 0.6250 4.7565 2.4583
N 1.0642 3.3906 1.1405
H 2.5373 3.8372 1.0566
O -1.8284 0.1324 1.5355
C -2.8875 -0.7405 1.0592
H -3.5128 -0.5298 2.4747
H -2.5837 -1.8015 1.6786
H -3.5564 -0.6706 0.7134

FeOMeImi2_CO

TE [hartree]: -2188.16389

ZPE [kJ/mol]: 650.82

G° [hartree]: -2187.91600

Coordinates [Å]:

N -0.1792 2.1583 0.4033
C 1.1236 2.1955 0.5722
C 1.9664 1.0488 0.1651
N 1.2070 0.2940 -0.7944
C 1.5942 -1.0895 -0.7937
C 0.4163 -1.8681 -1.0238
N -0.7935 -1.3601 -1.1466
Fe -0.7560 0.4560 -0.3968
C -2.4935 0.6109 -0.0066
H 2.1794 0.4681 1.0834
H 2.9387 1.4035 -0.2223
H 1.1177 -3.7303 -1.8889

H	2.4633	-1.3060	-1.4412	C	1.6167	-1.5258	-0.8350
H	1.8515	-1.4537	0.2199	C	0.3002	-1.9765	-1.3575
O	-3.5997	0.7299	0.2406	N	-0.7579	-1.2015	-1.2904
C	-1.6800	-2.3083	-1.5789	Fe	-0.3522	0.5581	-0.5160
H	-2.7427	-2.1341	-1.5977	C	-2.0004	1.1076	-0.2682
C	-0.7018	3.3129	0.9167	H	2.4375	-0.0202	1.0321
H	-1.7586	3.5211	0.9028	H	3.5042	0.6783	-0.2176
C	-0.9875	-3.4221	-1.9403	H	0.5979	-3.9165	-2.1074
H	-1.3085	-4.3741	-2.3254	H	2.4517	-1.9535	-1.4033
N	0.3369	-3.1218	-1.7204	H	1.6927	-1.8325	0.2107
C	0.3141	4.0708	1.4109	O	-3.0718	1.4839	-0.1423
H	0.3246	5.0348	1.8887	C	-1.8036	-1.8885	-1.8366
N	1.4613	3.3478	1.1794	H	-2.7867	-1.4564	-1.9151
H	2.3951	3.6239	1.4242	C	0.3046	3.3757	0.7137
C	-0.8842	1.1996	-2.0247	H	-0.6872	3.7939	0.6819
O	-0.9066	1.6561	-3.0654	C	-1.3665	-3.1142	-2.2380
O	-0.2881	-0.3390	1.2983	H	-1.0871	-3.9400	-2.7086
C	-1.1723	-1.1324	1.9867	N	-0.0270	-3.1506	-1.9297
H	-0.6719	-1.5863	2.8578	C	1.4581	3.9398	1.1664
H	-1.5776	-1.9753	1.3919	H	1.6701	4.9078	1.5858
H	-2.0502	-0.5860	2.3855	N	2.4338	2.9909	0.9775
FeOMeImi2_H_Pyr				C	0.1443	0.7313	-3.4712
TE [hartree]: -2284.82363				C	0.3029	1.6392	-4.5062
ZPE [kJ/mol]: 855.28				C	-0.0216	2.9020	-3.9753
G° [hartree]: -2284.49787				C	-0.3557	2.6891	-2.0648
Coordinates [Å]:				N	-0.2567	1.3729	-2.3330
N	0.5718	2.1147	0.2633	H	0.2306	-0.3457	-3.5113
C	1.8553	1.9031	0.4341	H	0.5954	1.4088	-5.5205
C	2.4658	0.5847	0.1221	H	-0.0208	3.8504	-4.4924
N	1.5961	-0.0651	-0.8535	H	-0.6517	3.4169	-1.9069
				H	1.7420	0.2975	-1.7964

H 3.4074 3.0936 1.2010
 O -0.0283 -0.3382 1.1770
 C -1.0782 -0.8496 1.8997
 H -0.7125 -1.4080 2.7785
 H -1.7639 -0.0727 2.2891
 H -1.7104 -1.5562 1.3249

FeOMeImi2_H_OMe

TE [hartree]: -2190.54674

ZPE [kJ/mol]: 771.92

G° [hartree]: -2190.25273

Coordinates [Å]:

N 0.4989 2.1133 0.2429
 C 1.7916 1.9246 0.3682
 C 2.4119 0.6138 0.0404
 N 1.5091 -0.0483 -0.8821
 C 1.5871 -1.4957 -0.9416
 C 0.2574 -1.9721 -1.4062
 N -0.8194 -1.2391 -1.2489
 Fe -0.4237 0.5248 -0.4699
 C -2.0704 1.0605 -0.2177
 H 2.4397 0.0137 0.9555
 H 3.4347 0.7276 -0.3433
 H 0.5743 -3.8835 -2.2203
 H 2.4000 -1.8685 -1.0579
 H 1.7446 -1.8557 0.0795
 O -3.1490 1.4173 -0.0695
 C -1.8732 -1.9522 -1.7419
 H -2.8761 -1.5600 -1.7368
 C 0.2292 3.3800 0.6749
 H -0.7703 3.7809 0.6692

C -1.4217 -3.1514 -2.2034
 H -1.9276 -3.9847 -2.6589
 N -0.0642 -3.1451 -1.9858
 C 1.3899 3.9710 1.0731
 H 1.6021 4.9499 1.4662
 N 2.3731 3.0326 0.8666
 C -0.6970 2.3636 -2.7470
 O -0.1703 1.1747 -2.3028
 H -1.8026 2.3622 -2.7798
 H -0.3560 2.5819 -3.7725
 H -0.4077 3.2379 -2.1314
 H 1.4268 0.4167 -1.7995
 H 3.3519 3.1513 1.0569
 O -0.0717 -0.3416 1.2281
 C -1.0937 -0.8969 1.9554
 H -0.6999 -1.4310 2.8378
 H -1.8166 -0.1515 2.3411
 H -1.6934 -1.6383 1.3886

RuOMeImi2_H_H

TE [hartree]: -907.78736

ZPE [kJ/mol]: 683.70

G° [hartree]: -907.52695

Coordinates [Å]:

N -0.2002 2.2098 0.4456
 C 1.1109 2.2288 0.5817
 C 1.9620 1.0535 0.2409
 N 1.2836 0.2874 -0.8119
 C 1.5943 -1.1460 -0.8534
 C 0.3953 -1.8751 -1.3587
 N -0.8295 -1.4024 -1.2344

Ru	-0.8734	0.4543	-0.3699	Coordinates [Å]:		
C	-2.6392	0.6581	-0.1120	N	0.0643	2.0307 0.9638
H	1.9796	0.4029	1.1192	C	1.3082	2.2642 0.5751
H	2.9818	1.3536	-0.0306	C	2.0141	1.3249 -0.3485
H	1.1503	-3.6711	-2.1468	N	1.2861	0.0857 -0.2916
H	2.4855	-1.3722	-1.4529	C	1.6243	-0.8877 -1.2890
H	1.7568	-1.4553	0.1810	C	0.5461	-1.9194 -1.2466
O	-3.7813	0.8141	0.0153	N	-0.6188	-1.6851 -0.6583
C	-1.6809	-2.3374	-1.7529	Ru	-0.6691	0.2410 0.1988
H	-2.7453	-2.1779	-1.7697	C	-1.4838	0.9669 -1.1763
C	-0.6737	3.4074	0.9009	H	3.0706	1.2226 -0.0458
H	-1.7257	3.6358	0.8901	H	2.0222	1.7718 -1.3636
C	-0.9559	-3.4018	-2.1965	H	1.2982	-3.5810 -2.2730
H	-1.2481	-4.3285	-2.6588	H	1.6543	-0.4632 -2.3138
N	0.3573	-3.0892	-1.9455	H	2.6072	-1.3632 -1.1235
C	0.3740	4.1672	1.3264	O	-2.0095	1.4530 -2.0956
H	0.4207	5.1555	1.7494	C	-1.3959	-2.8010 -0.8282
N	1.4977	3.4082	1.1091	H	-2.3970	-2.8531 -0.4358
H	2.4407	3.6757	1.3257	C	-0.3154	3.0451 1.7985
H	-1.1580	1.1619	-1.7943	H	-1.2931	3.0537 2.2496
H	1.4067	0.7164	-1.7200	C	-0.6883	-3.7291 -1.5263
O	-0.0375	-0.4917	1.3722	H	-0.9352	-4.7233 -1.8559
C	-0.8505	-1.3051	2.1232	N	0.5359	-3.1539 -1.7778
H	-0.2884	-1.7951	2.9405	C	0.7210	3.9184 1.9168
H	-1.6858	-0.7603	2.6016	H	0.8304	4.8342 2.4712
H	-1.3190	-2.1231	1.5385	N	1.7371	3.4062 1.1399
RuOMeImi2				H	2.6483	3.8110 1.0199
TE [hartree]: -906.58627				O	-2.0725	0.1387 1.6495
ZPE [kJ/mol]: 627.23				C	-3.1264	-0.7500 1.6481
G° [hartree]: -906.34737				H	-3.6836	-0.6783 2.5955
				H	-2.8136	-1.8081 1.5536

H -3.8490 -0.5550 0.8360

RuOMeImi2_CO

TE [hartree]: -1019.82295

ZPE [kJ/mol]: 650.88

G° [hartree]: -1019.57504

Coordinates [Å]:

