Supporting Information

Enhanced Catalytic Activity of Nickel Complexes of an Adaptive Diphosphine-Benzophenone Ligand in Alkyne Cyclotrimerization

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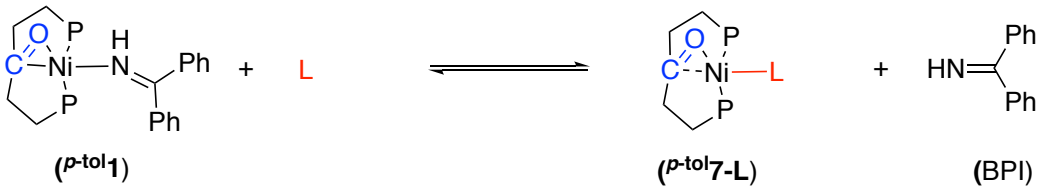
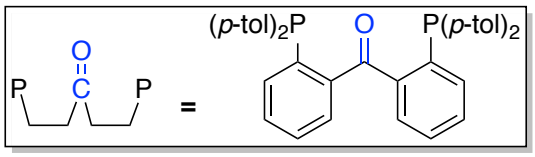
1. Ligand exchange reactions

Determination of the standard equilibrium constant (K_{eq}) and the standard Gibbs free energy of the reaction (Δ_rG°)

Consider the ligand exchange reaction between benzophenone imine (BPI) from $^{p\text{-tol}}$**1** and external co-ligand (L), as depicted below (Scheme S1).



($^{p\text{-tol}}$**1**) ($^{p\text{-tol}}$**7-L**) (BPI)



Scheme S1. Ligand exchange reaction: $^{p\text{-tol}}$**1** + L ⇔ $^{p\text{-tol}}$**7-L** + BPI. L = benzonitrile (PhCN), styrene (C_2H_3Ph), or diphenylacetylene (C_2Ph_2); BPI = benzophenone imine.

The Gibbs free energy of the reaction (Δ_rG) (left to right) is given by: $\mathbf{\Delta_rG = \Delta_rG^\circ + RTln(K_{eq})}$; With Δ_rG° = The Gibbs free energy of the reaction at the standard conditions, R = The gas constant, T = The temperature of the reaction, K_{eq} = The standard equilibrium constant = $\frac{\prod_n^{i=1} a(\text{product})_i}{\prod_n^{i=1} a(\text{reactant})_i} = \frac{a(\mathbf{7-L}) \times a(\text{BPI})}{a\left(^{p-\text{tol}}\mathbf{1}\right) \times a(\text{L})}$; with a = activity

When the equilibrium is reached, $\mathbf{\Delta_rG = 0 \Leftrightarrow \Delta_rG^\circ = -RTln(K_{eq}) = -RTln \frac{a\left(^{p-\text{tol}}\mathbf{7-L}\right) \times a(\text{BPI})}{a\left(^{p-\text{tol}}\mathbf{1}\right) \times a(\text{L})}}$

In solution $\frac{\prod_n^{i=1} a(\text{product})_i}{\prod_n^{i=1} a(\text{reactant})_i} \approx \frac{\prod_n^{i=1} C(\text{product})_i}{\prod_n^{i=1} C(\text{reactant})_i}$; with C = molar concentration

$$\mathbf{\Delta_rG^\circ = -RTln(K_{eq}) -RTln \frac{\prod_n^{i=1} C(product)_i}{\prod_n^{i=1} C(reactant)_i} = -RTln \frac{C(7-L) \times C(BPI)}{C\left(^{p-tol}1\right) \times C(L)}}$$

The relative concentration between the reactants and products were determined by ^{1}H and ^{31}P NMR at a temperature T = 298.15 K. Table S1 show the differences of the calculated parameters between the two NMR methods. In the Results and Discussion part of the paper the K_{eq} and $\Delta_rG^\circ_{298,15}$ are reported according to ^{1}H NMR.

Table S1. Determination of standard equilibrium constant (K_{eq}) and the standard Gibbs free energy of the reaction ($\Delta_rG^\circ_{298,15}$) for the ligand exchange reaction: $^{p\text{-tol}}$**1** + L ⇔ $^{p\text{-tol}}$**7-L** + BPI. L = benzonitrile (PhCN), styrene (C_2H_3Ph), or diphenylacetylene (C_2Ph_2); BPI = benzophenone imine.

Ligand	**Product**	**K_{eq} [-]**		**$\Delta_rG^\circ_{298,15}$ [kcal/mol]**	
		NMR		**NMR**	
		^{1}H	**^{31}P**	**^{1}H**	**^{31}P**
PhCN	**$^{p\text{-tol}}$7-PhCN**	$2.7\ 10^{-3}$	$3.6\ 10^{-3}$	3.5	3.3
Styrene	**$^{p\text{-tol}}$7-C_2H_3Ph**	$1.5\ 10^{-2}$	$1.0\ 10^{-2}$	2.4	2.7
Diphenyacetylene	**$^{p\text{-tol}}$7-C_2Ph_2**	$6.1\ 10^{-3}$	$3.4\ 10^{-3}$	3.1	3.3

NMR data

K_{eq} determination

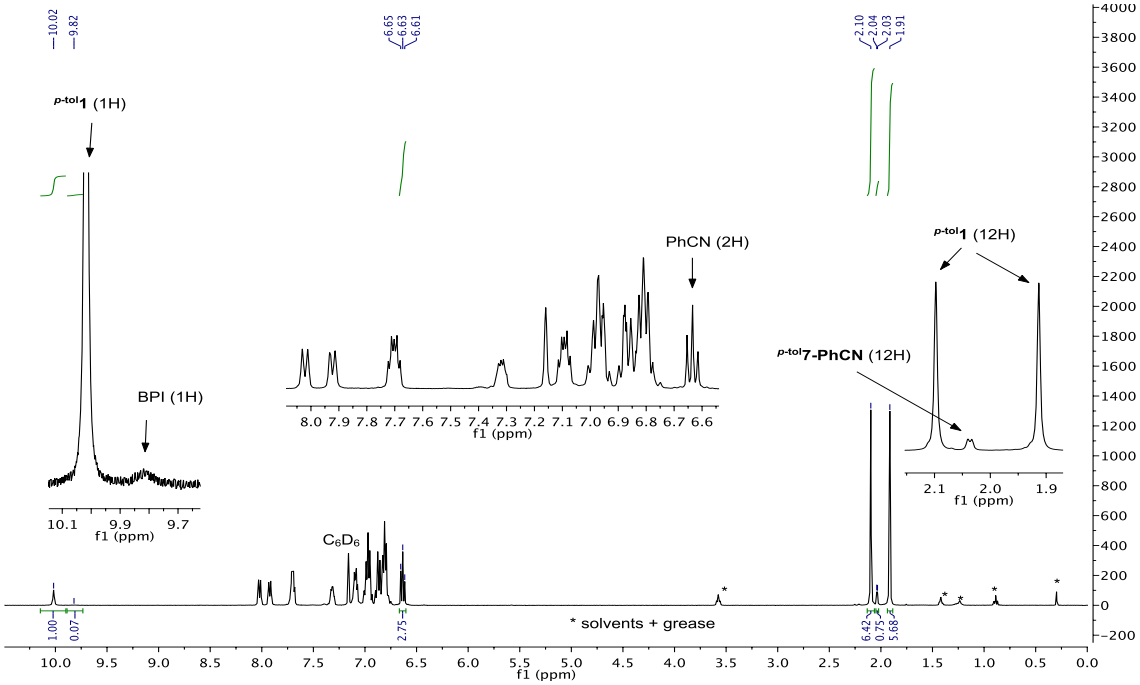


Figure S1. *In-situ* ^{1}H NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + PhCN ⇔ $^{p\text{-tol}}$**7-PhCN** + BPI. The values of the integrated peaks displayed in this spectrum were used to calculate the standard equilibrium constant (K_{eq}) and Gibbs free energy of the reaction ($\Delta_rG^{\circ}_{298,15}$).

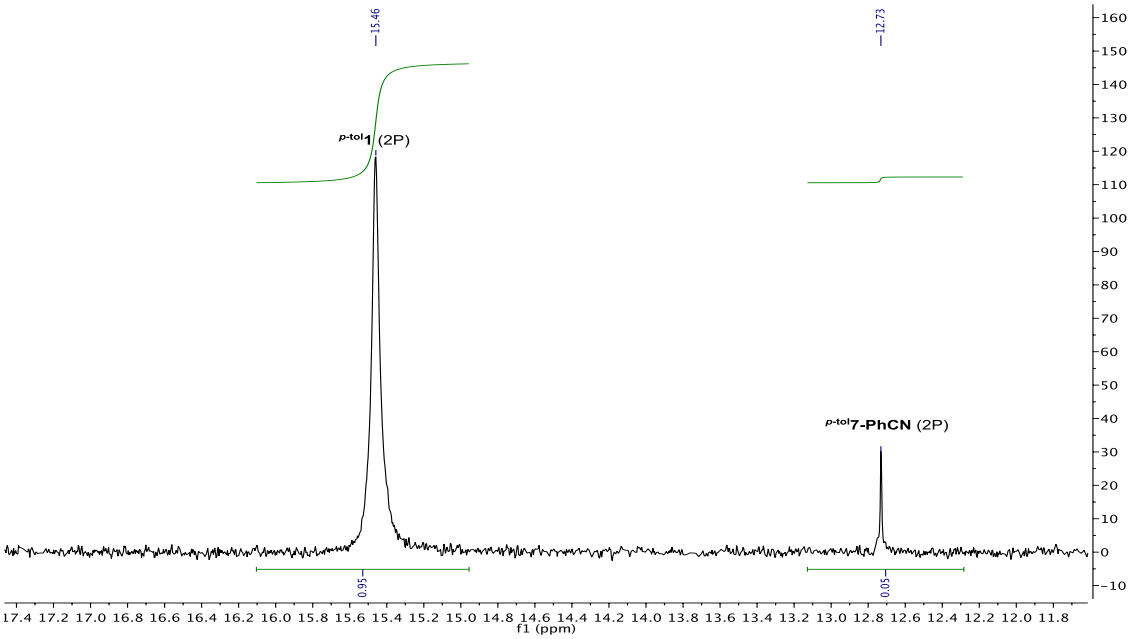


Figure S2. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + PhCN ⇔ $^{p\text{-tol}}$**7-PhCN** + BPI. The values of the integrated peaks shown in this spectrum were used to calculate the standard equilibrium constant (K_{eq}) and Gibbs free energy of the reaction ($\Delta_rG^{\circ}_{298,15}$).

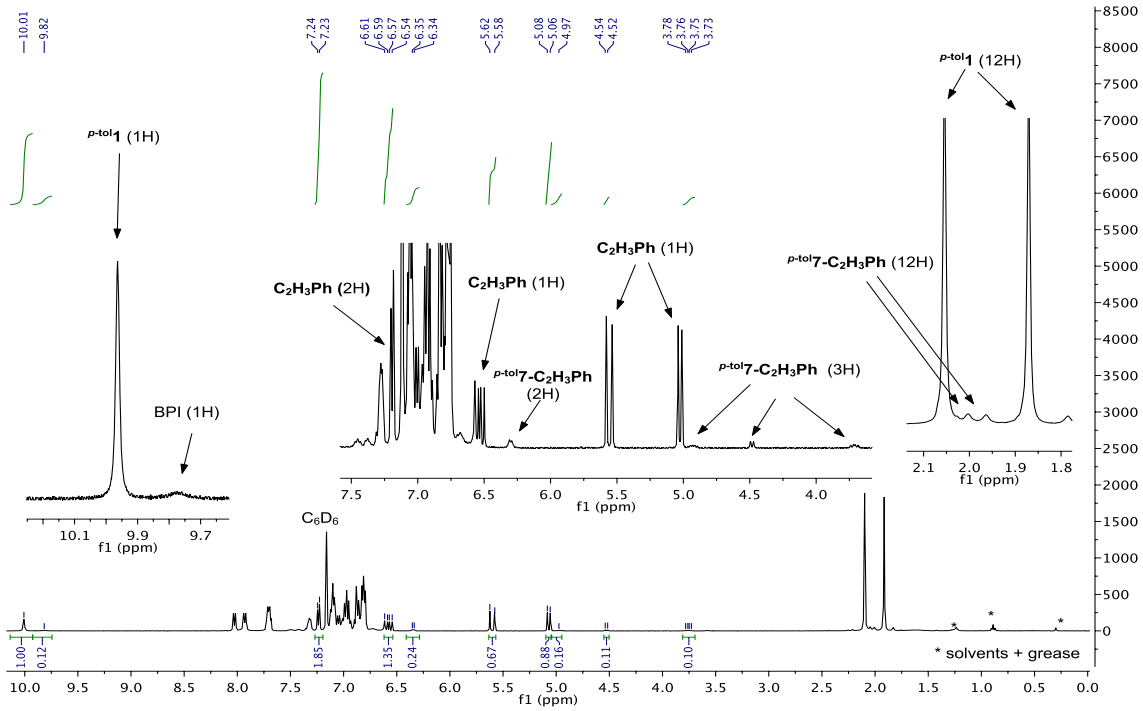


Figure S3. *In-situ* ^{1}H NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + C_2H_3Ph ⇔ $^{p\text{-tol}}$**7-C_2H_3Ph** + BPI. The values of the integrated peaks displayed in this spectrum were used to calculate the standard equilibrium constant (K_{eq}) and Gibbs free energy of the reaction ($\Delta_rG^\circ_{298,15}$).

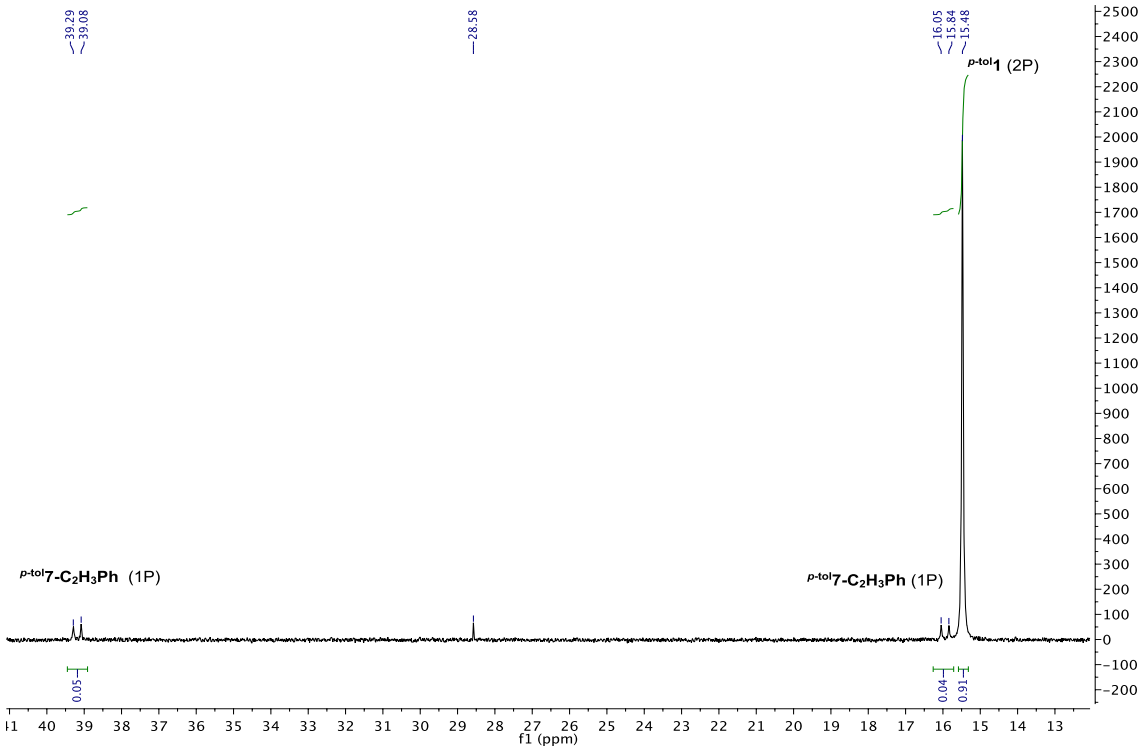


Figure S4. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + C_2H_3Ph ⇔ $^{p\text{-tol}}$**7-C_2H_3Ph** + BPI. The values of the integrated peaks displayed in this spectrum were used to calculate the standard equilibrium constant (K_{eq}) and Gibbs free energy of the reaction ($\Delta_rG^\circ_{298,15}$). The peak at 28.5 ppm is an unknown impurity.