N -0.1574 2.2226 0.4453

C 1.1522 2.2086 0.5981

C 1.9699 1.0359 0.2012

N 1.2215 0.2828 -0.7729

C 1.6008 -1.1063 -0.7732

C 0.4413 -1.9006 -1.2493

N -0.7918 -1.4359 -1.1858

Ru -0.8331 0.4782 -0.4215

C -2.6581 0.6332 -0.0244

H 2.1562 0.4544 1.1240

H 2.9543 1.3728 -0.1699

H 1.2173 -3.7269 -1.9116

H 2.4834 -1.3177 -1.4033

H 1.8375 -1.4745 0.2432

O -3.7726 0.7374 0.2207

C -1.6349 -2.4054 -1.6562

H -2.7007 -2.2606 -1.7020

C -0.6291 3.4064 0.9416

H -1.6771 3.6528 0.9305

C -0.8941 -3.4880 -2.0139

H -1.1717 -4.4437 -2.4227

N 0.4127 -3.1474 -1.7534

C 0.4227 4.1308 1.4086

H 0.4773 5.1024 1.8676

N 1.5376 3.3593 1.1779

H 2.4844 3.6049 1.4046

C -1.1080 1.2655 -2.0872

O -1.2791 1.7353 -3.1175

O -0.2982 -0.3846 1.3445

C -1.2069 -1.1367 2.0560

H -0.7151 -1.5950 2.9286

H -1.6457 -1.9681 1.4718

H -2.0571 -0.5469 2.4469

RuOMeImi2_H_Pyr

TE [hartree]: -1116.46018

ZPE [kJ/mol]: 854.49

G° [hartree]: -1116.13472

Coordinates [Å]:

N 0.5557 2.1803 0.3101

C 1.8451 1.9362 0.4297

C 2.4305 0.5975 0.1350

N 1.5812 -0.0603 -0.8591

C 1.5825 -1.5246 -0.8341

C 0.2723 -1.9927 -1.3706

N -0.8233 -1.2621 -1.2928

Ru -0.4647 0.5858 -0.4790

C -2.1599 1.1511 -0.1964

H 2.3637 -0.0002 1.0480

H 3.4793 0.6716 -0.1754

H 0.6461 -3.9027 -2.1593

H 2.4227 -1.9619 -1.3870

H 1.6435 -1.8206 0.2157

O -3.2390 1.5293 -0.0384

C -1.8381 -1.9809 -1.8586

H	-2.8369	-1.5858	-1.9285	N	0.4994	2.1822	0.2903
C	0.3417	3.4643	0.7243	C	1.7955	1.9556	0.3746
H	-0.6407	3.9041	0.7169	C	2.3901	0.6236	0.0639
C	-1.3468	-3.1781	-2.2822	N	1.5073	-0.0423	-0.8821
H	-1.8155	-4.0144	-2.7708	C	1.5598	-1.4955	-0.9344
N	-0.0092	-3.1656	-1.9702	C	0.2339	-1.9803	-1.4170
C	1.5301	4.0094	1.1038	N	-0.8740	-1.2853	-1.2521
H	1.7855	4.9851	1.4784	Ru	-0.5220	0.5609	-0.4363
N	2.4711	3.0295	0.9057	C	-2.2180	1.1232	-0.1698
C	0.1097	0.7682	-3.4924	H	2.3765	0.0281	0.9824
C	0.3749	1.6691	-4.5119	H	3.4256	0.7165	-0.2887
C	0.0890	2.9470	-3.9944	H	0.6129	-3.8633	-2.2670
C	-0.3318	2.7529	-2.6893	H	2.3775	-1.8802	-1.5577
N	-0.3234	1.4323	-2.3785	H	1.7027	-1.8493	0.0909
H	0.1310	-0.3120	-3.5304	O	-3.0304	1.4936	-0.0138
H	0.7063	1.4254	-5.5111	C	-1.9007	-2.0237	-1.7685
H	0.1654	3.8941	-4.5082	H	-2.9141	-1.6611	-1.7612
H	-0.6383	3.4891	-1.9614	C	0.2811	3.4654	0.7059
H	1.7331	0.3001	-1.8028	H	-0.7075	3.8906	0.7242
H	3.0456	3.1144	1.0822	C	-1.4039	-3.1969	-2.2489
O	-0.0423	-0.3722	1.2885	H	-1.8785	-4.0365	-2.7262
C	-1.0613	-0.9785	1.9904	N	-0.0503	-3.1507	-2.0219
H	-0.6585	-1.5173	2.8643	C	1.4725	4.0278	1.0501
H	-1.8059	-0.2589	2.3741	H	1.7250	5.0077	1.4160
H	-1.6256	-1.7202	1.3935	N	2.4211	3.0595	0.8289
RuOMeImi2_H_OMe				C	-0.6714	2.4145	-2.8170
TE [hartree]: -1022.17903				O	-0.1949	1.1990	-2.3759
ZPE [kJ/mol]: 771.48				H	-1.7736	2.4450	-2.8696
G° [hartree]: -1021.88518				H	-0.2965	2.6282	-3.8315
Coordinates [Å]:				H	-0.3654	3.2663	-2.1810
				H	1.4541	0.4143	-1.8043

H 3.4085 3.1548 0.9836
 O -0.1003 -0.3380 1.3552
 C -1.0920 -1.0123 2.0312
 H -0.6776 -1.5112 2.9238
 H -1.9005 -0.3469 2.3832
 H -1.5807 -1.8008 1.4269

MnCON_CH2PiPr2_H_H

TE [hartree]: -2746.40871

ZPE [kJ/mol]: 1422.80

G° [hartree]: -2745.86680

Coordinates [Å]:

C -3.1563 1.8508 0.2798
 N -1.7457 2.0143 0.6242
 C -1.2042 3.3515 0.3896
 C 0.2216 3.3879 0.9082
 P 1.1162 1.0918 0.2271
 Mn -0.5035 0.4521 -0.1418
 C 0.5675 -0.9203 -0.3853
 H -3.7723 2.6223 0.7632
 H -3.2500 1.9734 -0.8016
 H 0.7115 4.3355 0.6774
 H -1.2324 3.5372 -0.6868
 H -1.8206 4.1179 0.8809
 O 1.2754 -1.8295 -0.4845
 H 0.2123 3.2870 1.9989
 H -1.6407 1.8052 1.6123
 C 2.1336 2.5978 -1.1695
 C 2.4715 1.6217 1.4712
 C 3.1277 2.9003 1.9800
 H 2.4488 3.4579 2.6306

H 3.4501 3.5701 1.1812
 H 4.0118 2.6542 2.5747
 C 2.0250 0.7586 2.6392
 H 1.2155 1.2360 3.1994
 H 2.8613 0.6062 3.3283
 H 1.6570 -0.2095 2.3061
 H 3.2147 1.0552 0.8975
 C 2.7344 1.4448 -1.9649
 H 3.2853 0.7443 -1.3332
 H 3.4281 1.8295 -2.7177
 H 1.9552 0.8809 -2.4798
 C 1.3521 3.5365 -2.0769
 H 0.5011 3.0326 -2.5355
 H 1.9980 3.8878 -2.8869
 H 0.9891 4.4189 -1.5457
 H 2.9500 3.1682 -0.7142
 H -3.5758 0.3942 1.7979
 H -4.6145 0.2439 0.3858
 C -3.1713 -1.5019 -1.4360
 H -3.9561 -2.1670 -1.0613
 C -3.8247 -0.4703 -2.3439
 H -3.0969 0.2428 -2.7316
 H -4.6182 0.0833 -1.8376
 H -4.2779 -0.9724 -3.2036
 C -2.1547 -2.0339 -2.2023
 H -1.3838 -1.7054 -2.6429
 H -2.6501 -2.8826 -3.0118
 H -1.6550 -3.0729 -1.5661
 C -3.5937 0.4609 0.7046
 P -2.3536 -0.7514 0.0553
 C -2.4914 -2.1900 1.2309

H -2.0867 -3.0247 0.6459
 C -1.6289 -2.0298 2.4712
 H -0.5805 -1.8885 2.2166
 H -1.0727 -2.9151 3.1069
 H -1.9374 -1.1624 3.0625
 C -3.9252 -2.5275 1.6242
 H -4.3477 -1.7537 2.2703
 H -3.9462 -3.0464 2.1885
 H -4.5919 -2.6491 0.7689
 C -0.6805 0.7904 -1.8704
 H -0.3267 0.1263 1.4017
 O -0.7465 0.9494 -3.0206

MnCON_CH2PiPr2

TE [hartree]: -2745.22896

ZPE [kJ/mol]: 1366.39

G° [hartree]: -2744.70853

Coordinates [Å]:

C -3.0929 1.8192 0.4377
 N -1.6385 1.8558 0.4811
 C -1.2189 3.2458 0.5774
 C 0.2342 3.3628 0.9984
 P 1.1232 1.9218 0.2996
 Mn -0.5127 0.4227 0.0003
 C -0.0955 0.0035 -1.6442
 H -3.5081 2.5260 1.1717
 H -3.4531 2.1673 -0.5437
 H 0.6799 4.3148 0.6998
 H -1.3764 3.7591 -0.3847
 H -1.8504 3.7790 1.3039
 O 0.1528 -0.2382 -2.7510

H 0.3026 3.2878 2.0859
 C 0.4858 -0.9255 0.5510
 C 2.0672 2.6254 -1.1211
 C 2.4395 1.5249 1.5397
 C 3.4777 2.6196 1.7411
 H 3.0113 3.5515 2.0737
 H 4.0476 2.8310 0.8352
 H 4.1903 2.3189 2.5146
 C 1.8179 1.1222 2.8719
 H 1.3966 1.9869 3.3909
 H 2.5826 0.6917 3.5234
 H 1.0232 0.3857 2.7487
 H 2.9290 0.6382 1.1212
 C 3.0141 1.5959 -1.7223
 H 3.7466 1.2342 -0.9975
 H 3.5651 2.0392 -2.5565
 H 2.4673 0.7343 -2.1080
 C 1.1175 3.1924 -2.1679
 H 0.4655 2.4176 -2.5731
 H 1.6903 3.6162 -2.9975
 H 0.4876 3.9857 -1.7606
 H 2.6560 3.4525 -0.7086
 H -3.7015 0.2835 1.8064
 H -4.6219 0.2683 0.3010
 C -3.1884 -1.4832 -1.4134
 H -4.1677 -1.8567 -1.0936
 C -3.4101 -0.3987 -2.4590
 H -2.4644 0.0269 -2.7961
 H -4.0302 0.4148 -2.0771
 H -3.9172 -0.8210 -3.3311
 C -2.3715 -2.6420 -1.9663

H -1.3672 -2.3188 -2.2442
 H -2.8507 -3.0446 -2.8631
 H -2.2761 -3.4583 -1.2475
 C -3.6284 0.4285 0.7264
 P -2.3994 -0.7762 0.0982
 C -2.4536 -2.1794 1.3060
 H -1.6961 -2.8758 0.9290
 C -2.0053 -1.7159 2.0687
 H -1.0745 -1.1494 2.6461
 H -1.8505 -2.5810 3.3368
 H -2.7615 -1.0839 3.1597
 C -3.7950 -2.8936 1.3867
 H -4.5952 -2.2010 1.6636
 H -3.7583 -3.6718 2.1544
 H -4.0734 -3.3730 0.4471
 O 1.1368 -1.8057 0.9276

MnCON_CH2PiPr2_CO

TE [hartree]: -2858.49225

ZPE [kJ/mol]: 1390.32

G° [hartree]: -2857.96270

Coordinates [Å]:

C -2.5452 1.3263 1.9420
 N -1.1136 1.3711 1.8904
 C -0.6310 2.7205 1.9262
 C 0.8859 2.7104 1.9790
 P 1.4738 1.6046 0.6422
 Mn -0.2321 0.1404 0.4325
 C 0.5135 -0.8958 -0.7992
 H -2.9099 1.8665 2.8323
 H -3.0421 1.8161 1.0776

H 1.3245 3.7088 1.9342
 H -0.9624 3.3388 1.0651
 H -1.0160 3.2374 2.8218
 O 0.9920 -1.5585 -1.6135
 H 1.2020 2.2385 2.9146
 O 0.8560 -1.2691 2.7950
 C 2.0025 2.6755 -0.7829
 C 3.0800 0.9705 1.3172
 C 3.7730 0.0008 0.3721
 H 4.1710 0.5170 -0.0505
 H 3.1009 -0.7855 0.0269
 H 4.6172 -0.4744 0.8789
 C 4.0310 2.0634 1.7843
 H 4.4289 2.6410 0.9468
 H 4.8862 1.6134 2.2965
 H 3.5567 2.7573 2.4802
 H 2.7550 0.4092 2.1999
 C 2.0190 1.8898 -2.0889
 H 2.5867 0.9617 -2.0202
 H 2.4644 2.4995 -2.8802
 H 1.0064 1.6305 -2.4011
 C 1.1738 3.9448 -0.9341
 H 0.1290 3.7239 -1.1526
 H 1.5654 4.5324 -1.7695
 H 1.2078 4.5744 -0.0447
 H 3.0295 2.9736 -0.5464
 H -2.6489 -0.5439 2.9718
 H -4.0841 -0.2316 1.9825
 C -3.3180 -1.2939 -0.6965
 H -3.8988 -2.1815 -0.4247
 C -4.2952 -0.1403 -0.8842

H	-3.7831	0.7909	-1.1257	C	0.9424	2.7041	1.9926
H	-4.9126	0.0315	-0.0021	P	1.5439	1.6248	0.6204
H	-4.9660	-0.3708	-1.7169	Mn	-0.2030	0.2052	0.3570
C	-2.5779	-1.5862	-1.9967	C	0.5214	-0.7726	-0.9248
H	-2.0338	-0.7062	-2.3434	H	-2.9483	1.8480	2.7900
H	-3.2954	-1.8614	-2.7750	H	-2.9405	1.7630	1.0242
H	-1.8566	-2.3979	-1.9009	H	1.3875	3.7000	1.9869
C	-2.9995	-0.1200	2.0256	H	-0.9142	3.2820	1.0404
P	-2.1274	-1.0505	0.7094	H	-0.9749	3.2992	2.8066
C	-1.9911	-2.7484	1.4414	O	0.9721	-1.3804	-1.7957
H	-1.3600	-2.5736	2.3195	H	1.2527	2.2131	2.9206
C	-3.3149	-3.3213	1.9286	C	2.0637	2.7924	-0.7264
H	-3.8401	-2.6408	2.6008	C	3.1350	0.9762	1.3053
H	-3.1341	-4.2519	2.4739	C	3.9114	0.1686	0.2753
H	-3.9839	-3.5629	1.0993	H	4.3742	0.8166	-0.4739
C	-1.2672	-3.7290	0.5309	H	3.2807	-0.5584	-0.2362
H	-1.8778	-3.9895	-0.3370	H	4.7130	-0.3826	0.7730
H	-1.0611	-4.6564	1.0718	C	4.0196	2.0398	1.9402
H	-0.3179	-3.3313	0.1698	H	4.3785	2.7661	1.2055
C	-1.0636	1.2366	-0.7420	H	4.9014	1.5653	2.3798
C	0.4525	-0.7480	1.8591	H	3.5136	2.5867	2.7375
O	-1.6166	1.9690	-1.4304	H	2.7880	0.2870	2.0834
MnCON_CH2PiPr2_H_Pyr				C	2.1590	2.0650	-2.0634
TE [hartree]: -2955.21486				H	2.7607	1.1584	-2.0106
ZPE [kJ/mol]: 1597.27				H	2.6079	2.7251	-2.8111
G° [hartree]: -2954.60649				H	1.1678	1.7842	-2.4217
Coordinates [Å]:				C	1.1569	4.0094	-0.8593
C	-2.5457	1.2964	1.9296	H	0.1359	3.7213	-1.1157
N	-1.0849	1.3916	1.8925	H	1.5236	4.6470	-1.6688
C	-0.5707	2.7624	1.9376	H	1.1304	4.6180	0.0458
				H	3.0635	3.1410	-0.4441

H	-2.5494	-0.5904	2.9423
H	-4.0038	-0.3119	1.9900
C	-3.3018	-1.2995	-0.6952
H	-3.9053	-2.1635	-0.3948
C	-4.2329	-0.1058	-0.8634
H	-3.6813	0.7942	-1.1387
H	-4.8174	0.1039	0.0336
H	-4.9407	-0.3099	-1.6718
C	-2.6176	-1.6181	-2.0209
H	-2.0803	-0.7470	-2.3983
H	-3.3693	-1.8933	-2.7663
H	-1.9037	-2.4377	-1.9450
C	-2.9225	-0.1700	2.0024
P	-2.0445	-1.0764	0.6528
C	-1.8607	-2.7686	1.3777
H	-1.1010	-2.6112	2.1505
C	-3.1269	-3.3122	2.0238
H	-3.5096	-2.6626	2.8126
H	-2.9161	-4.2850	2.4769
H	-3.9259	-3.4649	1.2928
C	-1.3025	-3.7583	0.3645
H	-2.0523	-4.0241	-0.3853
H	-1.0065	-4.6775	0.8759
H	-0.4226	-3.3676	-0.1466
C	-0.9570	1.1890	-0.8835
H	-0.7372	0.9153	2.7181
N	0.6760	-0.9259	1.8865
C	0.6380	-0.8041	3.2481
C	1.4762	-1.9991	1.6370
C	1.9446	-2.5581	2.8131
C	1.4027	-1.7853	3.8564

H	1.5436	-1.9175	4.9191
H	0.0866	-0.0367	3.7763
H	2.5953	-3.4156	2.9001
H	1.6800	-2.3180	0.6269
O	-1.4503	1.8330	-1.7136

MnCON_CH2PiPr2_H_OMe

TE [hartree]: -2860.88267

ZPE [kJ/mol]: 1514.90

G° [hartree]: -2860.30567

Coordinates [Å]:

C	-2.5560	1.2261	1.9495
N	-1.1076	1.3300	1.8101
C	-0.6076	2.6986	1.8928
C	0.9062	2.6657	1.8851
P	1.4751	1.6005	0.4901
Mn	-0.2568	0.1468	0.2685
C	0.5338	-0.9374	-0.8803
H	-2.8981	1.7379	2.8600
H	-3.0186	1.7314	1.0972
H	1.3340	3.6691	1.8632
H	-0.9931	3.2541	1.0335
H	-0.9790	3.1955	2.8001
O	1.0437	-1.6353	-1.6460
H	1.2576	2.1741	2.7972
C	1.9489	2.7767	-0.8642
C	3.0943	0.9908	1.1464
C	3.8560	0.1485	0.1330
H	4.3025	0.7737	-0.6446
H	3.2214	-0.5948	-0.3503
H	4.6735	-0.3804	0.6308