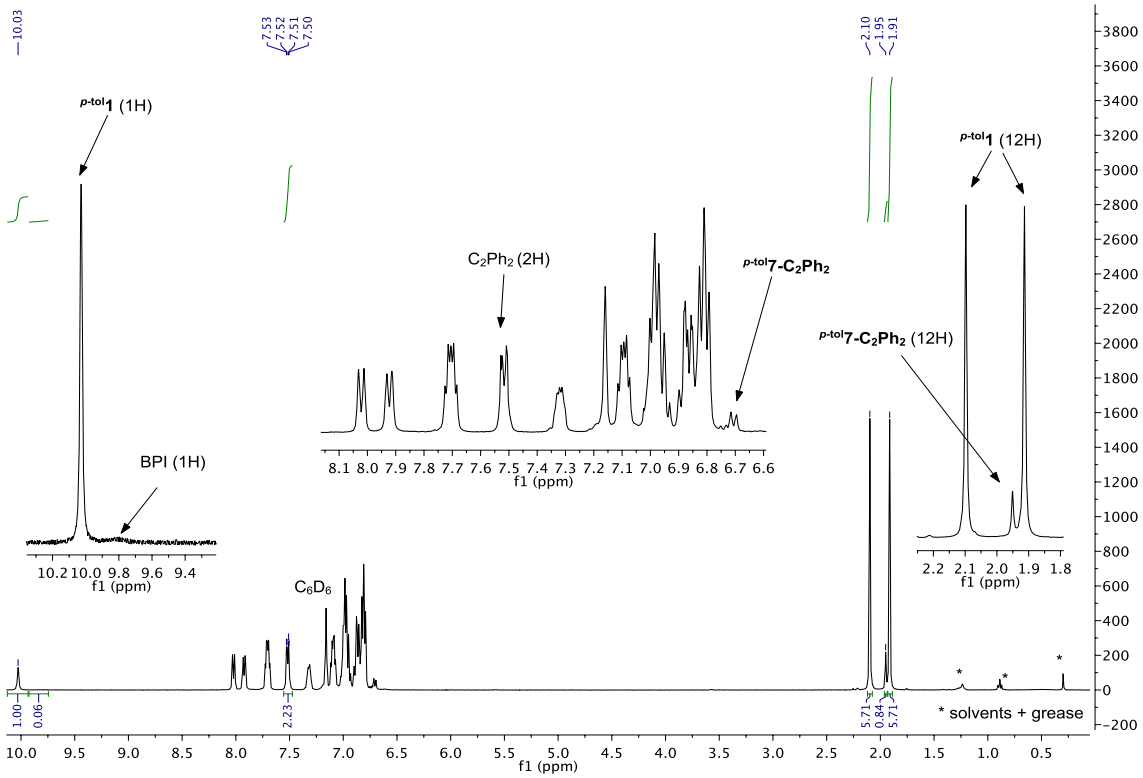


Figure S5. *In-situ* ^{1}H NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + C_2Ph_2 ⇔ $^{p\text{-tol}}$**7-C_2Ph$_2$** + BPI. The values of the integrated peaks displayed in this spectrum were used to calculate the standard equilibrium constant (K_{eq}) and Gibbs free energy of the reaction ($\Delta_rG^\circ_{298,15}$).

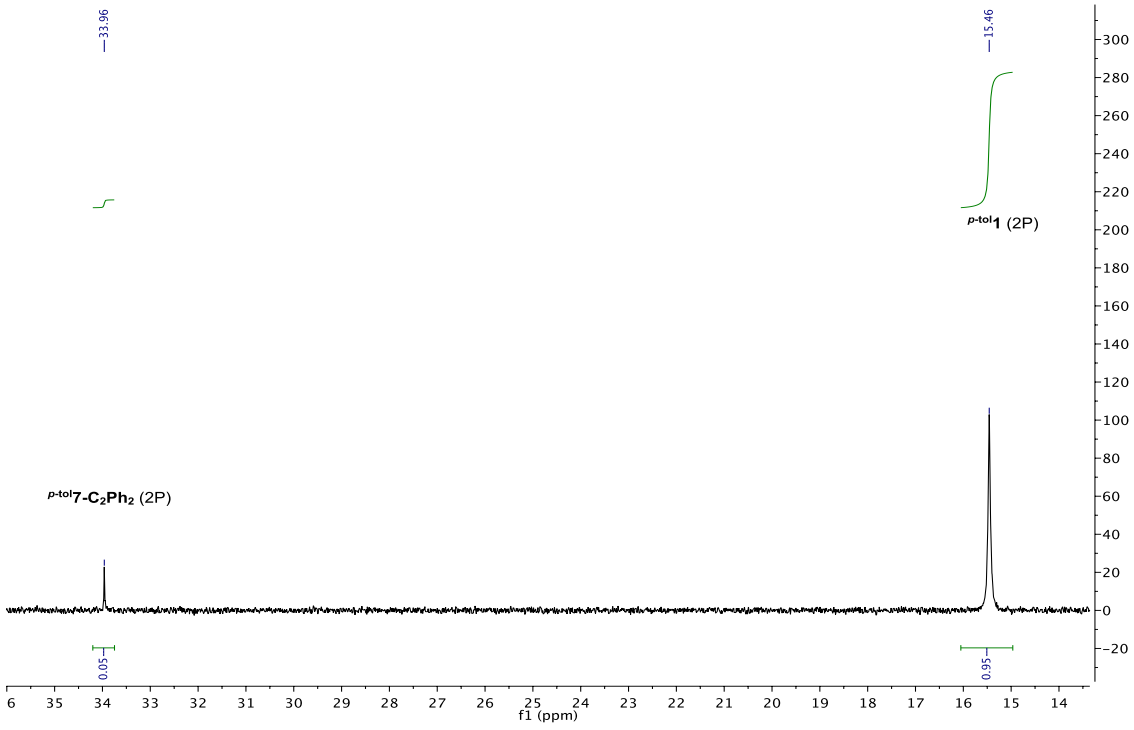


Figure S6. *in-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + C_2Ph_2 ⇔ $^{p\text{-tol}}$**7-C_2Ph$_2$** + BPI. The values of the integrated peaks displayed in this spectrum were used to calculate the standard equilibrium constant (K_{eq}) and Gibbs free energy of the reaction ($\Delta_rG^\circ_{298,15}$).

NMR at different stoichiometry and ^{13}C-NMR

p-tol7-PhCN

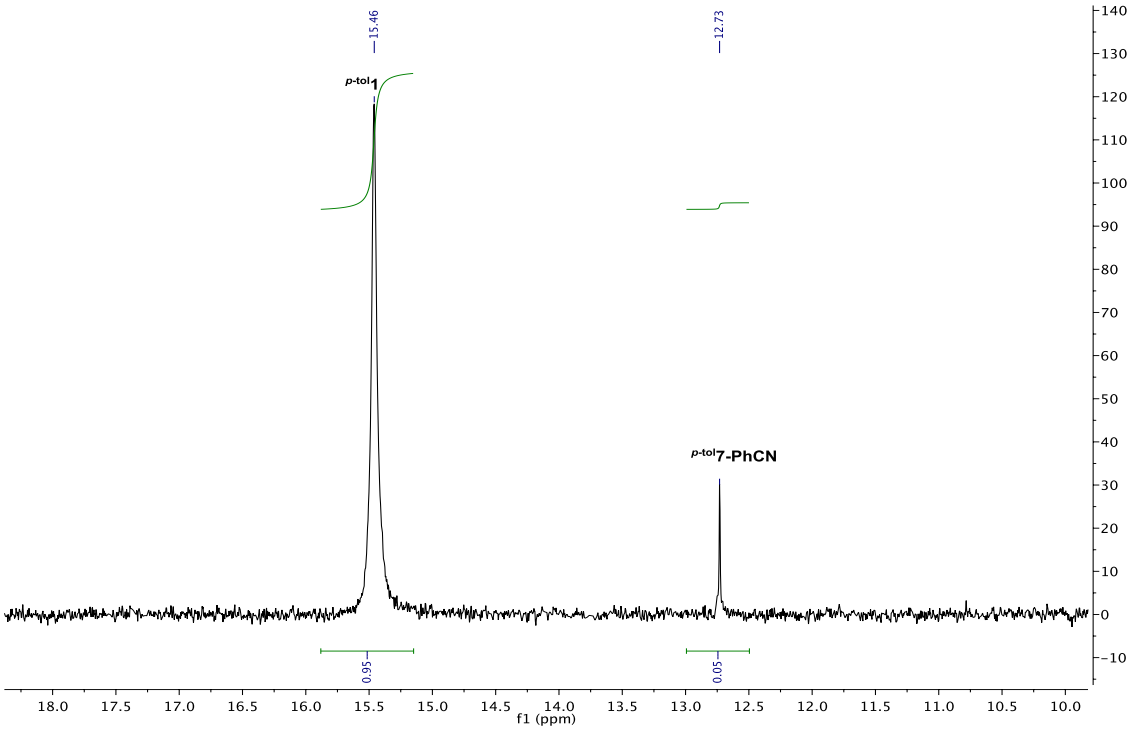


Figure S7. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x PhCN ⇔ $^{p\text{-tol}}$**7-PhCN** + BPI. x = 1 equivalent.

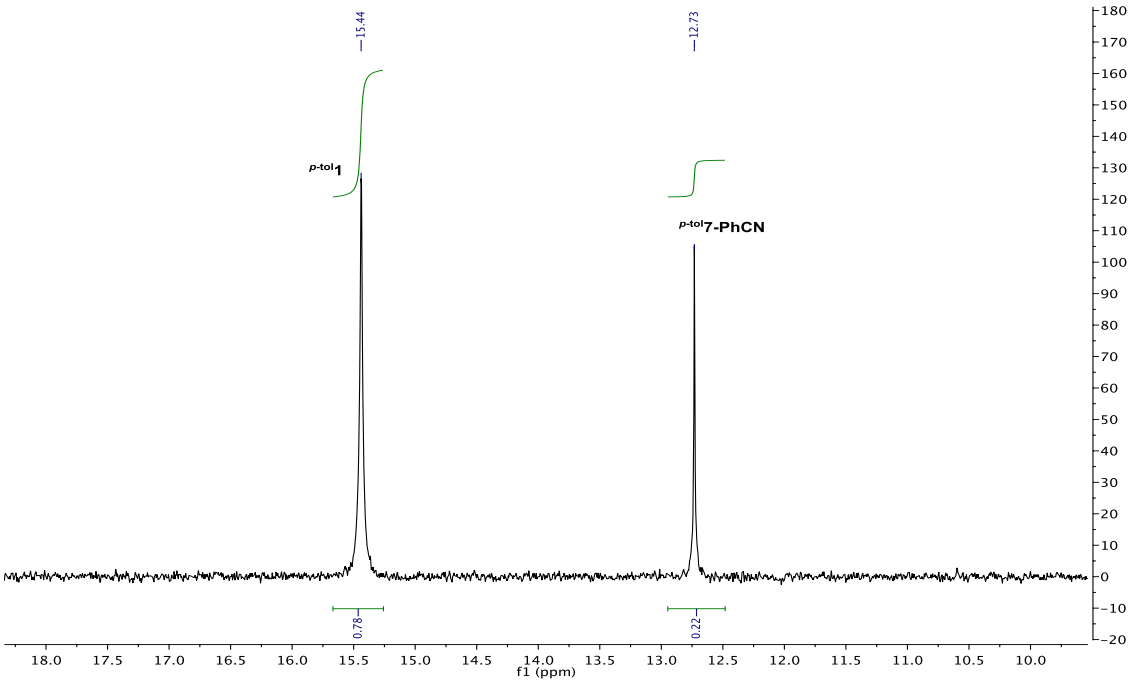


Figure S8. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x PhCN ⇔ $^{p\text{-tol}}$**7-PhCN** + BPI. x = 50 equivalents.

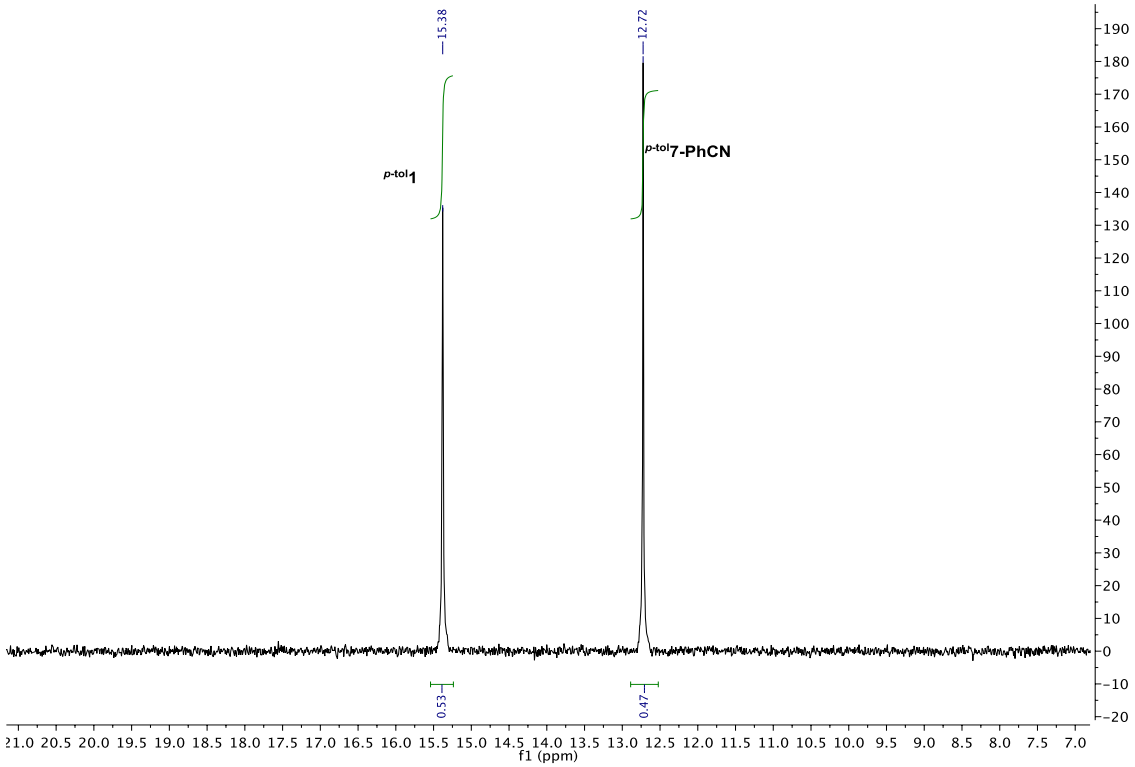


Figure S9. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x PhCN ⇔ $^{p\text{-tol}}$**7-PhCN** + BPI. x = 200 equivalents.

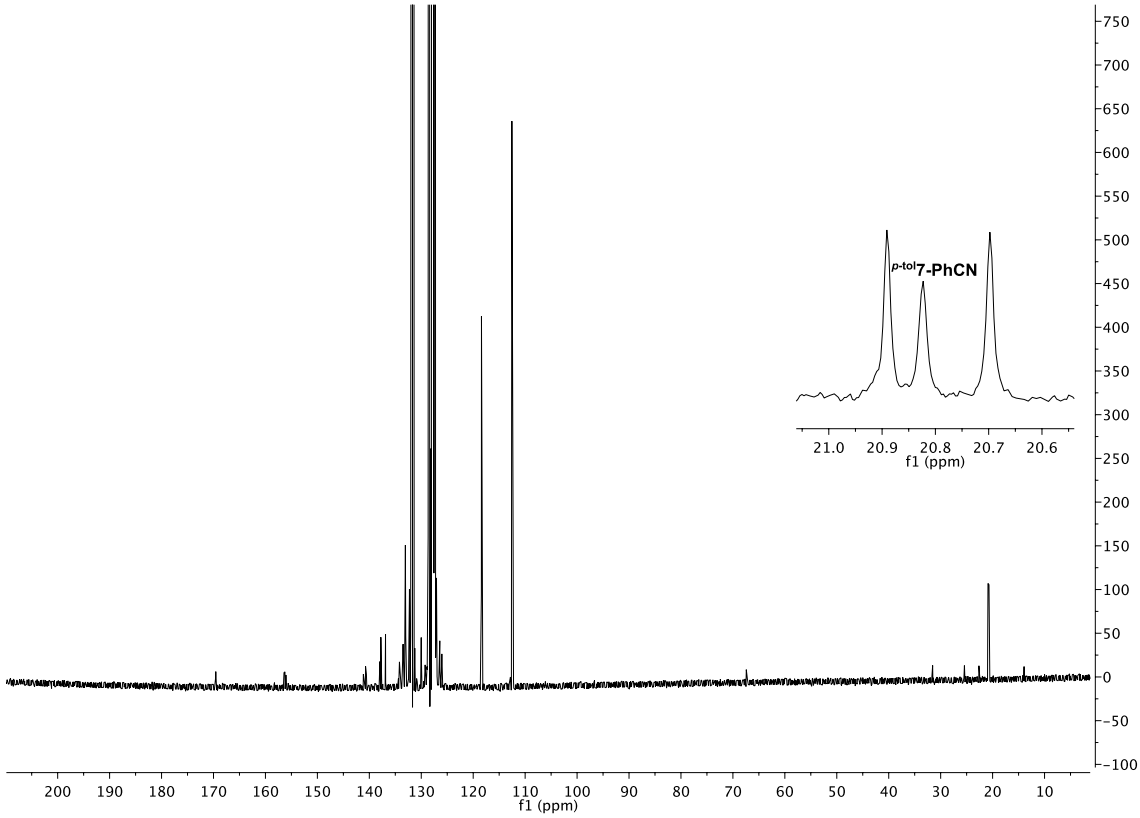


Figure S10. *In-situ* ^{13}C NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x PhCN ⇔ $^{p\text{-tol}}$**7-PhCN** + BPI. x = 50 equivalents. No carbonyl peals have been detected around 200 ppm.