C	3.9916	2.0749	1.7275	H	-3.6202	-2.7168	2.6971
H	4.3387	2.7694	0.9581	H	-2.9905	-4.3349	2.4033
H	4.8815	1.6172	2.1696	H	-3.9829	-3.5515	1.1820
H	3.5003	2.6554	2.5099	C	-1.3502	-3.8087	0.3070
H	2.7565	0.3395	1.9590	H	-2.0845	-4.0799	-0.4558
C	2.0715	2.0406	-2.1946	H	-1.0656	-4.7288	0.8248
H	2.7143	1.1629	-2.1338	H	-0.4645	-3.4192	-0.1955
H	2.4872	2.7116	-2.9519	C	-0.9797	1.0519	-1.0436
H	1.0933	1.7094	-2.5441	H	-0.6453	0.7473	2.5200
C	0.9916	3.9544	-1.0001	O	0.4331	-0.6723	2.0057
H	-0.0188	3.6218	-1.2420	C	1.2679	-1.7636	2.0921
H	1.3236	4.6003	-1.8181	H	1.5495	-1.9559	3.1406
H	0.9492	4.5674	-0.0982	H	0.8206	-2.6998	1.7125
H	2.9339	3.1702	-0.5883	H	2.2103	-1.6481	1.5287
H	-2.5375	-0.6882	2.9001	O	-1.4596	1.6555	-1.9133
H	-4.0210	-0.3741	1.9988				
C	-3.4043	-1.3077	-0.7212	FeOMeN_CH2PiPr2_H_H			
H	-4.0360	-2.1425	-0.3968	TE [hartree]:	-2859.53329		
C	-4.2887	-0.0773	-0.8747	ZPE [kJ/mol]:	1510.02		
H	-3.7073	0.7966	-1.1716	G° [hartree]:	-2858.95815		
H	-4.8357	0.1620	0.0386	Coordinates [Å]:			
H	-5.0286	-0.2556	-1.6604	C	-2.6729	1.3507	1.5310
C	-2.7652	-1.6689	-2.0586	N	-1.2113	1.3560	1.5613
H	-2.2056	-0.8235	-2.4600	C	-0.6219	2.6917	1.4909
H	-3.5432	-1.9277	-2.7827	C	0.8814	2.5506	1.6336
H	-2.0801	-2.5133	-1.9862	P	1.4290	1.3053	0.3859
C	-2.9387	-0.2390	1.9865	Fe	-0.3896	0.0610	0.1383
P	-2.1062	-1.1162	0.5914	C	0.3833	-1.1416	-0.8213
C	-1.9353	-2.8163	1.3021	H	-3.0841	2.0011	2.3152
H	-1.1987	-2.6374	2.0919	H	-2.9651	1.7452	0.5567
C	-3.2058	-3.3725	1.9299	H	1.3918	3.5089	1.5260

H -0.8872 3.0963 0.5131
H -1.0359 3.3457 2.2704
O 0.9302 -1.9888 -1.3818
H 1.1264 2.1626 2.6283
H -0.9097 0.9199 2.4271
C 2.1106 2.3238 -1.0008
C 2.9947 0.6018 1.0989
C 3.9091 1.6569 1.7113
H 3.4714 2.0755 2.6212
H 4.1264 2.4834 1.0337
H 4.8640 1.2040 1.9917
C 2.7425 -0.5174 2.0969
H 2.1709 -0.1593 2.9584
H 3.6967 -0.9011 2.4700
H 2.1800 -1.3356 1.6518
H 3.4978 0.1686 0.2262
C 2.3950 1.4237 -2.1966
H 3.0590 0.5932 -1.9455
H 2.8736 2.0009 -2.9927
H 1.4706 1.0034 -2.5914
C 1.1881 3.4775 -1.3744
H 0.1732 3.1156 -1.5439
H 1.5501 3.9597 -2.2867
H 1.1566 4.2413 -0.5941
H 3.0603 2.7396 -0.6469
H -2.8555 -0.4510 2.6936
H -4.2276 -0.1657 1.6273
C -3.5052 -1.3055 -0.9144
H -4.2659 -1.9947 -0.5318
C -4.1874 0.0059 -1.2817
H -3.4449 0.7771 -1.4906

H -4.8394 0.3619 -0.4808
H -4.8119 -0.1375 -2.1680
C -2.8383 -1.9515 -2.1225
H -2.0986 -1.2826 -2.5611
H -3.5880 -2.1768 -2.8861
H -2.3334 -2.8868 -1.8690
C -3.1425 -0.0812 1.7031
P -2.2593 -1.0936 0.4391
C -2.2328 -2.8059 1.1604
H -2.0485 -3.4455 0.2890
C -1.0902 -3.0148 2.1419
H -0.1238 -2.8249 1.6796
H -1.1102 -4.0412 2.5197
H -1.1777 -2.3443 3.0020
C -3.5549 -3.2218 1.7952
H -3.7580 -2.6392 2.6975
H -3.5090 -4.2727 2.0939
H -4.4087 -3.1111 1.1256
H 0.1391 -0.7174 1.3228
O -1.2408 1.3181 -1.1799
C -1.1610 1.1770 -2.5438
H -0.6512 2.0272 -3.0378
H -0.6181 0.2746 -2.8763
H -2.1558 1.1200 -3.0279

FeOMeN_CH2PiPr2

TE [hartree]: -2858.32509

ZPE [kJ/mol]: 1452.32

G° [hartree]: -2857.77193

Coordinates [Å]:

C -2.8709 -1.5116 -0.6055

N	-1.4254	-1.5125	-0.4668	H	2.4369	-3.0029	1.4540
C	-0.9696	-2.8908	-0.5231	H	-3.3765	0.0721	-1.9563
C	0.5265	-2.9873	-0.7581	H	-4.4523	-0.0100	-0.5570
P	1.3092	-1.5107	-0.0189	C	-3.0735	1.4417	1.5376
Fe	-0.3623	-0.0317	-0.0908	H	-4.1231	1.6636	1.3102
H	-3.1691	-2.1861	-1.4230	C	-3.0087	0.2101	2.4322
H	-3.3372	-1.9287	0.3007	H	-1.9663	-0.0519	2.6193
H	0.9484	-3.9206	-0.3773	H	-3.5162	-0.6496	1.9917
H	-1.2426	-3.4154	0.4055	H	-3.4926	0.4258	3.3892
H	-1.4956	-3.4273	-1.3277	C	-2.4469	2.6394	2.2362
H	0.7256	-2.9407	-1.8305	H	-1.4170	2.4121	2.5063
C	0.5142	1.1389	-1.0056	H	-3.0015	2.8595	3.1531
C	1.8765	-2.0792	1.6419	H	-2.4534	3.5429	1.6228
C	2.8716	-1.2729	-0.9820	C	-3.4153	-0.1222	-0.8825
C	3.9062	-2.3722	-0.7781	P	-2.2935	1.0878	-0.0977
H	3.5113	-3.3440	-1.0877	C	-2.5404	2.6487	-1.0593
H	4.2366	-2.4554	0.2573	H	-1.7994	3.3365	-0.6357
H	4.7884	-2.1696	-1.3921	C	-2.2083	2.4522	-2.5341
C	2.5805	-1.0972	-2.4686	H	-1.2570	1.9451	-2.6874
H	2.3361	-2.0557	-2.9332	H	-2.1538	3.4240	-3.0314
H	3.4666	-0.7082	-2.9763	H	-2.9867	1.8744	-3.0385
H	1.7578	-0.4093	-2.6592	C	-3.9291	3.2577	-0.9104
H	3.2724	-0.3268	-0.5995	H	-4.7013	2.5656	-1.2580
C	2.7869	-1.0686	2.3236	H	-4.0047	4.1618	-1.5214
H	3.6426	-0.7820	1.7087	H	-4.1619	3.5332	0.1183
H	3.1760	-1.4938	3.2533	O	1.0824	1.8882	-1.6729
H	2.2221	-0.1709	2.5684	O	0.1075	0.6851	1.6292
C	0.6758	-2.3962	2.5245	C	0.8962	1.8017	1.7671
H	0.0783	-1.4942	2.6664	H	1.0388	2.0379	2.8351
H	1.0201	-2.7457	3.5022	H	0.4686	2.7087	1.2981
H	0.0436	-3.1772	2.0984	H	1.9076	1.6889	1.3319

				H	3.7938	2.9215	2.0463
				H	2.7920	0.6281	2.2697
FeOMeN_CH2PiPr2_CO				C	2.3255	2.0599	-2.0197
TE [hartree]: -2971.53565				H	3.1388	1.3481	-1.8750
ZPE [kJ/mol]: 1478.15				H	2.6371	2.7670	-2.7934
G° [hartree]: -2970.97265				H	1.4632	1.5126	-2.3979
Coordinates [Å]:				C	0.9202	3.8845	-0.9789
C	-2.4633	1.3357	1.9593	H	-0.0624	3.4359	-1.1205
N	-1.0265	1.3580	1.9291	H	1.1828	4.4659	-1.8673
C	-0.5707	2.7213	1.9341	H	0.8561	4.5782	-0.1394
C	0.9439	2.7478	1.9818	H	2.8891	3.3147	-0.3827
P	1.5113	1.6689	0.6229	H	-2.6017	-0.5391	2.9911
Fe	-0.2130	0.2140	0.4523	H	-4.0290	-0.1949	1.9959
C	0.5092	-0.8019	-0.8012	C	-3.3550	-1.1618	-0.6440
H	-2.8269	1.8924	2.8392	H	-4.0798	-1.8870	-0.2570
H	-2.9119	1.8217	1.0759	C	-4.0909	0.1487	-0.8992
H	1.3591	3.7549	1.9099	H	-3.3890	0.9607	-1.0850
H	-0.9233	3.2874	1.0550	H	-4.7170	0.4310	-0.0515
H	-0.9683	3.2446	2.8200	H	-4.7455	0.0320	-1.7676
O	0.9802	-1.4625	-1.6073	C	-2.7416	-1.7280	-1.9174
H	1.2869	2.2960	2.9171	H	-1.9888	-1.0549	-2.3249
O	0.8505	-1.1556	2.7702	H	-3.5196	-1.8567	-2.6749
C	1.9825	2.8160	-0.7434	H	-2.2722	-2.6992	-1.7569
C	3.1077	0.9921	1.2852	C	-2.9429	-0.0999	2.0492
C	3.6594	-0.1991	0.5160	P	-2.1017	-0.9994	0.7020
H	4.0231	0.0853	-0.4726	C	-1.9083	-2.7032	1.4131
H	2.9150	-0.9843	0.3848	H	-1.4495	-2.4795	2.3834
H	4.5037	-0.6301	1.0613	C	-3.2314	-3.4081	1.6787
C	4.1770	2.0526	1.5070	H	-3.9443	-2.7685	2.2034
H	4.6004	2.3977	0.5609	H	-3.0625	-4.2943	2.2966
H	4.9989	1.6339	2.0943	H	-3.6973	-3.7467	0.7503