$^{p\text{-tol}}$7-C_2H_3Ph

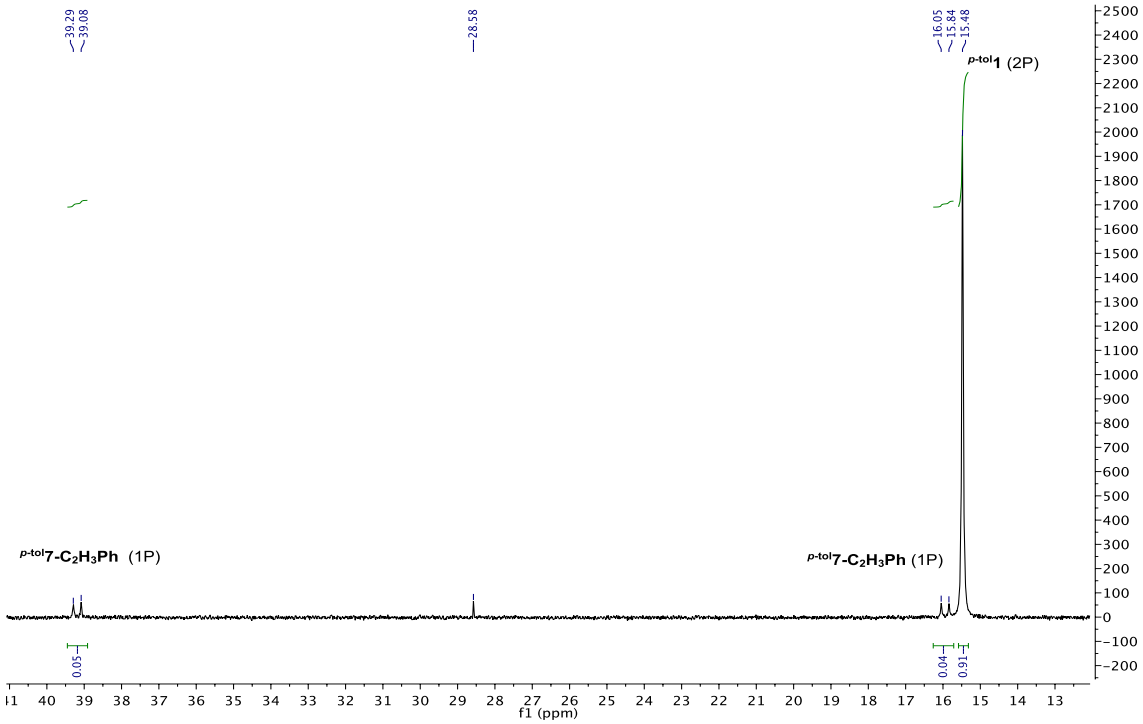


Figure S11. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2H_3Ph ⇔ $^{p\text{-tol}}$**7-C_2H_3Ph** + BPI. X = 1 equivalent. The peak at 28.5 ppm is an unknown impurity.

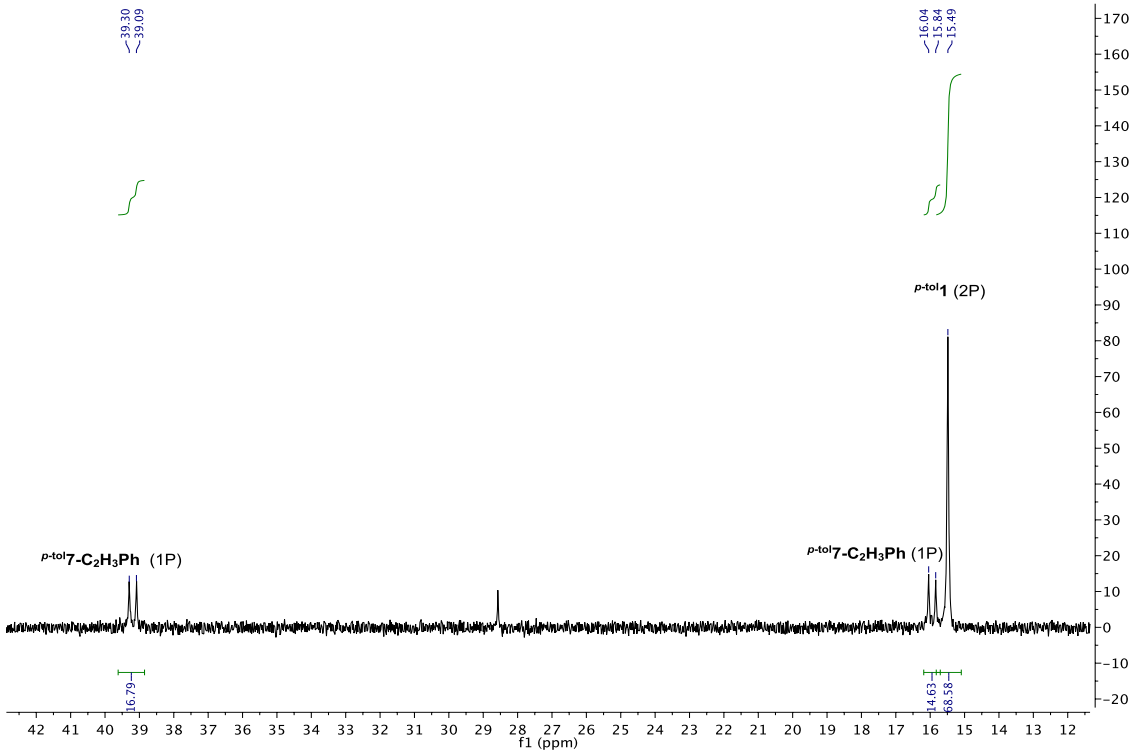


Figure S12. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2H_3Ph ⇔ $^{p\text{-tol}}$**7-C_2H_3Ph** + BPI. x= = 50 equivalents. The peak at 28.5 ppm is an unknown impurity.

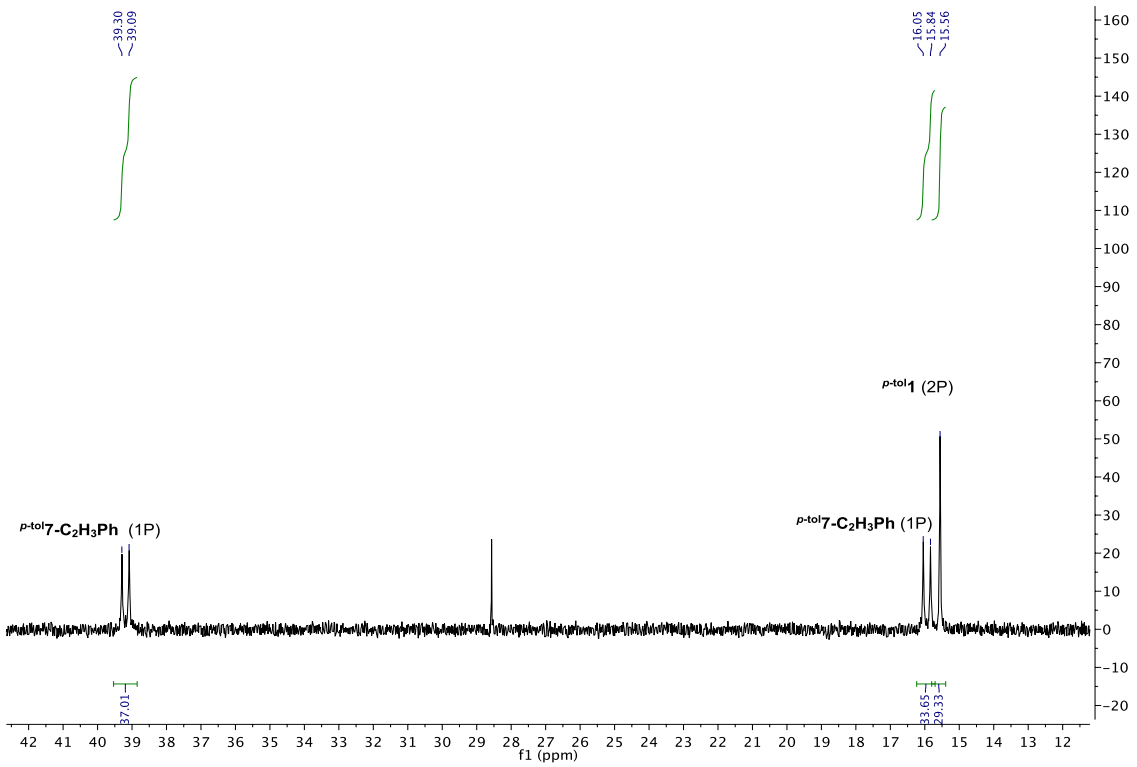


Figure S13. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2H_3Ph ⇔ $^{p\text{-tol}}$**7-C_2H_3Ph** + BPI. x = 200 equivalents. The peak at 28.5 ppm is an unknown impurity.

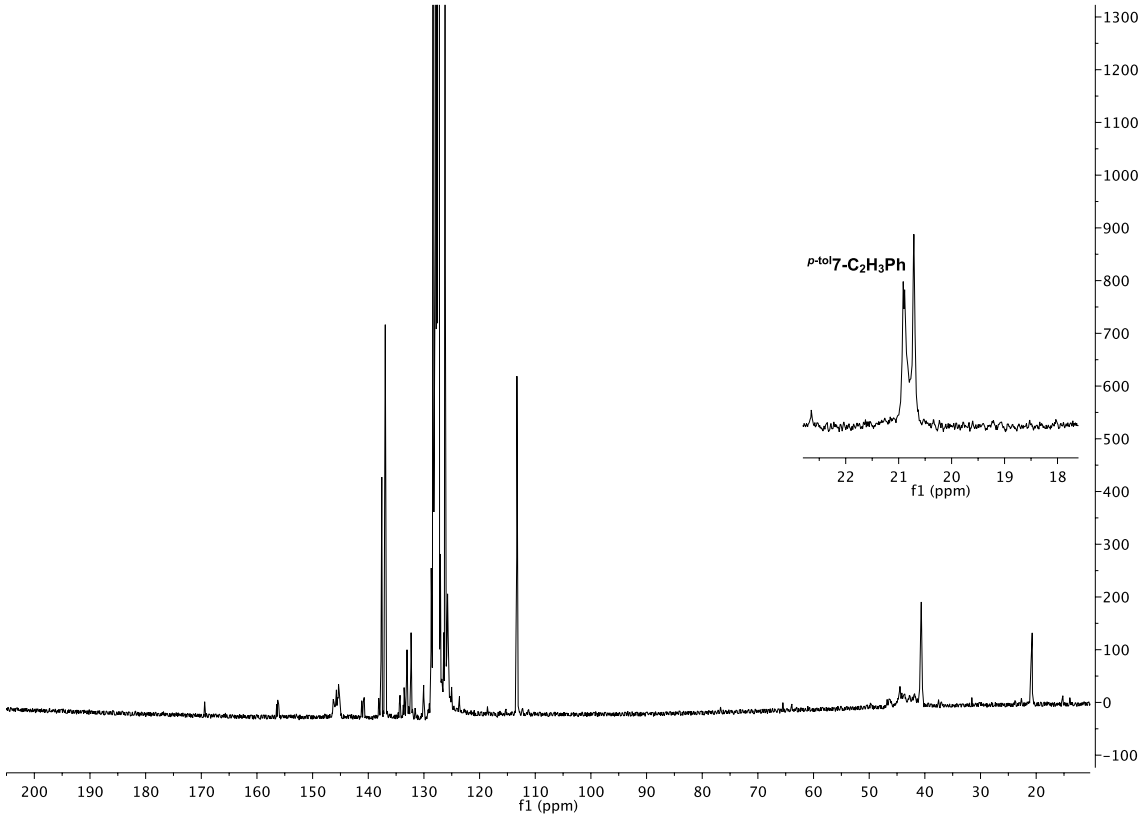


Figure S14. *In-situ* ^{13}C NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2H_3Ph ⇔ $^{p\text{-tol}}$**7-C_2H_3Ph** + BPI. x = 50 equivalents. No carbonyl peals have been detected around 200 ppm.

p-tol7-C_2Ph_2

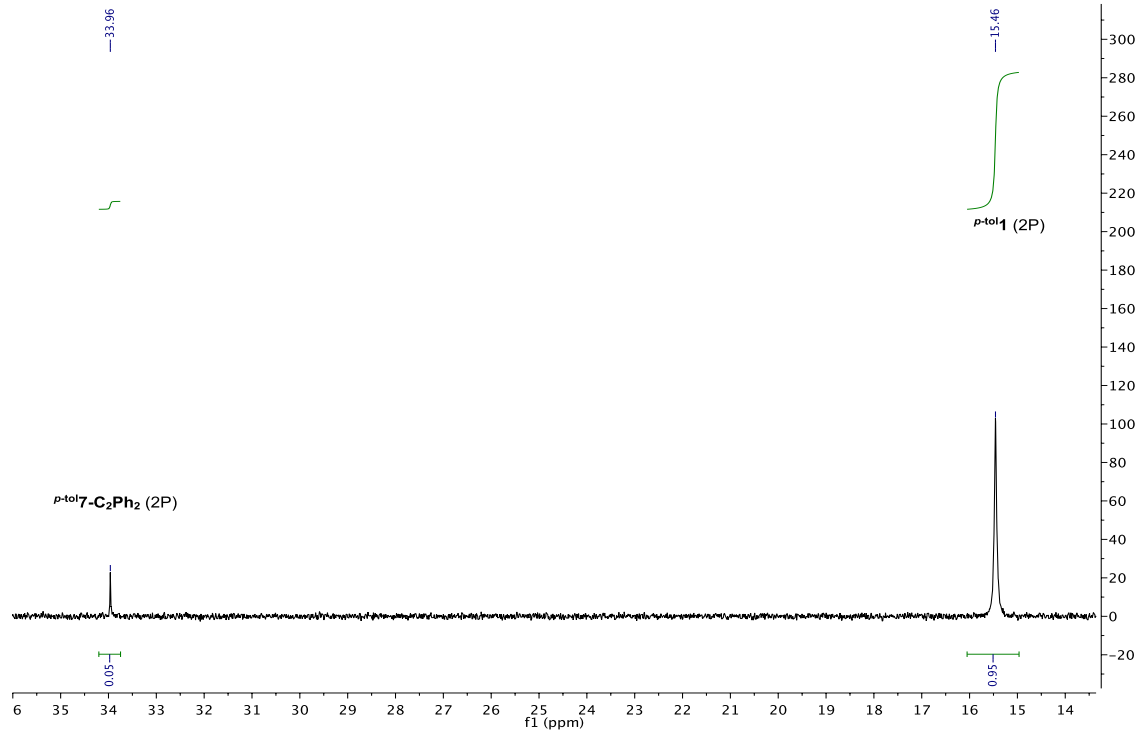


Figure S15. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2Ph_2 ⇔ $^{p\text{-tol}}$**7-C_2Ph_2** + BPI + BPI. x = 1 equivalent.