C -0.9452 -3.6021 0.6518
 H -1.3447 -3.8998 -0.3190
 H -0.7658 -4.5170 1.2231
 H 0.0187 -3.1223 0.4836
 C 0.4471 -0.6366 1.8347
 C -1.1047 1.3501 -2.1988
 O -1.1377 1.4053 -0.8240
 H -2.1135 1.2391 -2.6366
 H -0.5085 0.5251 -2.6257
 H -0.6923 2.2724 -2.6470

FeOMeN_CH2PiPr2_H_Pyr

TE [hartree]: -3068.19740

ZPE [kJ/mol]: 1683.81

G° [hartree]: -3067.55607

Coordinates [Å]:

C -2.5365 1.2913 1.8334
 N -1.0755 1.3848 1.8488
 C -0.5875 2.7650 1.8103
 C 0.9221 2.7326 1.9177
 P 1.5624 1.6241 0.5935
 Fe -0.1919 0.1946 0.3782
 C 0.4894 -0.7369 -0.9266
 H -2.9690 1.8856 2.6490
 H -2.8663 1.7075 0.8814
 H 1.3574 3.7320 1.8821
 H -0.9123 3.1837 0.8576
 H -1.0303 3.3530 2.0625
 O 0.9232 -1.3313 -1.8062
 H 1.2160 2.2805 2.8707
 C 2.1074 2.7621 -0.7619

C 3.1314 0.9803 1.3301
 C 3.9456 0.1648 0.3359
 H 4.4370 0.8075 -0.3991
 H 3.3349 -0.5665 -0.1936
 H 4.7262 -0.3845 0.8675
 C 3.9943 2.0525 1.9813
 H 4.3718 2.7742 1.2513
 H 4.8639 1.5834 2.4501
 H 3.4642 2.6039 2.7594
 H 2.7654 0.2983 2.1051
 C 2.2909 2.0010 -2.0694
 H 2.9270 1.1232 -1.9609
 H 2.7482 2.6561 -2.8164
 H 1.3296 1.6694 -2.4591
 C 1.1602 3.9398 -0.9518
 H 0.1417 3.5902 -1.1235
 H 1.4726 4.5270 -1.8200
 H 1.1542 4.6102 -0.0910
 H 3.0825 3.1469 -0.4406
 H -2.5498 -0.5654 2.9139
 H -3.9969 -0.3140 1.9411
 C -3.2990 -1.3272 -0.7059
 H -3.9296 -2.1595 -0.3712
 C -4.1814 -0.1011 -0.9004
 H -3.5742 0.7812 -1.1033
 H -4.8081 0.1028 -0.0307
 H -4.8484 -0.2616 -1.7521
 C -2.6306 -1.7195 -2.0187
 H -2.0513 -0.8885 -2.4183
 H -3.3944 -1.9813 -2.7564
 H -1.9609 -2.5725 -1.9147

C -2.0916 -0.1692 1.9608
 P -2.0405 -1.0986 0.6336
 C -1.8397 -2.7785 1.3792
 H -1.0786 -2.6065 2.1477
 C -3.1013 -3.3152 2.0409
 H -3.4802 -2.6542 2.8218
 H -2.8851 -4.2806 2.5070
 H -3.9041 -3.4802 1.3169
 C -1.2842 -3.0788 0.3839
 H -2.0395 -4.0777 -0.3509
 H -0.9760 -4.6920 0.9146
 H -0.4112 -3.4056 -0.1453
 H -0.7532 0.9720 2.7166
 N 0.6799 -0.9318 1.8141
 C 0.6253 -0.8333 3.1771
 C 1.4881 -1.9966 1.5541
 C 1.9463 -2.5736 2.7250
 C 1.3886 -1.8216 3.7749
 H 1.5178 -1.9715 4.8365
 H 0.0599 -0.0816 3.7096
 H 2.6003 -3.4292 2.8035
 H 1.7058 -2.2989 0.5418
 O -1.1707 1.4718 -0.7719
 C -1.2219 1.5291 -2.1449
 H -2.2517 1.4249 -2.5336
 H -0.6303 0.7568 -2.6638
 H -0.8588 2.4957 -2.5403

FeOMeN_CH2PiPr2_H_OMe

TE [hartree]: -2973.91958

ZPE [kJ/mol]: 1601.93

G° [hartree]: -2973.30943

Coordinates [Å]:

C -2.4580 1.2819 1.9049
 N -1.0035 1.3592 1.8385
 C -0.5112 2.7315 1.8704
 C 1.0003 2.7006 1.9017
 P 1.5843 1.6383 0.5172
 Fe -0.1613 0.1861 0.3391
 C 0.5816 -0.8438 -0.8458
 H -2.8397 1.8435 2.7686
 H -2.8437 1.7453 0.9947
 H 1.4311 3.7027 1.8747
 H -0.8791 3.2240 0.9686
 H -0.9093 3.2677 2.0743
 O 1.0792 -1.5297 -1.6219
 H 1.3365 2.2165 2.8238
 C 2.0538 2.8283 -0.8184
 C 3.1909 1.0150 1.1879
 C 3.9760 0.1808 0.1847
 H 4.4708 0.8170 -0.5532
 H 3.3488 -0.5337 -0.3493
 H 4.7576 -0.3817 0.7026
 C 4.0782 2.0952 1.7921
 H 4.4312 2.7991 1.0340
 H 4.9640 1.6353 2.2402
 H 3.5751 2.6654 2.5743
 H 2.8384 0.3585 1.9901
 C 2.2891 2.1008 -2.1374
 H 3.0360 1.3119 -2.0564
 H 2.6336 2.8117 -2.8941
 H 1.3666 1.6491 -2.4985

C 1.0198 3.9357 -0.9873
H 0.0278 3.0512 -1.1482

RuOMeN_CH2PPh2

TE [hartree]: -2142.89905

ZPE [kJ/mol]: 1473.22

G° [hartree]: -2142.33793

Coordinates [Å]:

C -2.9166 1.5188 0.2531
N -1.6054 1.8114 0.8475
C -1.1034 3.1268 0.4279
C 0.2893 3.3630 0.9780
P 1.3598 1.9262 0.5356
Ru -0.1487 0.2270 0.3434
C 1.0601 -1.0947 0.0368
H -3.6602 2.2601 0.5744
H -2.7681 1.6059 -0.8247
H 0.7038 4.3066 0.6165
H -1.0808 3.0893 -0.6628
H -1.7900 3.9219 0.7472
O 1.8308 -1.9401 -0.1179
H 0.2766 3.4087 2.0712
H -3.5148 0.0201 1.6946
H -4.3062 -0.1384 0.1276
C -3.3625 0.1159 0.6153
P -2.0181 -1.0716 0.1808
O -0.6517 1.0137 -1.5859
C -2.3382 -2.4944 1.2655
C -1.4216 -2.8120 2.2614
C -1.6606 -3.8792 3.1159
C -2.8168 -4.6312 2.9822

C -3.7356 -4.3204 1.9874
C -3.4958 -3.2606 1.1295
H -0.5261 -2.2078 2.3540
H -0.9377 -4.1244 3.8855
H -4.6377 -4.9112 1.8768
H -4.2032 -3.0360 0.3385
H -3.0028 -5.4655 3.6491
C -2.4490 -1.7170 -1.4581
C -1.9311 -2.9519 -1.8460
C -2.1428 -3.4317 -3.1270
C -2.8662 -2.6783 -4.0409
C -3.3763 -1.4454 -3.6655
C -3.1686 -0.9656 -2.3815
H -1.3558 -3.5409 -1.1399
H -1.7353 -4.3940 -3.4145
H -3.9319 -0.8469 -4.3782
H -3.5523 0.0100 -2.1138
H -3.0265 -3.0504 -5.0463
C 2.6654 1.9718 1.7990
C 3.5518 3.0460 1.8768
C 4.5176 3.0833 2.8677
C 4.6139 2.0425 3.7832
C 3.7421 0.9681 3.7048
C 2.7678 0.9327 2.7167
H 3.4949 3.8482 1.1488
H 5.2024 3.9218 2.9232
H 3.8203 0.1507 4.4125
H 2.0712 0.1051 2.6432
H 5.3749 2.0695 4.5548
C 2.2497 2.4246 -0.9641
C 3.4594 1.7979 -1.2591

C	4.1214	2.0071	-2.4437	H	-1.2911	3.4944	-0.4101
C	3.5780	2.9671	-3.3536	H	-1.8224	3.7127	1.2480
C	2.3708	3.5869	-3.0718	O	1.7046	-2.0221	0.8624
C	1.7081	3.3165	-1.8842	H	0.3414	3.3323	2.1495
H	3.8853	1.0900	-0.5564	H	-3.5300	-0.0264	1.7051
H	5.0613	1.5766	-2.6601	H	-4.3450	-0.0537	0.1346
H	1.9352	4.2786	-3.7836	C	-3.3957	0.1499	0.6347
H	0.7536	3.7891	-1.6923	P	-2.0838	-1.0374	0.1327
H	4.0934	3.1768	-4.2838	O	-0.0353	0.2981	-1.6542
C	-0.0490	0.4676	-2.7013	C	-2.4345	-2.4792	1.1805
H	1.0499	0.5774	-2.6999	C	-1.5168	-2.8832	2.1432
H	-0.4137	0.9625	-3.6176	C	-1.8066	-3.9486	2.9843
H	-0.2541	-0.6106	-2.8228	C	-3.0174	-4.6126	2.8729
H	-0.0141	-0.1125	1.9237	C	-3.9423	-4.2114	1.9171
H	-1.6791	1.7842	1.8596	C	-3.6525	-3.1520	1.0750
RuOMeN_CH2PPH2_oH2				H	-0.5732	-2.3598	2.2324
TE [hartree]: -2141.66104				H	-1.0808	-4.2591	3.7268
ZPE [kJ/mol]: 1415.56				H	-4.8910	-4.7282	1.8277
G° [hartree]: -2141.12188				H	-4.3720	-2.8501	0.3216
Coordinates [Å]:				H	-3.2432	-5.4448	3.5298
C	-2.9139	1.5692	0.4085	C	-2.4789	-1.6048	-1.5423
N	-1.5009	1.7146	0.6919	C	-2.3293	-2.9394	-1.9089
C	-1.1450	3.1166	0.6168	C	-2.5374	-3.3336	-3.2220
C	0.2837	3.3603	1.0582	C	-2.8895	-2.3977	-4.1820
P	1.3513	1.9691	0.4997	C	-3.0245	-1.0630	-3.8267
Ru	-0.1847	0.2515	0.3313	C	-2.8117	-0.6663	-2.5175
C	0.9902	-1.1499	0.6041	H	-2.0496	-3.6763	-1.1652
H	-3.4991	2.2514	1.0445	H	-2.4211	-4.3763	-3.4942
H	-3.1267	1.8801	-0.6293	H	-3.2828	-0.3242	-4.5766
H	0.6640	4.3262	0.7192	H	-2.8799	0.3823	-2.2579
				H	-3.0515	-2.7063	-5.2085