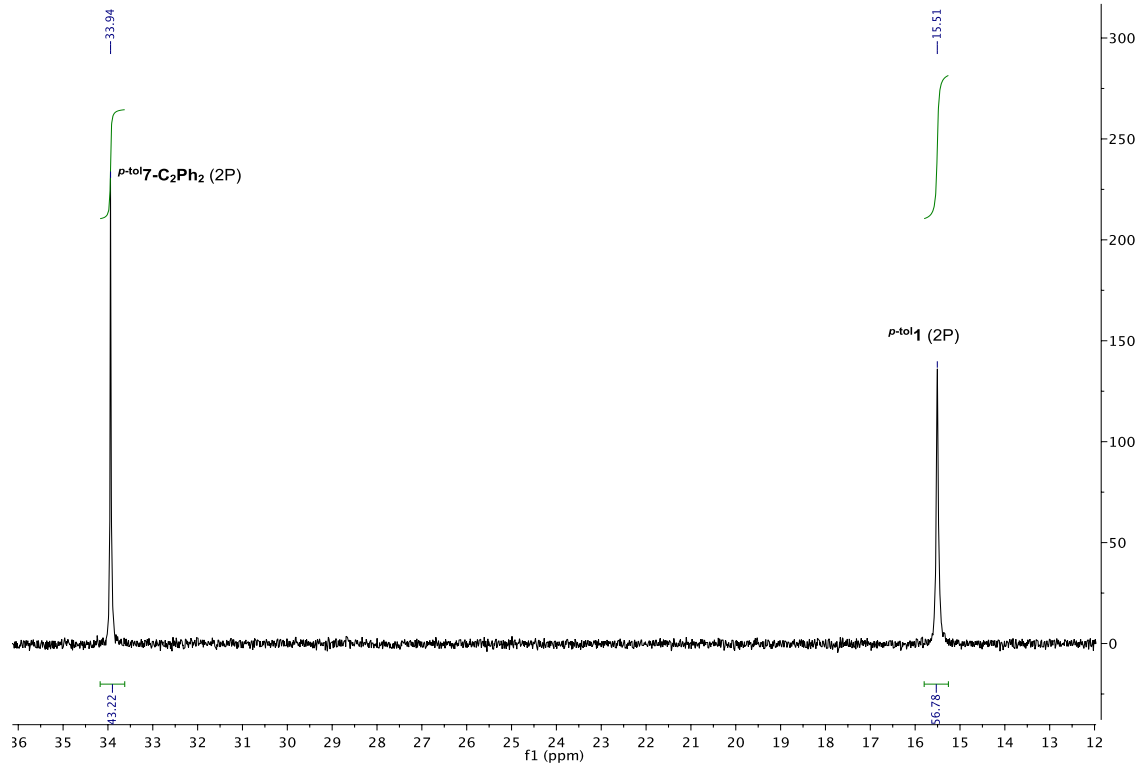


Figure S16. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2Ph_2 ⇔ $^{p\text{-tol}}$**7-C_2Ph_2** + BPI + BPI. x = 50 equivalents.

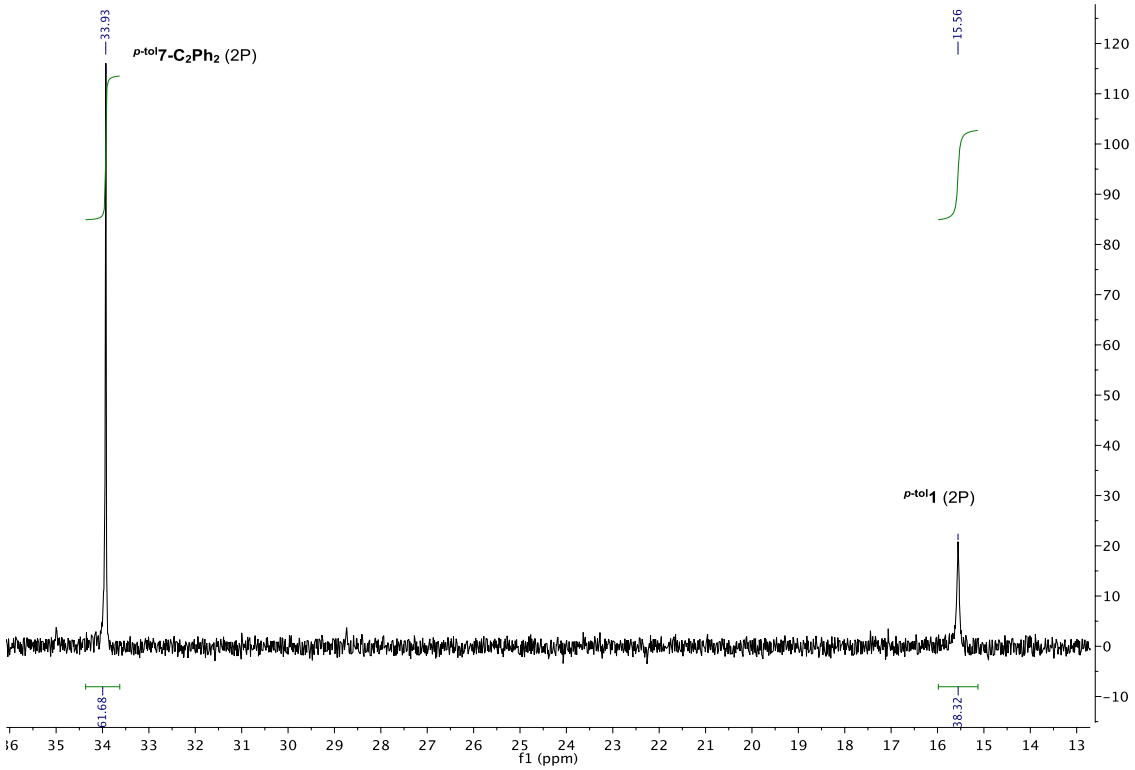


Figure S17. *In-situ* ^{31}P NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2Ph_2 ⇔ $^{p\text{-tol}}$**7-C_2Ph_2** + BPI + BPI. x = 200 equivalents.

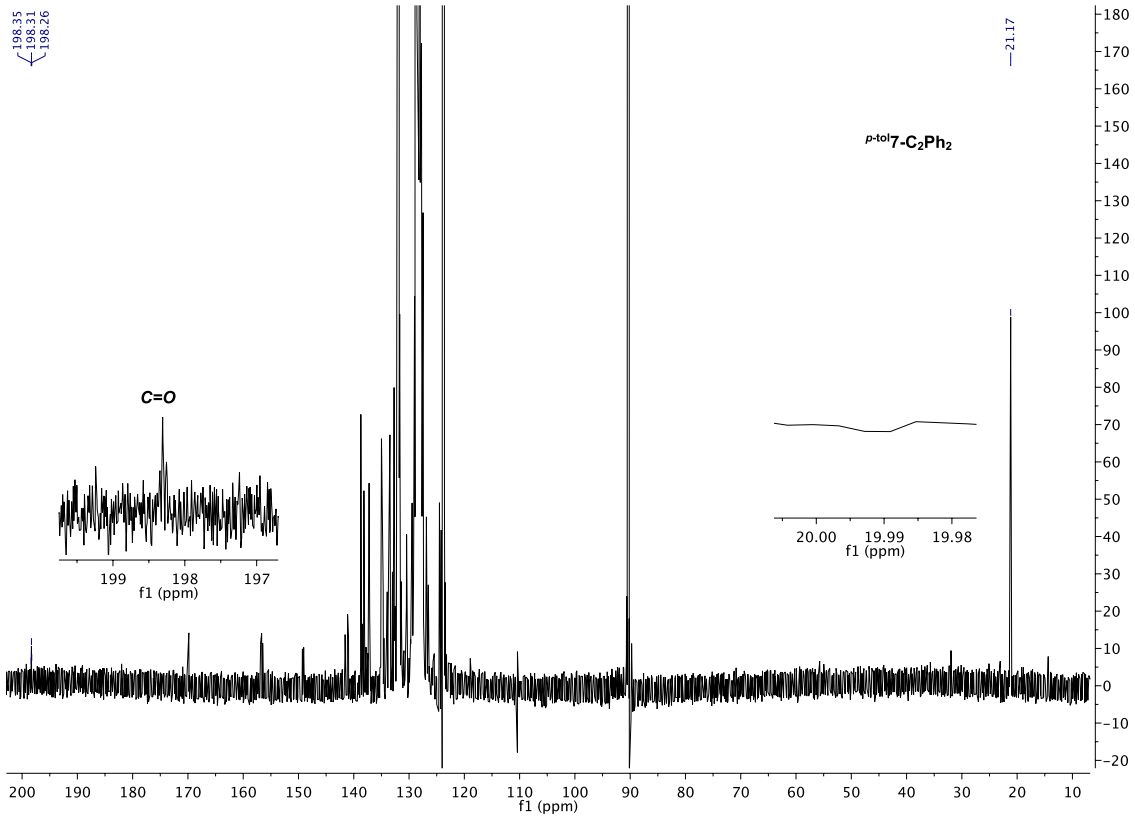


Figure S18. *In-situ* ^{13}C NMR (C_6D_6) of the ligand exchange reaction: $^{p\text{-tol}}$**1** + x C_2Ph_2 ⇔ $^{p\text{-tol}}$**7-C_2Ph_2** + BPI + BPI. x = 50 equivalents.

[($^{p\text{-tol}}$L1)Ni(PPh$_3$)] ($^{p\text{-tol}}$7-PPh$_3$)

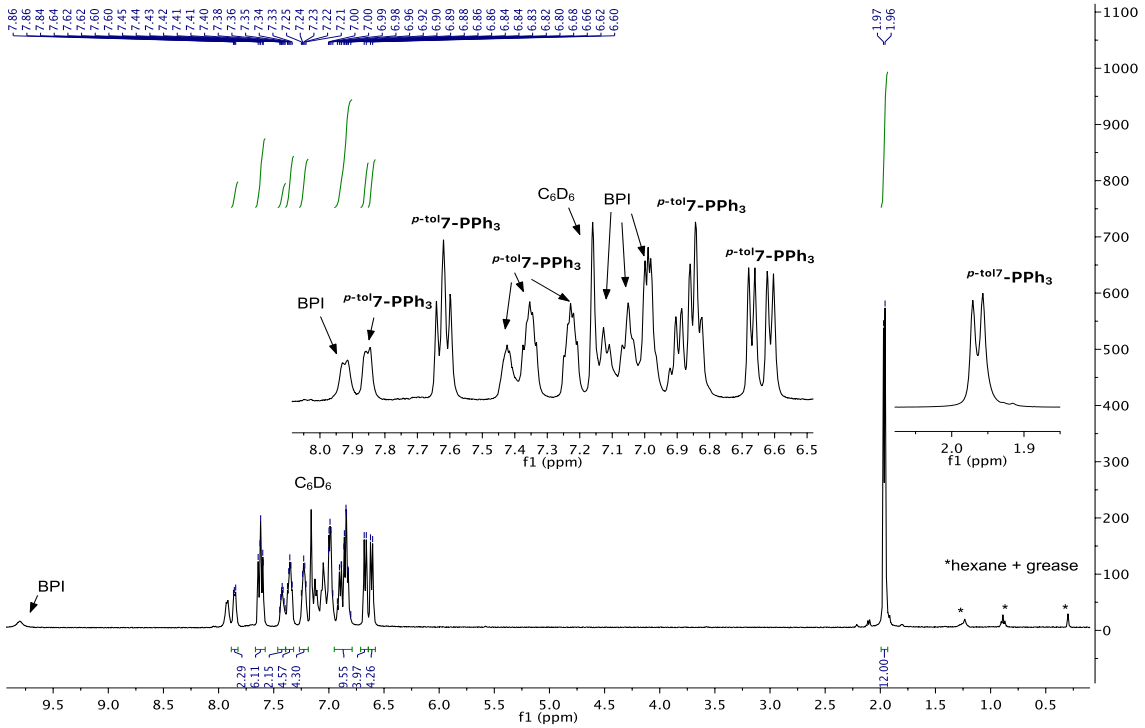


Figure S19. *In-situ* ^{1}H NMR (C_6D_6) of [($^{p\text{-tol}}$**L1**)Ni(PPh$_3$)] ($^{p\text{-tol}}$**7-PPh$_3$**) from the reaction of $^{p\text{-tol}}$**1** + equivalent of PPh$_3$. The sample contains a mixture of $^{p\text{-tol}}$**7-PPh$_3$** and BPI.

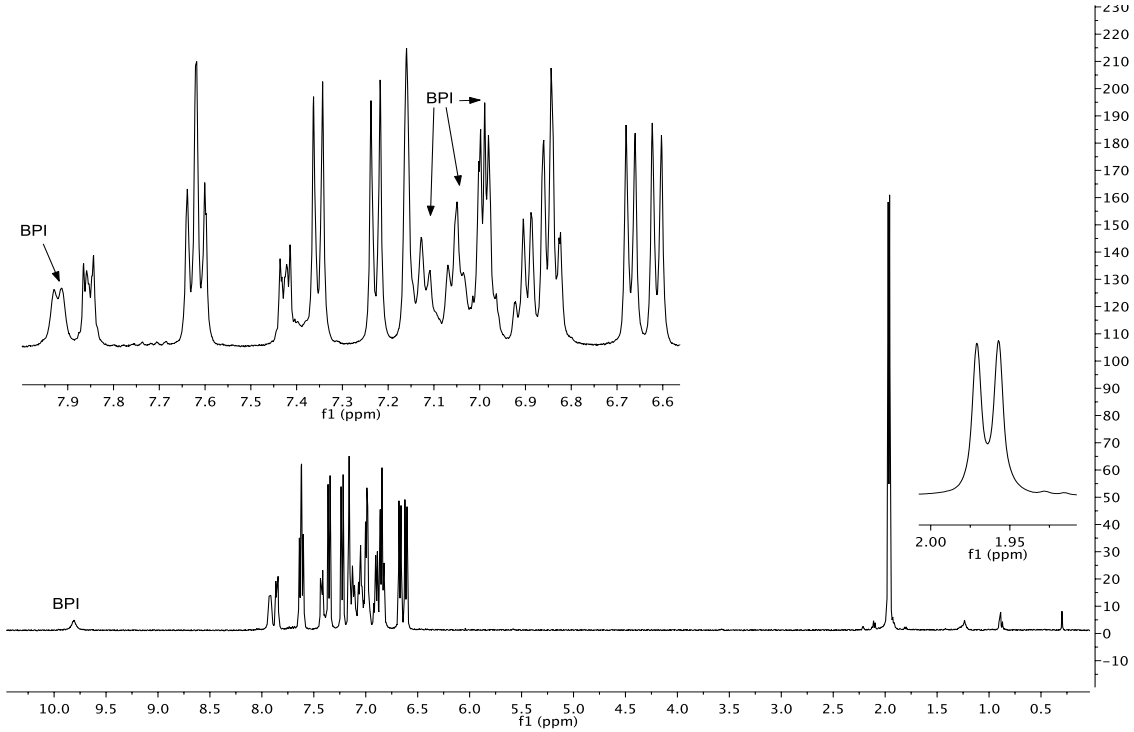


Figure S20. *In-situ* selective ^{1}H-{^{31}P} NMR (C_6D_6) of [($^{p\text{-tol}}$**L1**)Ni(PPh$_3$)] ($^{p\text{-tol}}$**7-PPh$_3$**) from the reaction of $^{p\text{-tol}}$**1** + equivalent of PPh$_3$. The sample contains a mixture of $^{p\text{-tol}}$**7-PPh$_3$** and BPI.

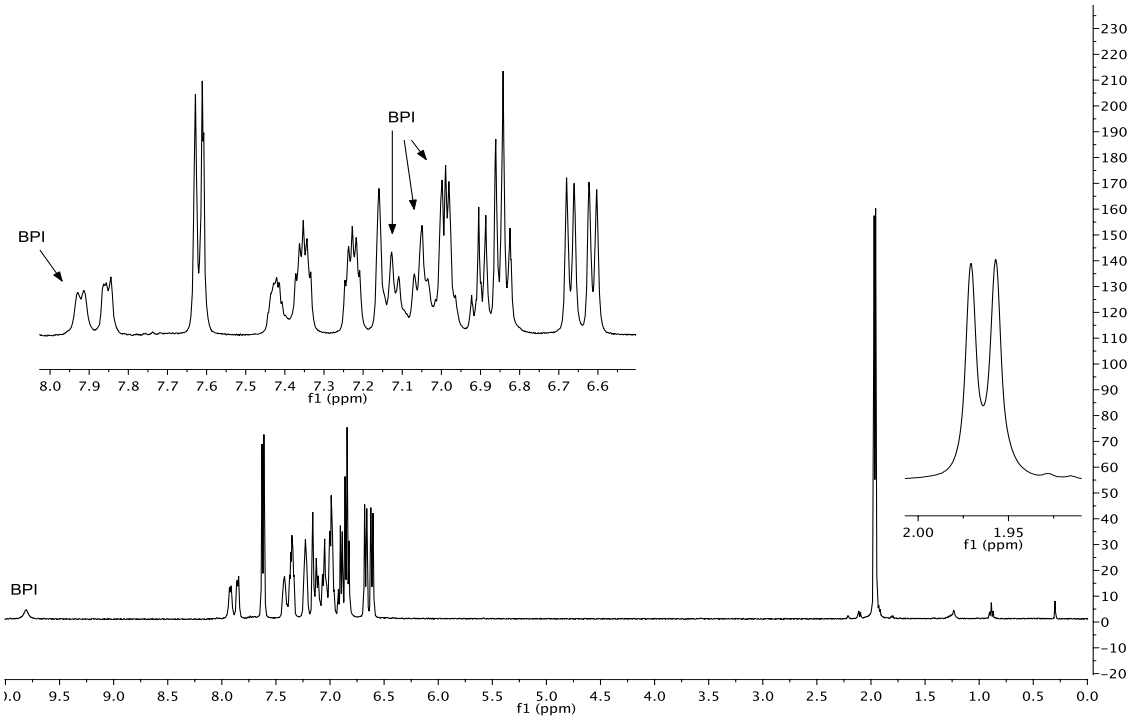


Figure S21. *In-situ* selective ^{1}H $\{^{31}P\}$ NMR (C_6D_6) of [(**$^{p\text{-tol}}$L1**)Ni(PPh_3)] (**$^{p\text{-tol}}$7-PPh$_3$**) from the reaction of **$^{p\text{-tol}}$1** + equivalent of PPh_3. The sample contains a mixture of **$^{p\text{-tol}}$7-PPh$_3$** and BPI. The ^{31}P-decoupling NMR is performed with the phosphorus atoms appearing at 38.5 The ^{31}P-decoupling NMR is performed with the phosphorus atoms appearing at 17.1 ppm as a doublet in ^{31}P NMR. ppm as a doublet in ^{31}P NMR.

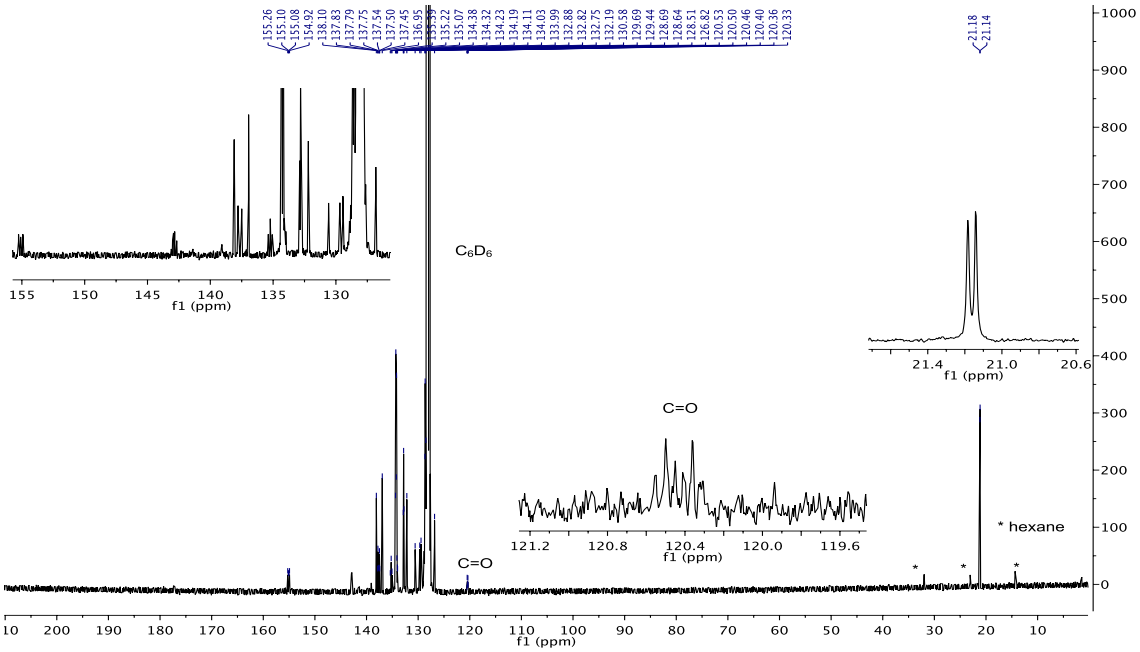


Figure S22. *In-situ* ^{13}C NMR (C_6D_6) of [(**$^{p\text{-tol}}$L1**)Ni(PPh_3)] (**$^{p\text{-tol}}$7-PPh$_3$**) from the reaction of **$^{p\text{-tol}}$1** + equivalent of PPh_3. The sample contains a mixture of **$^{p\text{-tol}}$7-PPh$_3$** and BPI.

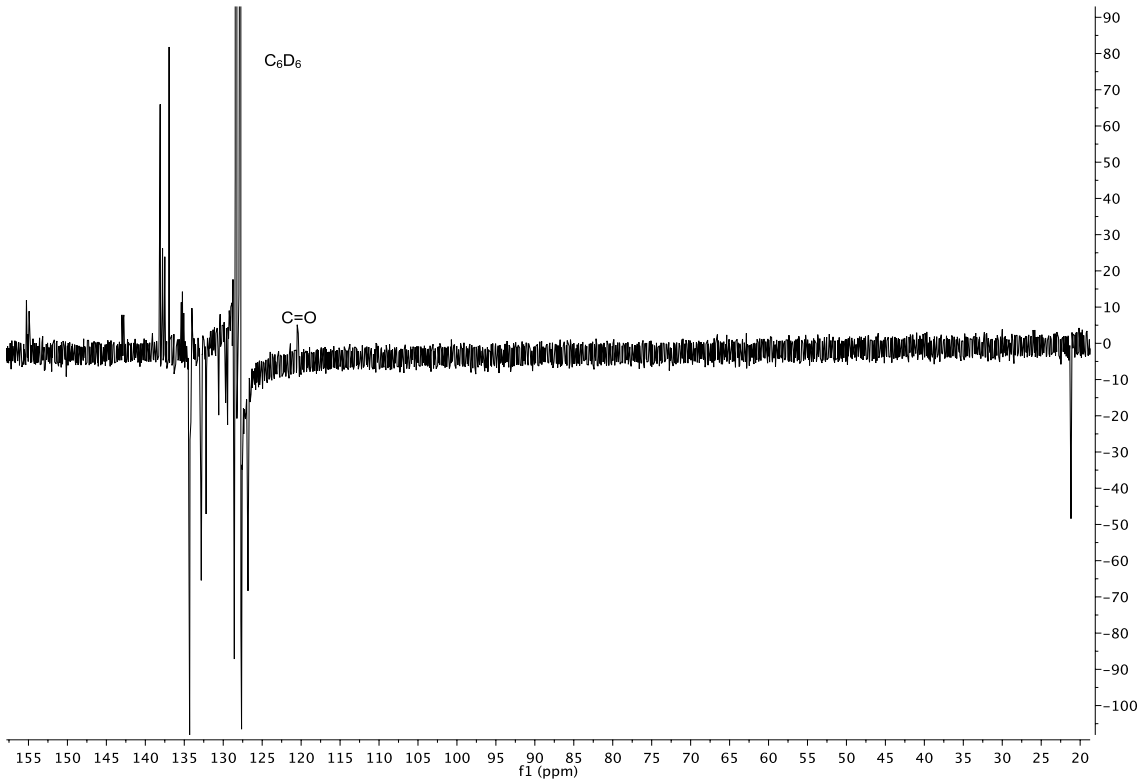


Figure S23. *In-situ* APT ^{13}C NMR (C_6D_6) of [(**$^{p\text{-tol}}$L1**)Ni(PPh_3)] (**$^{p\text{-tol}}$7-PPh$_3$**) from the reaction of **$^{p\text{-tol}}$1** + equivalent of PPh_3. The sample contains a mixture of **$^{p\text{-tol}}$7-PPh$_3$** and BPI.

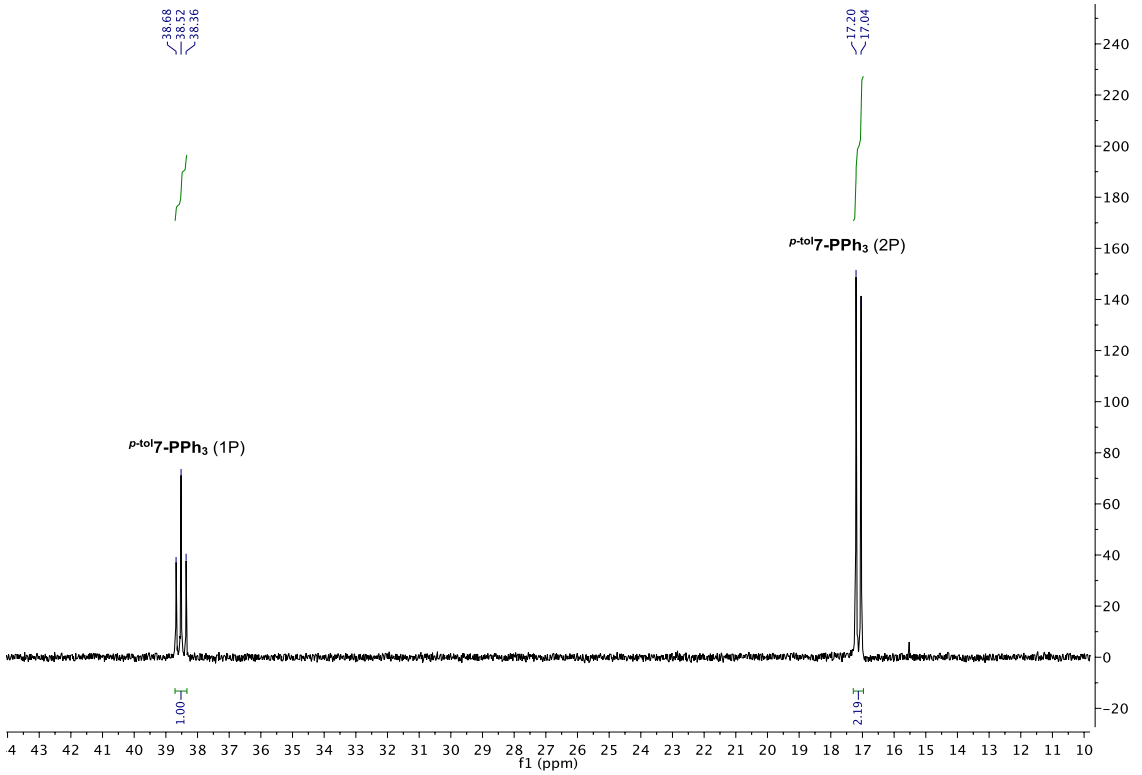
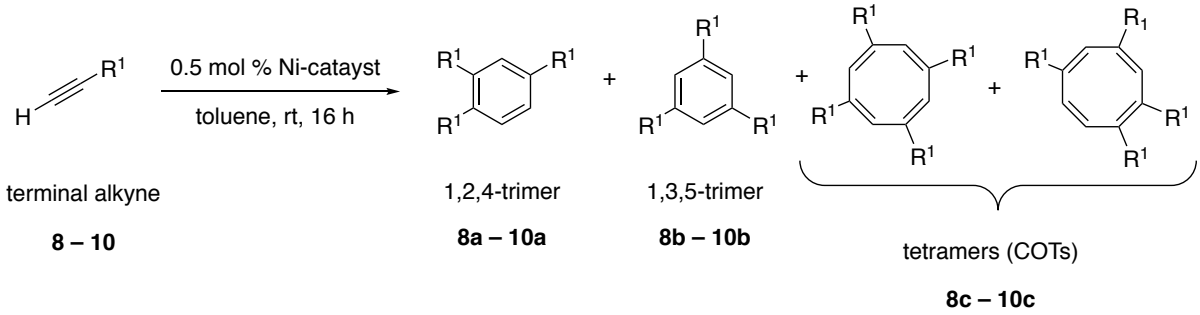


Figure S24. *In-situ* ^{31}P NMR (C_6D_6) of [(**$^{p\text{-tol}}$L1**)Ni(PPh_3)] (**$^{p\text{-tol}}$7-PPh$_3$**) from the reaction of **$^{p\text{-tol}}$1** + equivalent of PPh_3. The sample contains a mixture of **$^{p\text{-tol}}$7-PPh$_3$** and BPI

2. Catalytic comparison data



Scheme S2. Ni-catalyzed (*p*-tol**1** – Ph**L4**) oligomerization of terminal alkynes. COTs = cyclooctatetraenes.

Yields

Table S2. Catalyst (*p*-tol**1** – Ph**L4**) comparison data for the cyclotrimerization of phenyl acetylene (**8**), methyl propiolate (**9**), and methyl propargyl ether (**10**). Cyclotrimerization (and cyclotetramerization) products were isolated and the ratio between the different isomers was calculated by ^{1}H NMR. Average values are reported in Table 3. [a]For *p*-tol**2**, Ph**3**, and Ph**L4**, only trace amounts of catalytic products **10a** and **10b** were detected in which an accurate determination of the ratio between the two regio-isomers was not possible.

Substrate ***(-R¹)***	**Catalyst**	**Yield 1,2,4- (a) [%]**			**Yield 1,3,5- (b) [%]**			**Yield COTs (c) [%]**		
		Run 1	**Run 2**	**Avg.**	**Run 1**	**Run 2**	**Avg.**	**Run 1**	**Run 2**	**Avg.**
Phenyl acetylene **8** *(-Ph)*	*p*-tol**1**	87.3	86.4	**86.9**	2.7	3.6	**3.2**	0	0	**0**
	p-tol**2**	3.1	3.1	**3.1**	1.9	1.9	**1.9**	0	0	**0**
	Ph**3**	3.7	1.9	**2.8**	0.3	0.1	**0.2**	0	0	**0**
	Ph**L4** + $Ni(cod)_2$	5.2	4.0	**4.6**	1.8	2.0	**1.9**	0	0	**0**
Methyl propiolate **9** *(-CO_2Me)*	*p*-tol**1**	89.3	91.1	**90.2**	5.7	6.9	**6.3**	4	< 1	**2.5**
	p-tol**2**	26.7	22.3	**24.5**	2.3	1.7	**2.0**	10	5	**7.5**
	Ph**3**	68.8	61.1	**65.0**	11.2	13.4	**12.3**	7	6	**6.5**
	Ph**L4** + $Ni(cod)_2$	13.6	14.3	**14.0**	3.4	2.7	**3.0**	29	33	**31**
Methyl propargyl ether **10** *(-CH_2OMe)*[a]	*p*-tol**1**	69.3	73.8	**71.6**	5.7	8.2	**6.9**	0	0	**0**
	p-tol**2**	< 1	< 1	**< 1**	< 1	< 1	**< 1**	0	0	**0**
	Ph**3**	< 1	< 1	**< 1**	< 1	< 1	**< 1**	0	0	**0**
	Ph**L4** + $Ni(cod)_2$	< 1	< 1	**< 1**	< 1	< 1	**< 1**	0	0	**0**

Regioselectivity and chemoselectivity

Table S3. Catalyst ($^{p\text{-tol}}$**1** – ^{Ph}**L4**) comparison data for the cyclotrimerization of phenyl acetylene (**8**), methyl propiolate (**9**), and methyl propargyl ether (**10**). Cyclotrimerization (and cyclotetramerization) products were isolated and the ratio between the different isomers was calculated by ^{1}H NMR. Average values are reported in Table 3. [a]For $^{p\text{-tol}}$**2**, ^{Ph}**3**, and ^{Ph}**L4**, only trace amounts of catalytic products **10a** and **10b** were detected in which an accurate determination of the ratio between the two regio-isomers was not possible.