C 2.7074 2.0134 1.7079
 C 3.4493 3.1817 1.8887
 C 4.4476 3.2372 2.8455
 C 4.7179 2.1248 3.6324
 C 3.9858 0.9616 3.4593
 C 2.9816 0.9062 2.5022
 H 3.2500 4.0494 1.2692
 H 5.0180 4.1494 2.9783
 H 4.1936 0.0907 4.0699
 H 2.4066 -0.0013 2.3714
 H 5.5013 2.1680 4.3804
 C 2.1282 2.4966 -1.0513
 C 3.4950 2.3602 -1.2778
 C 4.0394 2.7000 -2.5072
 C 3.2235 3.1731 -3.5229
 C 1.8574 3.2945 -3.3098
 C 1.3099 2.9489 -2.0863
 H 4.1399 1.9869 -0.4913
 H 5.1057 2.5923 -2.6699
 H 1.2119 3.6467 -4.1062
 H 0.2389 3.0005 -1.9429
 H 3.6497 3.4390 -4.4835
 C 0.8402 -0.5246 -2.3306
 H 1.8931 -0.3570 -2.0483
 H 0.7514 -0.3154 -3.4066
 H 0.6222 -1.5956 -2.1839

RuOMeN_CH2PPh2_CO

TE [hartree]: -2254.90724

ZPE [kJ/mol]: 1439.54

G° [hartree]: -2254.35894

Coordinates [Å]:

C -2.8888 1.5786 0.2421
 N -1.5911 1.8136 0.8201
 C -1.1523 3.1198 0.4018
 C 0.2223 3.4428 0.9580
 P 1.3210 2.0379 0.5689
 Ru -0.1798 0.2597 0.4906
 C 1.0644 -1.1097 0.1561
 H -3.6034 2.3353 0.6073
 H -2.8714 1.6846 -0.8580
 H 0.6198 4.3861 0.5773
 H -1.1353 3.2130 -0.6995
 H -1.8622 3.8844 0.7596
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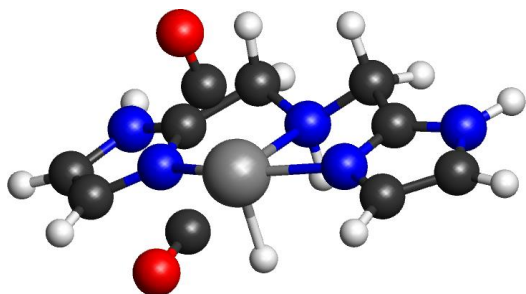
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H	-1.5273	-3.5756	-1.0166	O	-0.2554	0.5049	2.6007
H	-1.8559	-4.3976	-3.3053	C	-0.3763	-0.5419	3.4882
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H	-3.2781	0.1781	-2.1223	H	0.4273	-1.2941	3.3852
H	-2.9077	-2.9419	-5.0122	H	-1.3253	-1.0970	3.3940
C	2.6742	2.1963	1.8150	H	-1.5723	1.7852	1.8508
C	3.6102	3.2270	1.7421				
C	4.6023	3.3357	2.7017	RuOMeN_CH2PPh2_H_Pyr			
C	4.6688	2.4122	3.7370	TE [hartree]: -2353.08288			
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C	0.6453	3.0536	1.2681	C	-3.5524	-1.5320	-3.5485
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H	-3.4275	0.1240	1.7042	C	5.1308	0.1655	1.5503
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O	-0.6767	0.6850	-1.6402	H	5.8315	-0.5505	1.1371
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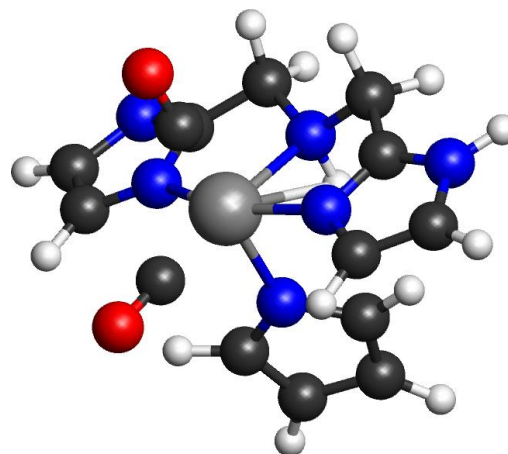
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C	-0.0177	-0.4899	4.5230
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H	0.9392	0.1742	-2.8450
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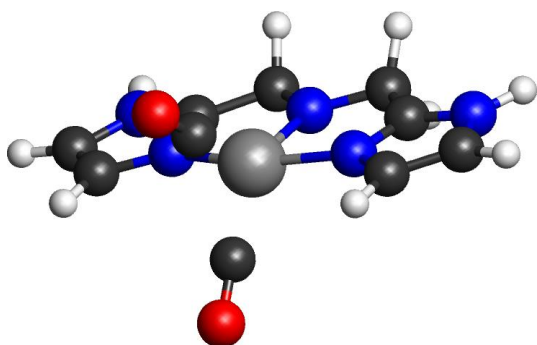
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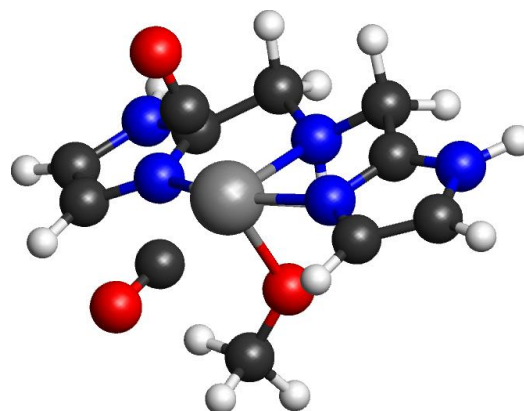
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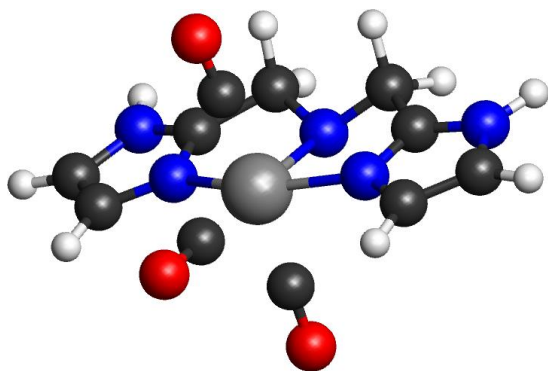
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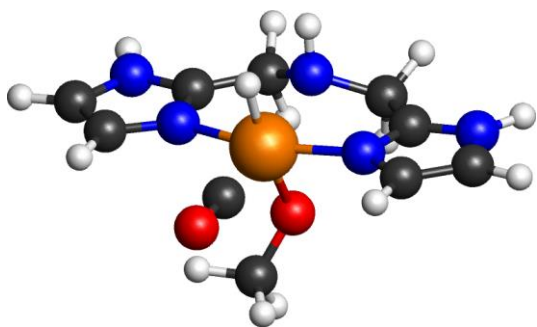
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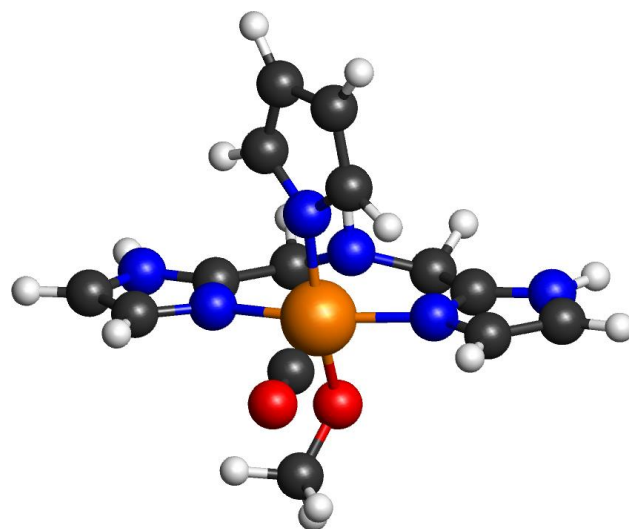
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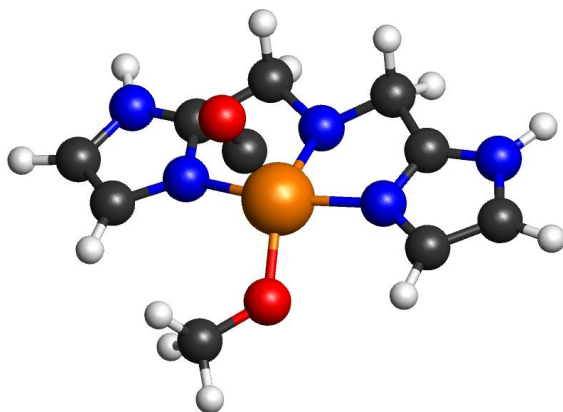
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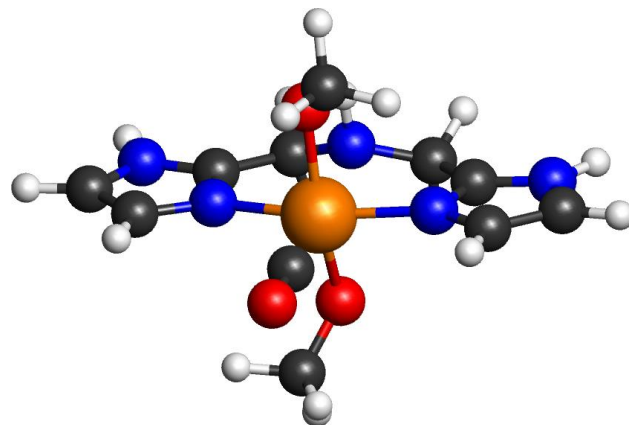
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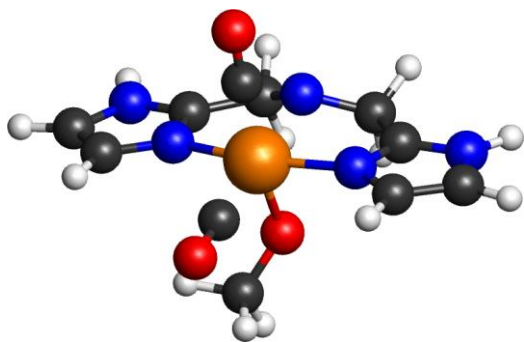
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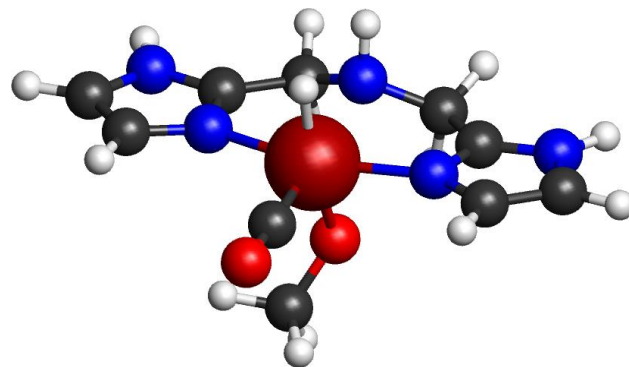
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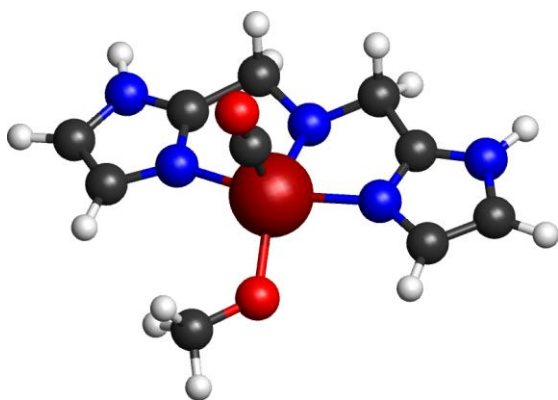
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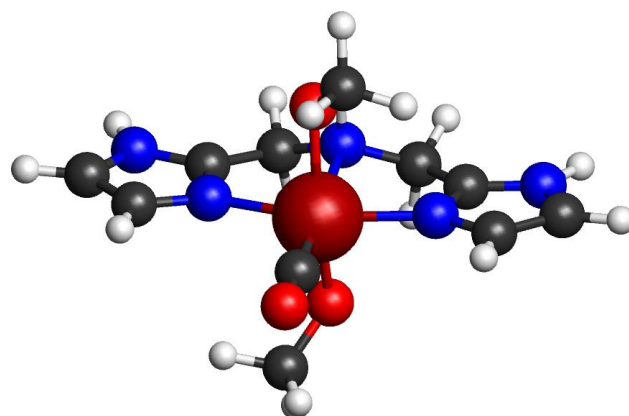
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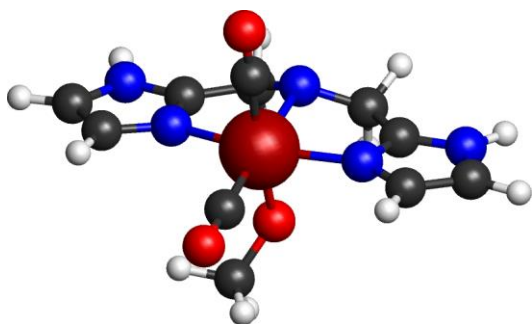
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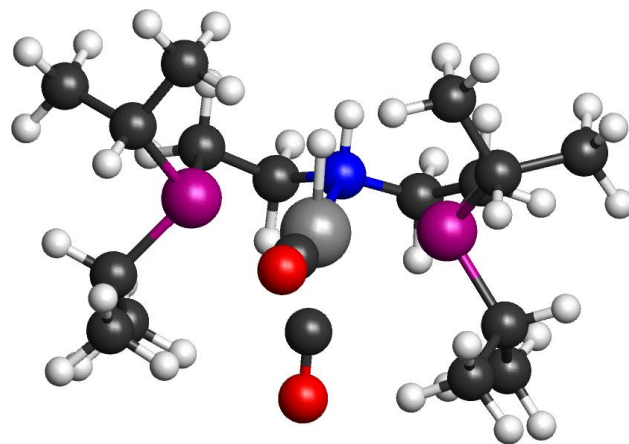
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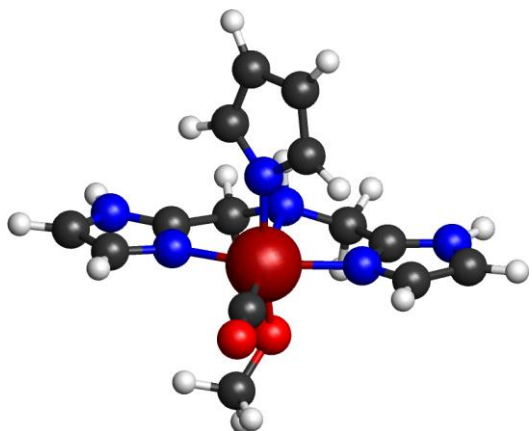
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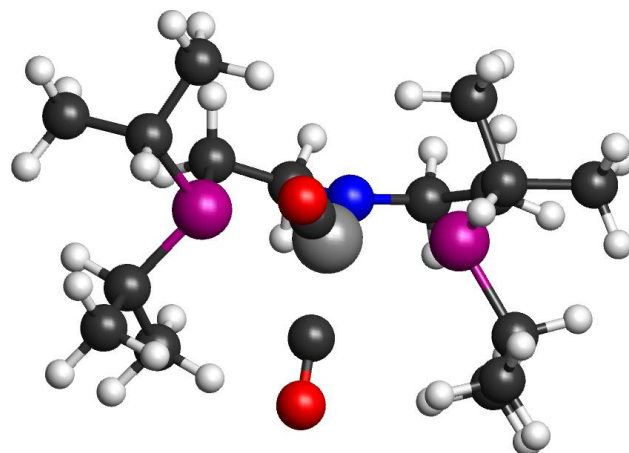
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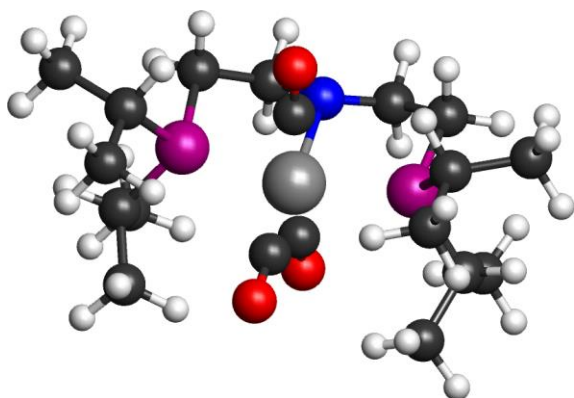
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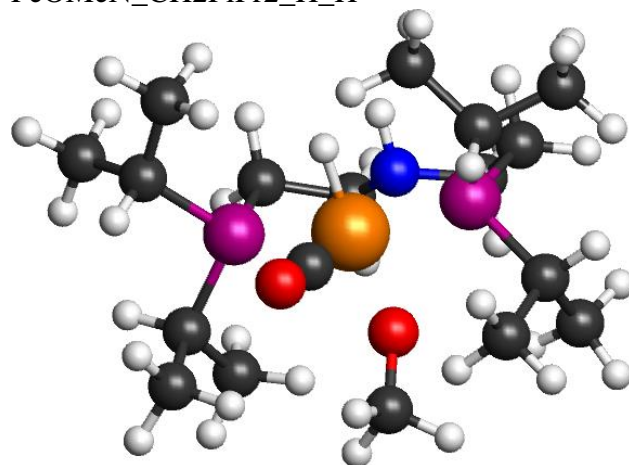
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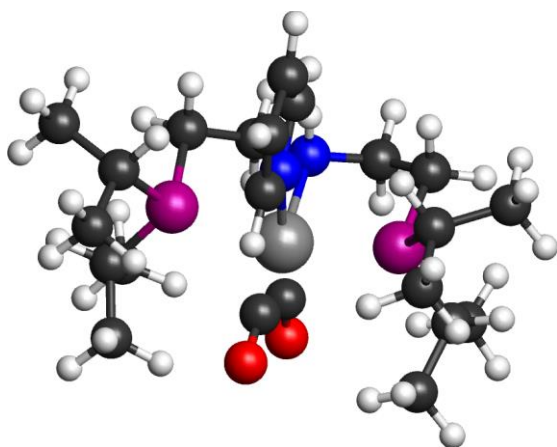
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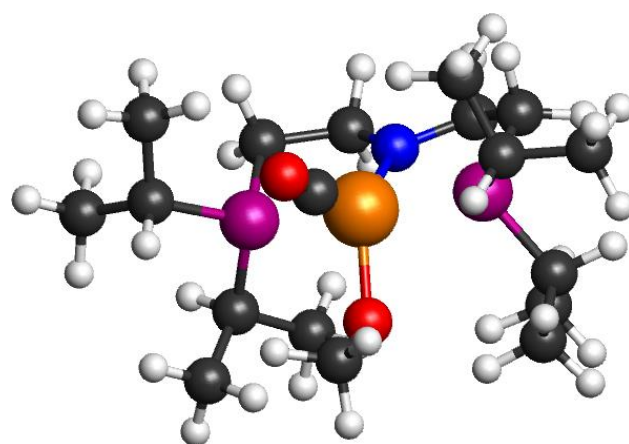
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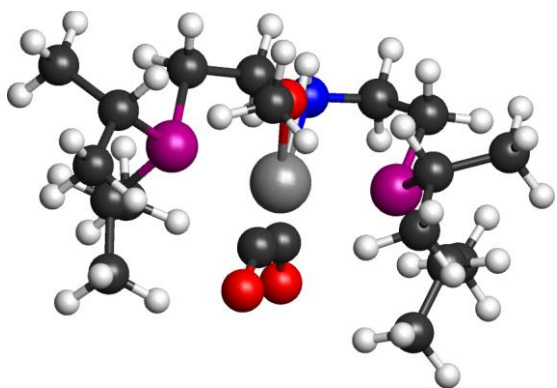
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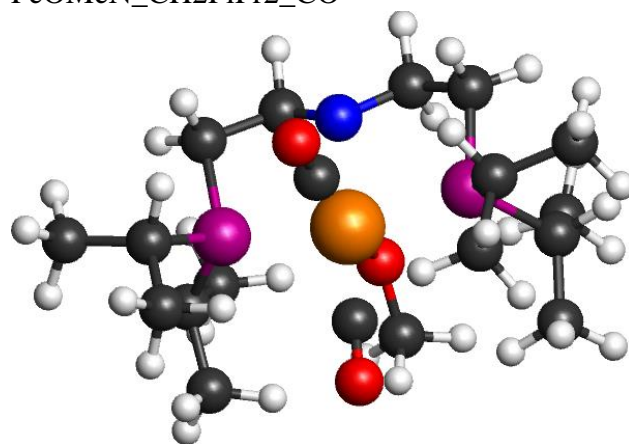
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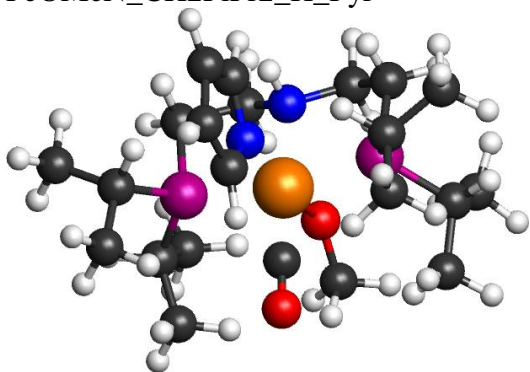
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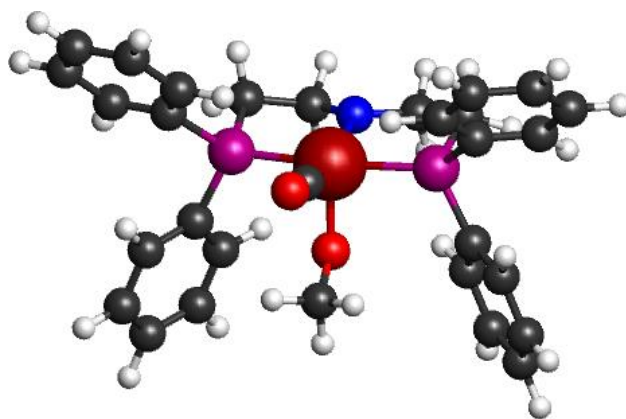
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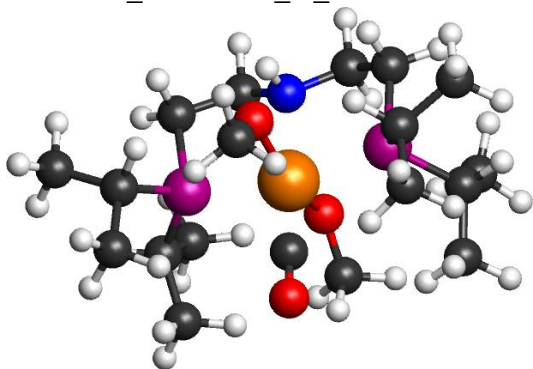
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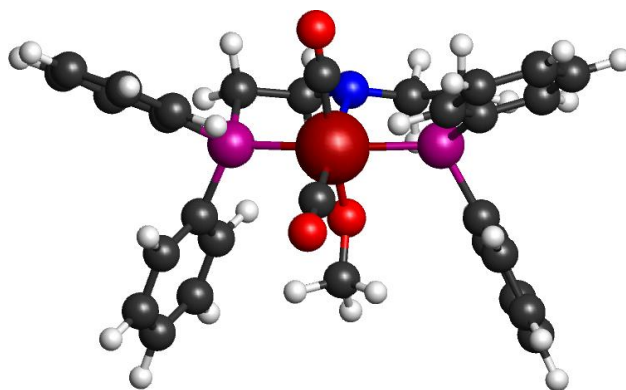
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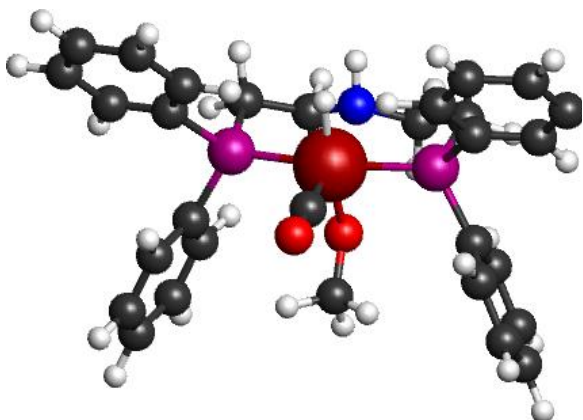
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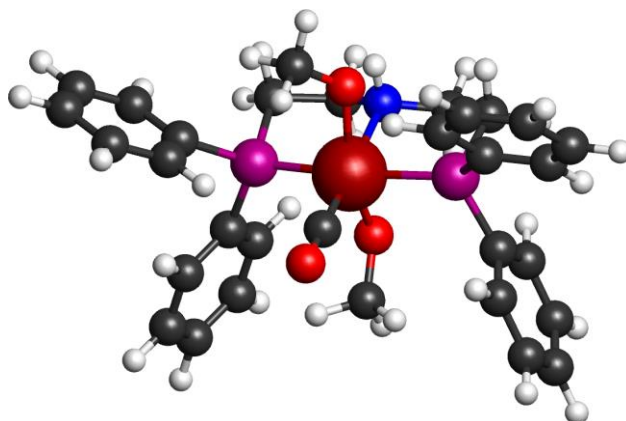
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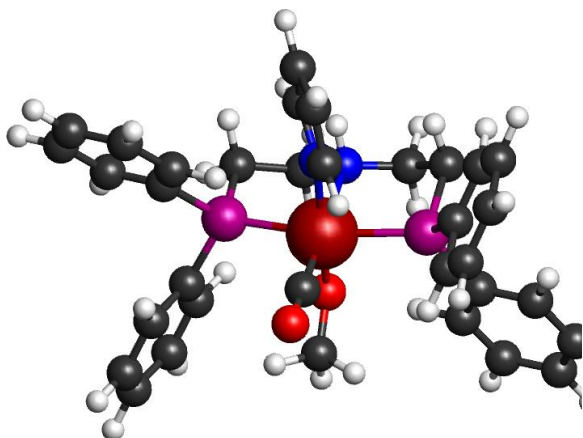
RuOMeN_CH2PPh2_H_H