Substrate *(-R¹)*	**Catalyst**	**1,2,4- (a):1,3,5- (b) ratio**			**Trimers:Tetramers ratio**		
		Run 1	**Run 2**	**Avg.**	**Run 1**	**Run 2**	**Avg.**
Phenyl acetylene **8** *(-Ph)*	$^{p\text{-tol}}$**1**	97:3	96:4	**97:3**	100:0	100:0	**100:0**
	$^{p\text{-tol}}$**2**	62:38	62:38	**62:38**	100:0	100:0	**100:0**
	^{Ph}**3**	93:7	94:6	**94:6**	100:0	100:0	**100:0**
	^{Ph}**L4** + $Ni(cod)_2$	76:24	66:34	**70:30**	100:0	100:0	**100:0**
Methyl propiolate **9** *(-CO_2Me)*	$^{p\text{-tol}}$**1**	94:6	93:7	**93:7**	97:3	< 99:1	**98:2**
	$^{p\text{-tol}}$**2**	92:8	93:7	**92:8**	75:25	83:17	**78:22**
	^{Ph}**3**	86:14	82:18	**84:16**	92:8	92:8	**92:8**
	^{Ph}**L4** + $Ni(cod)_2$	80:20	84:16	**82:18**	37:63	33:67	**35:65**
Methyl propargyl ether **10** *(-CH_2OMe)[a]*	$^{p\text{-tol}}$**1**	90:10	90:10	**90:10**	100:0	100:0	**100:0**
	$^{p\text{-tol}}$**2**	n/a	n/a	**n/a**	100:0	100:0	**100:0**
	^{Ph}**3**	n/a	n/a	**n/a**	100:0	100:0	**100:0**
	^{Ph}**L4** + $Ni(cod)_2$	n/a	n/a	**n/a**	100:0	100:0	**100:0**

Comparison of the catalytic methods

Table S4. Catalytic method (*A Vs B*) comparison. **Method *A*.** 0.5 mol% of nickel-benzophenone imine complex ($^{p\text{-tol}}$**1** – ^{Ph}**3**) is mixed with the corresponding terminal alkyne. **Method *B*.** The active catalyst is generated *in-situ* using 0.5 mol% of the ligand ($^{p\text{-tol}}$**L1** – ^{Ph}**L3**) + 0.5 mol% of $Ni(cod)_2$ + the corresponding terminal alkyne. Cyclotrimerization (and cyclotetramerization) products were isolated and the ratio between the different isomers was calculated by ^{1}H NMR. Values from method *A* are taken from Table S2.

Substrate ***(-R¹)***	**Catalyst**	**Yield 1,2,4- (a) [%]**		**Yield 1,2,4- (b) [%]**		**Yield COTs (c) [%]**	
		Method		**Method**		**Method**	
		A	***B***	***A***	***B***	***A***	***B***
Phenyl acetylene **8** *(-Ph)*	$^{p\text{-tol}}$**1**	86.9	85.4	3.2	3.6	0	0
	$^{p\text{-tol}}$**2**	3.1	3.1	1.9	1.9	0	0
	^{Ph}**3**	2.8	4.6	0.2	0.4	0	0
Methyl propiolate **9** *(-CO_2Me)*	$^{p\text{-tol}}$**1**	90.2	90.1	6.3	5.9	2.5	3
	$^{p\text{-tol}}$**2**	24.5	26.9	2.0	2.3	7.5	10
	^{Ph}**3**	65.0	64.4	12.3	11.0	6.5	7

General conditions and characterizations

Cyclotrimerization of phenyl acetylene (8) (Table 3; Entry 1). **Conditions:** room temperature; 16 hours. Triphenylbenzene was obtained as a mixture of 1,2,4- (**8a**) and 1,3,5-regioisomers (**8b**). The ratio between the two isomers was determined by integration ^{1}H NMR. **1,2,4-Triphenylbenzene (8a). ^{1}H NMR** (400 MHz, C_6D_6, 25 °C): δ_H 7.69 (Ar*H*, d, $^4J_{H,H}$ = 1.9 Hz, 1H); 7.5 (Ar*H*, td, $^3J_{H,H}$ = 7.8 Hz, $^4J_{H,H}$ = 1.3 Hz, 3H); 7.40 (Ar*H*, d, $^3J_{H,H}$ = 7.9 Hz, 1H); 7.27 – 7.18 (Ar*H*, m, 7H); 7.08 – 6.96 (Ar*H*, m, 6H). **LRMS (EI+):** m/z: calcd for $[M]^+$ 306; Found 306. NMR characterization values correspond to literature.[S1]

Cyclotrimerization of methyl propiolate (9) (Table 3; Entry 2). **Conditions:** room temperature; 16 hours. Trimethyl benzene-tricarboxylate obtained as a mixture of 1,2,4- (**9a**) to 1,3,5-regioisomers (**9b**) in addition to a minor amount of tetramethyl-cyclooctatetraene-tetracarboxylate (**9c**) (two isomers detected). For the catalysis with the *rac*-BINAP system (^{Ph}**L4**), the substituted cyclooctatetraene (**9c**) is obtained in majority. The ratio between the two isomers was determined by ^{1}H NMR. **Trimethyl benzene-1,2,4-tricarboxylate (9a). ^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): δ_H 8.42 (Ar*H*, d, $^4J_{H,H}$ = 2.0 Hz, 1H); 8,19 (Ar*H*, dd, $^3J_{HH}$ = 8.0 Hz, $^4J_{H,H}$ = 2.0 Hz, 1H); 7.75 (Ar*H*, d, $^3J_{H,H}$ = 8.0 Hz, 1H); 3.96 (CH_3, 3H); 3.93 (CH_3, 6H). **LRMS (EI+):** m/z: calcd for $[M]^+$ 252; Found 252. NMR characterization values correspond to literature.[S2]

Cyclotrimerization of methyl propargyl ether (10) (Table 3; Entry 3). **Conditions:** room temperature; 16 hours. Isolated by column chromatography (SiO_2; 100 % EtOAc). Tris(methoxymethyl)benzene was obtained as a mixture of 1,2,4- (**10a**) to 1,3,5-regioisomers (**10b**). The ratio between the two isomers was determined by ^{1}H NMR. **1,2,4-Tris(methoxymethyl)benzene (10a). ^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C): 7.51 (Ar*H*, s, 1H), 7.39 (Ar*H*, d, $^3J_{H,H}$ = 7.7 Hz, 1H), 7.23 (Ar*H*, d, $^3J_{H,H}$ = 7.7 Hz, 1H), 4.42 (C*H*$_2$, s, 2H), 4.40 (C*H*$_2$, s, 2H), 4.27 (C*H*$_2$, s, 2H), 3.15 (C*H*$_3$, s, 3H), 3.14 (C*H*$_3$, s, 6H); **LRMS (EI+):** m/z: calcd for $[M]^+$ 210; Found 210. NMR characterization values correspond to literature.[S1]

NMR data of catalytic products

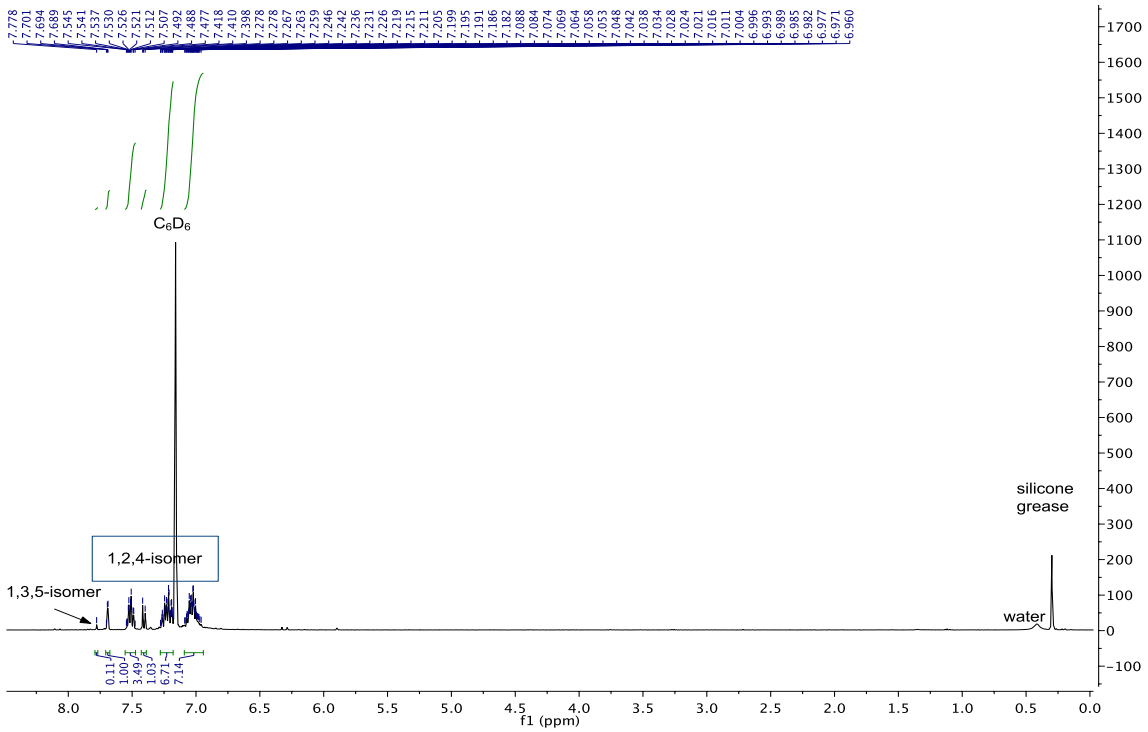


Figure S25. ^{1}H NMR (C_6D_6) from the cyclotrimerization of phenylacetylene catalyzed by [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**) yielding to a mixture of 1,2,4- (major product) and 1,3,5-triphenylbenzene. Spectrum from run 1.

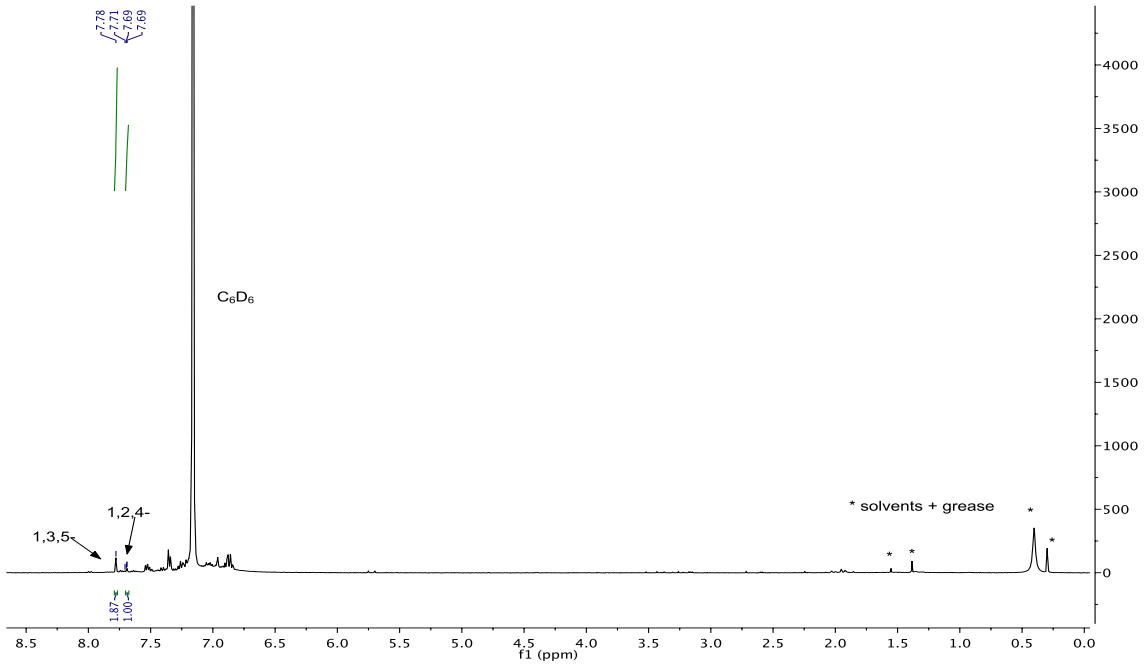


Figure S26. ^{1}H NMR (C_6D_6) from the cyclotrimerization of phenylacetylene catalyzed by [(*p*-tol**L2**)Ni(BPI)] (*p*-tol**2**) yielding to a mixture of 1,2,4- (major product) and 1,3,5-triphenylbenzene. Spectrum from run 1.

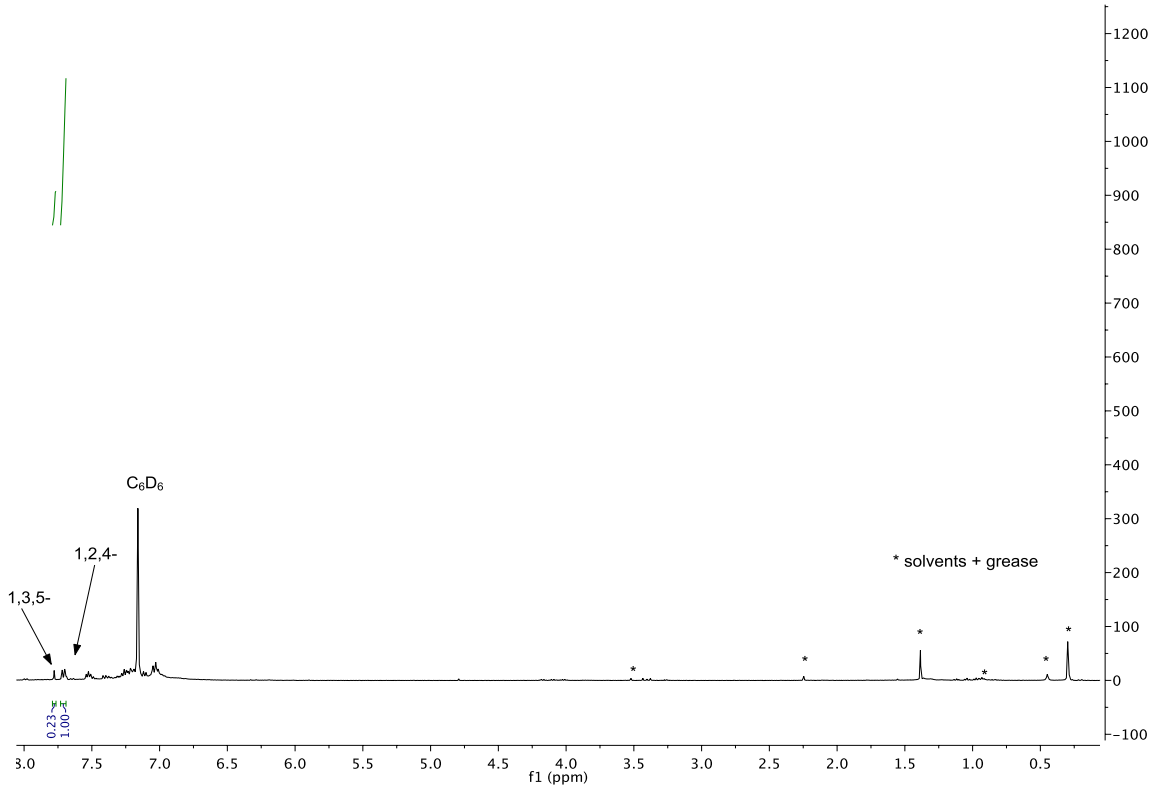


Figure S27. ^{1}H NMR (C_6D_6) from the cyclotrimerization of phenylacetylene catalyzed by [(**^{Ph}L3**)Ni(BPI)] (**^{Ph}3**) yielding to a mixture of 1,2,4- (major product) and 1,3,5-triphenylbenzene. Spectrum from run 1.

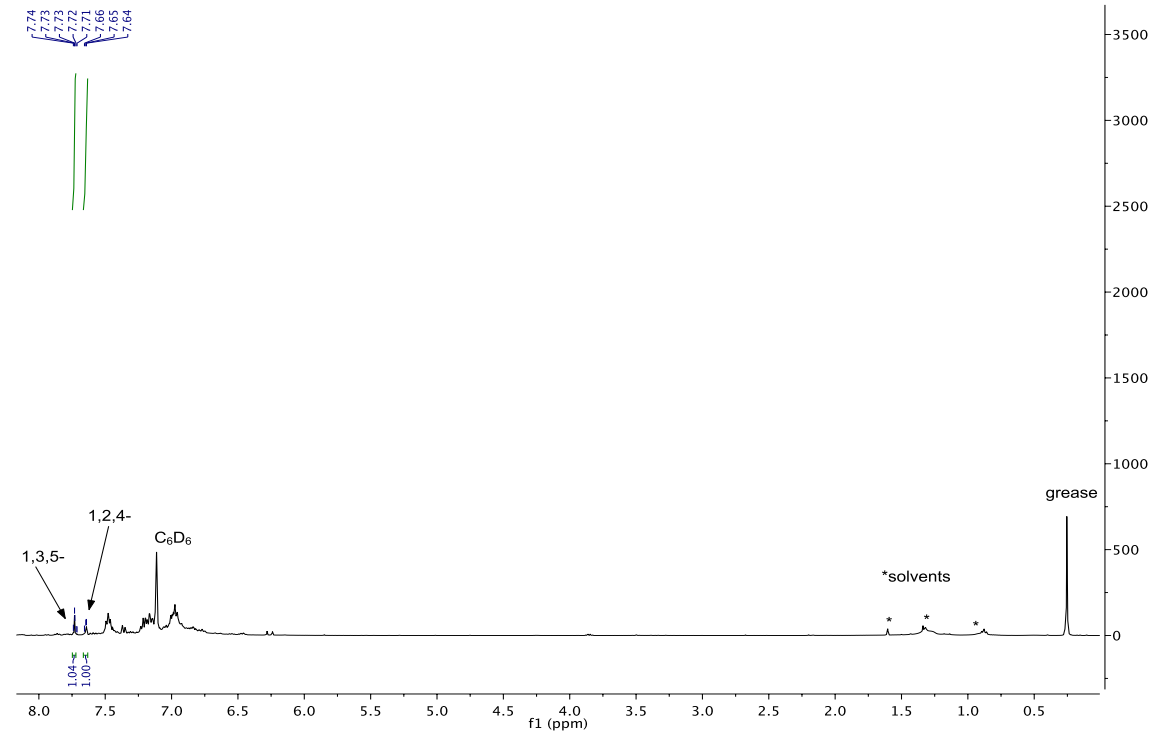


Figure S28. ^{1}H NMR (C_6D_6) from the cyclotrimerization of phenylacetylene catalyzed by **^{Ph}L4** system (**^{Ph}L4**) yielding to a mixture of 1,2,4- (major product) and 1,3,5-triphenylbenzene. Spectrum from run 1.

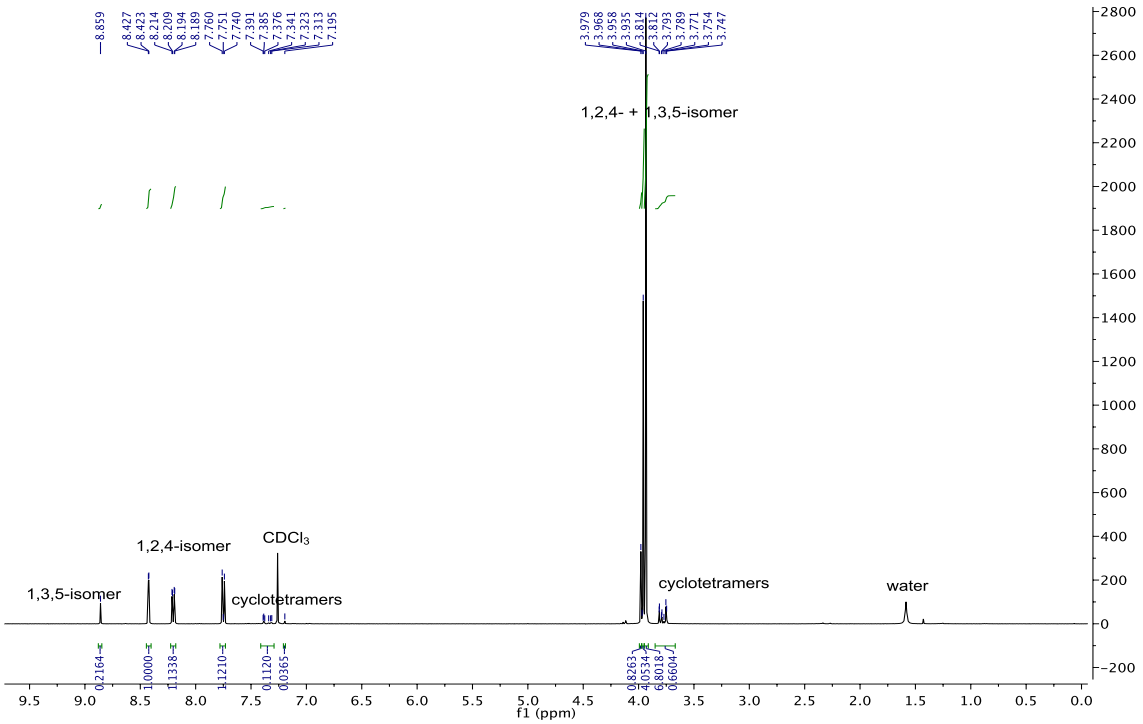


Figure S29. ^{1}H NMR ($CDCl_3$) from the oligomerization of methyl propiolate catalyzed by [($^{p\text{-}tol}$**L1**)Ni(BPI)] ($^{p\text{-}tol}$**1**) yielding to a mixture of trimethyl benzene-1,2,4- (major product) and 1,3,5-tricarboxylate. Cyclotetramerization products are also present in a minor amount. Spectrum from run 1.

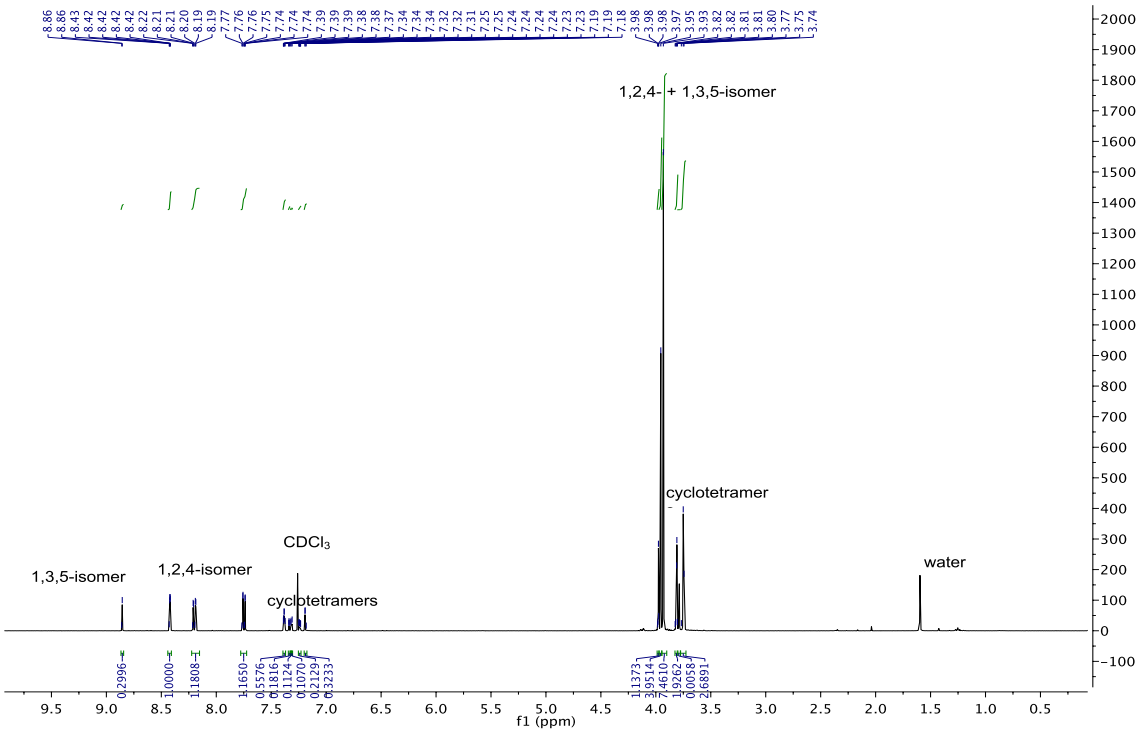


Figure S30. H NMR (C_6D_6) from the oligomerization of methyl propiolate catalyzed by [($^{p\text{-}tol}$**L2**)Ni(BPI)] ($^{p\text{-}tol}$**2**) yielding to a mixture of trimethyl benzene-1,2,4- (major product) and 1,3,5-tricarboxylate. Cyclotetramerization products are also present in a minor amount. Spectrum from run 1.

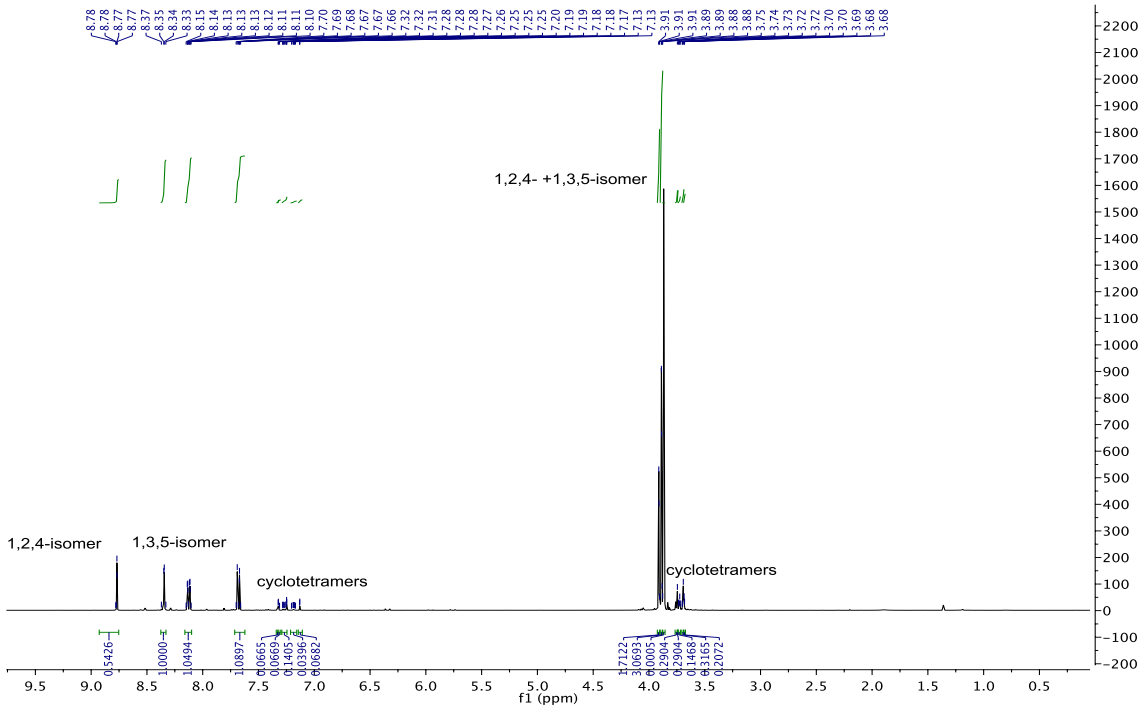


Figure S31. ^{1}H NMR ($CDCl_3$) from the oligomerization of methyl propiolate catalyzed by [(^{Ph}**L3**)Ni(BPI)] (^{Ph}**3**) yielding to a mixture of trimethyl benzene-1,2,4- (major product) and 1,3,5-tricarboxylate. Cyclotetramerization products are also present in a minor amount. Spectrum from run 1.

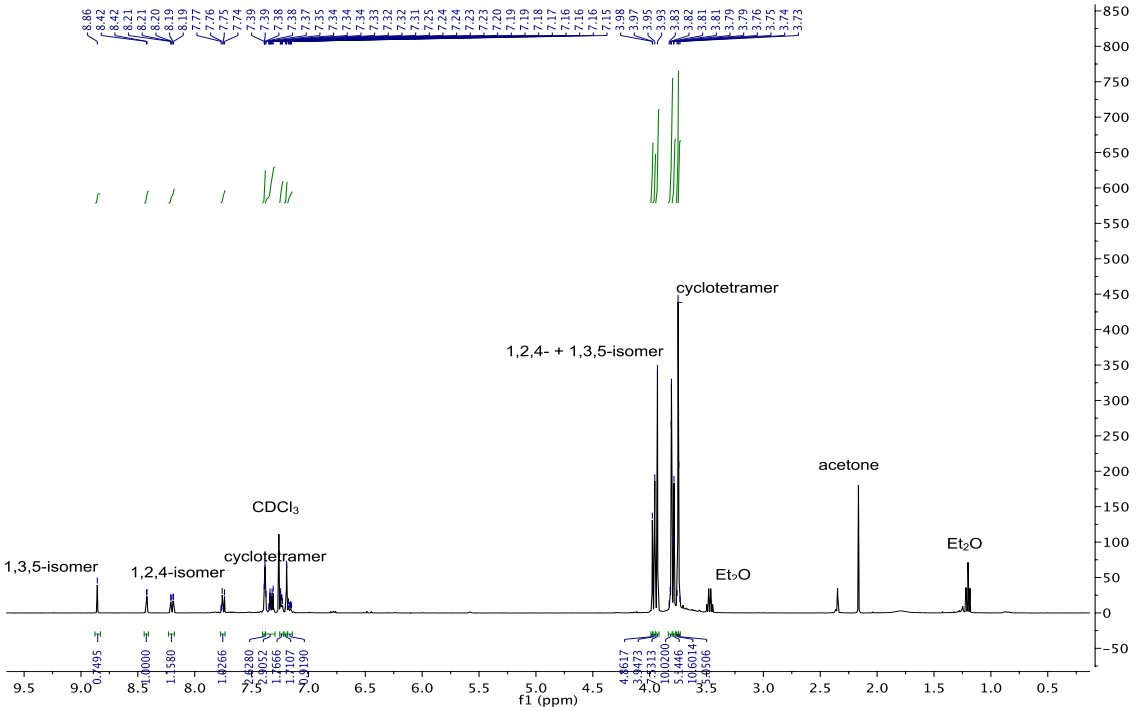


Figure S32. ^{1}H NMR ($CDCl_3$) from the oligomerization of methyl propiolate catalyzed by *rac*-BINAP-system (^{Ph}**L4**) yielding to a mixture of trimethyl benzene-1,2,4- and 1,3,5-tricarboxylate in addition to 1,2,4,6- (major product) and 1,3,5,7- substituted octatetraene. Cyclotetramerization products are the major species formed compared to the cyclotrimerization products. Spectrum from run 1.

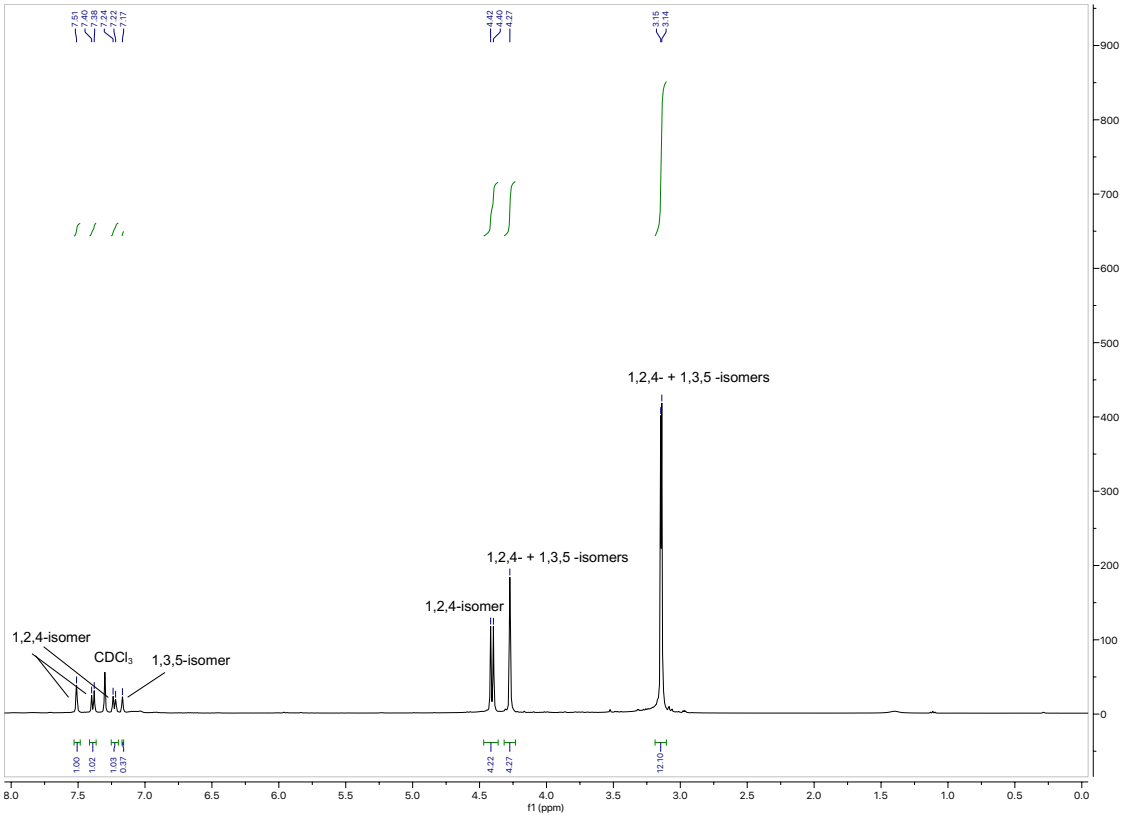
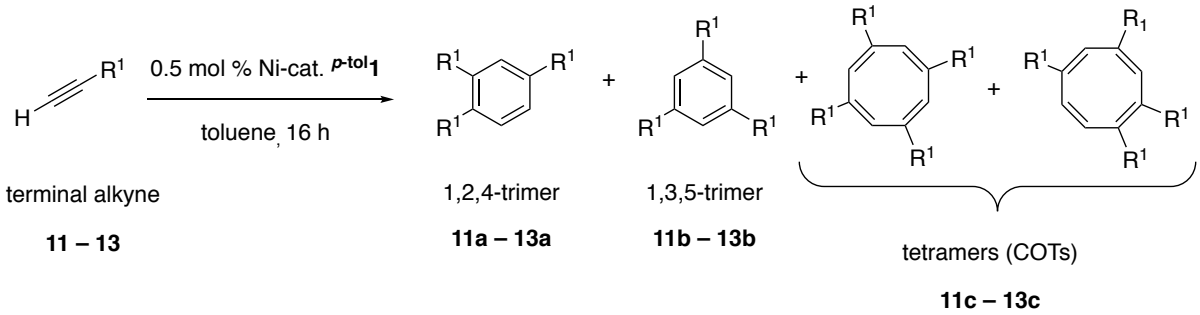


Figure S33. ^{1}H NMR ($CDCl_3$) from the cyclotrimerization of methyl propargyl ether catalyzed by [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**) yielding to a mixture of 1,2,4- (major product) and 1,3,5-tris(methoxymethyl)benzene. Spectrum from run 1.