RuOMeN_CH2PPh2_H_OMe



RuOMeN_CH2PPh2_H_Pyr



not accurate and we choose for the +H₂ reaction the value of B3LYP5-NL/def2-QZVP.

	+H ₂	+CO	+MeOH
DSD-PBE-NL/def2-QZVP	-27,8	-35,7	-9,8
B3LYP5-NL/def2-QZVP	14,8	-12,6	-17,1
DSD-PBE-NL/def2-TZVP	-22,3	-36,1	-13,9
B3LYP5-NL/def2-TZVP	14,7	-15,2	-23,6
PBE0-D3(BJ) / def2-TZVP	7,7	-15,8	-3,7

Determination of ³¹P NMR shifts:

³¹P NMR shifts were determined with the GIAO Method. Reference is H₃PO₄ the structures were computed at the same level of theory (PBE0-D3BJ/def2-TZVP).

Integrity check:

The H₂ addition reaction showed for DSD-PBE-NL a surprising high value. Because the difference to B3LYP5-NL is around 40 kJ/mol, and the value is negative, and it is too far away from the Mn-Imi2, this has to be a wrong description of the MnCON_CH2PiPr2_H_H complex. That's why we believe that this value is

	Exp. (THF- <i>d</i> 8) ³¹ P ppm	Calc. (Gas) ³¹ P, ppm	Δ, ppm
Mn-AM	+113.4	+105.1	8.3
Cis-Mn-DH	+109.6	+105.7	3.9
trans-Mn-DH	+107.5	+101.6	6
Mn-CO	+94.9	+87.0	7

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