3. Alkyne cyclotrimerization catalyzed by $^{p\text{-tol}}$1 (additional substrates)



Scheme S3. $^{p\text{-tol}}$**1**-catalyzed alkyne cyclotrimerization. COTs = cyclooctatetraenes.

Yields

Table S5. $^{p\text{-tol}}$**1**-catalyzed cyclotrimerization of ethyl propiolate (**11**), 1-ethynyl-4-fluorobenzene (**12**), 4-ethynilanisole (**13**). The temperature of reaction time is room temperature for ethyl propiolate (**11**), 50 ˚C for ethynyl-4-fluorobenzene (**12**) and 4-ethynilanisole (**13**). Cyclotrimerization (and cyclotetramerization) products were isolated and the ratio between the different isomers was calculated by ^{1}H NMR. Average values are reported in Table 4.

Substrate *(-R¹)*	**Yield 1,2,4- (a) [%]**			**Yield 1,3,5- (b) [%]**			**Yield COT (c) [%]**		
	Run 1	**Run 2**	**Avg.**	**Run 1**	**Run 2**	**Avg.**	**Run 1**	**Run 2**	**Avg.**
11 *(-CO_2Et)*	90.2	89.3	**89.8**	6.8	6.7	**6.8**	2	3	**2.5**
12 *(-p-F-C_6H_4)*	92.2	94.0	**93.1**	4.8	5.0	**4.9**	0	0	**0**
13 *(-p-OMe-C_6H_4)*	66.5	63.6	**65.0**	3.5	3.4	**3.5**	0	0	**0**

Regioselectivity and chemoselectivity

Table S6. $^{p\text{-tol}}$**1**-catalyzed cyclotrimerization of ethyl propiolate (**11**), 1-ethynyl-4-fluorobenzene (**12**), 4-ethynilanisole (**13**). The temperature of reaction time is room temperature for ethyl propiolate (**11**), 50 ˚C for ethynyl-4-fluorobenzene (**12**) and, 4-ethynilanisole (**13**). Cyclotrimerization (and cyclotetramerization) products were isolated and the ratio between the different isomers was calculated by ^{1}H NMR. Average values are reported in Table 4.

Substrate *(-R^1)*	**1,2,4- (a):1,3,5- (b) ratio**			**Trimers:Tetramers ratio**		
	Run 1	**Run 2**	**Avg.**	**Run 1**	**Run 2**	**Avg.**
11 *(-CO_2Et)*	93:7	93:7	**93:7**	98:2	98:2	**98:2**
12 *(-p-F-C_6H_4)*	95:5	95:5	**95:5**	100:0	100:0	**100:0**
13 *(-p-OMe-C_6H_4)*	95:5	95:5	**95:5**	100:0	100:0	**100:0**

General conditions and characterizations

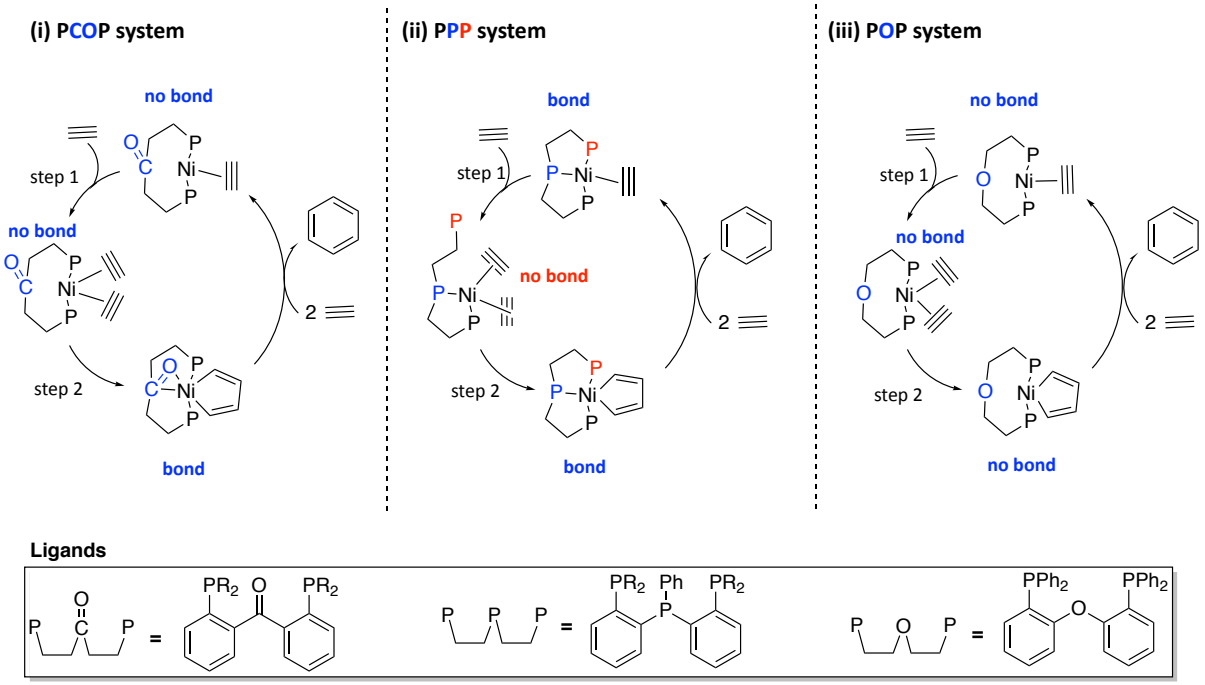
Cyclotrimerization of ethyl propiolate (11) (Table 4; Entry 1). **Conditions:** room temperature; 16 hours. triethyl benzene-tricarboxylate was obtained as a mixture of 1,2,4- (**11a**) to 1,3,5- (**11b**) regioisomers in addition to a minor amount of tetraethyl-cyclooctatetraene-tetracarboxylate (**11c**) (two isomers detected) in an average (2 runs) combined yield of 99.1%. **Triethyl benzene-1,2,4-tricarboxylate (11a). ^{1}H NMR** (400 MHz, C_6D_6, 25 °C): δ_H 8.62 (Ar*H*, d, $^4J_{H,H}$ = 2.0 Hz, 1H); 7.99 (Ar*H*, dd, $^3J_{H,H}$ = 8.0 Hz, $^4J_{H,H}$ = 2.0 Hz, 1H); 7.48 (Ar*H*, d, $^3J_{H,H}$ = 8.0 Hz, 1H); 4.17 (CH_2, q, $^3J_{H,H}$ = 7.2 Hz, 2H); 4.10 (CH_2, q, $^4J_{H,H}$ = 7.2 Hz, 2H); 4.02 (CH_2, q, $^4J_{H,H}$ = 7.2 Hz, 2H); 1.04 (CH_3, t, $^3J_{H,H}$ = 6.8 Hz, 3H); 0.98 (CH_3, t, $^3J_{H,H}$ = 6.8 Hz, 3H); 0.94 (CH_3, t, $^3J_{H,H}$ = 6.8 Hz, 3H). **LRMS (EI+):** m/z: calcd for $[M]^+$ 294; Found 294. NMR characterization values correspond to literature.[S2]

Cyclotrimerization of 1-ethynyl-4-fluorobenzene (12) (Table 4; Entry 2). **Conditions:** 50 ˚C; 16 hours. Tris(4-fluorophenyl)benzene was obtained as a 95:5 mixture of 1,2,4- (**12a**) to 1,3,5- (**12b**) regioisomers in an average (2 runs) combined yield of 98.0 %. **1,2,4-Tris(4-fluorophenyl)benzene (12a). ^{1}H NMR** (400 MHz, C_6D_6, 25 °C): δ_H 7.41 (Ar*H*, s, 1 H), 7.37–7.19 (Ar*H*, m, 4 H), 6.95–6.86 (Ar*H*, m, 6 H), 6.70 (Ar*H*, t, $^3J_{H,H}$ = 8.6 Hz, 4 H). **^{19}F NMR** (400 MHz, C_6D_6, 25 °C): δ_F –114.97 (Ar*F*, m, 1F); –115.25 (Ar*F*, m, 1F); –115.36 (Ar*F*, m, 1F); **LRMS (EI+):** m/z: calcd for $[M]^+$ 360; Found 360. NMR characterization values correspond to literature.[S1]

Cyclotrimerization of 4-ethynylanisole (13) (Table 4; Entry 3). **Conditions:** 50 ˚C; 16 hours. Tris(4-dimethylaminophenyl)benzene was obtained as a 95:5 mixture of 1,2,4- (**13a**) to 1,3,5- (**13b**) regioisomers in an average (2 runs) combined yield of 68.5 %. **1,2,4-Tris(4-dimethylaminophenyl)benzene (13a). ^{1}H NMR** (400 MHz, C_6D_6, 25 °C): δ 7.99 (Ar*H*, d,

$^{3}J_{H,H}$ = 1.9 Hz, 1H), 7.76–7.62 (Ar*H*, m, 4 H), 7.42–7.38 (Ar*H*, m, 4 H), 6.73–6.66 (Ar*H*, m, 2 H), 6.58–6.46 (Ar*H*, m, 4 H), 2.56 (NC*H*$_3$, s, 6 H), 2.47 (NC*H*$_3$, s, 6 H), 2.46 (NC*H*$_3$, s, 6 H). **LRMS (EI+):** m/z: calcd for $[M]^+$ 396; Found 396. NMR characterization values correspond to literature.[S1]

4. Proposed catalytic cycles



Scheme S4. Proposed simplified catalytic cycle for the cyclotrimerization of acetylene catalyzed by $^{p\text{-tol}}$**1** (i), $^{p\text{-tol}}$**2** (ii), and ^{Ph}**3** (iii). R = *para*-tolyl.

5. NMR of isolated ligand, complexes, and generated alkyne complexes

bis(2-di(*para* -tolyl)phosphinophenyl) phenylphosphine (*p*-tolL2)

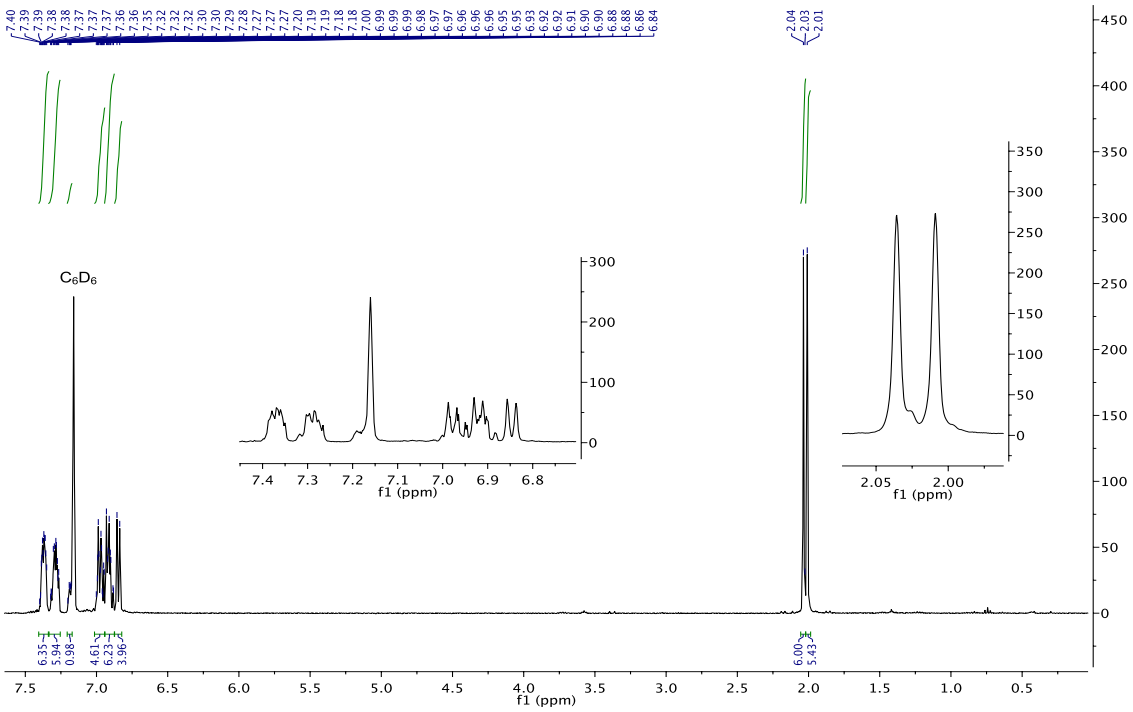


Figure S34. ^{1}H NMR (C_6D_6) of bis(2-di(*para* -tolyl)phosphinophenyl) phenylphosphine (*p*-tolL2).

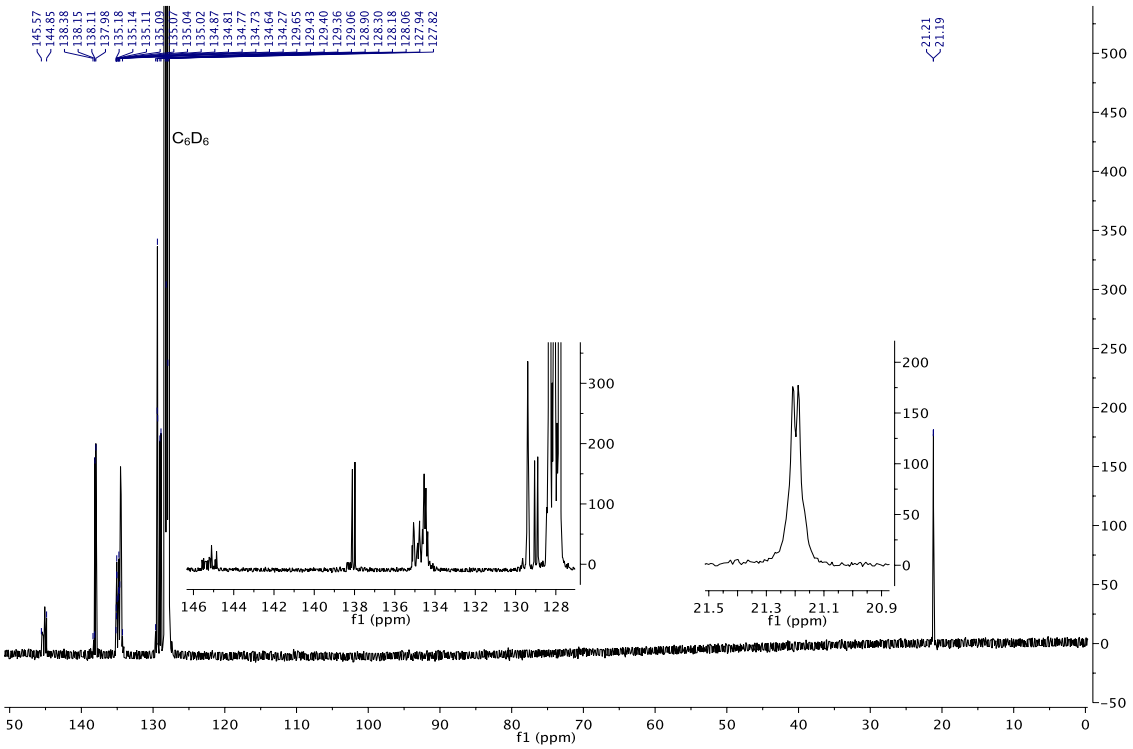


Figure S35. ^{13}C NMR (C_6D_6) of bis(2-di(*para* -tolyl)phosphinophenyl) phenylphosphine (*p*-tolL2).

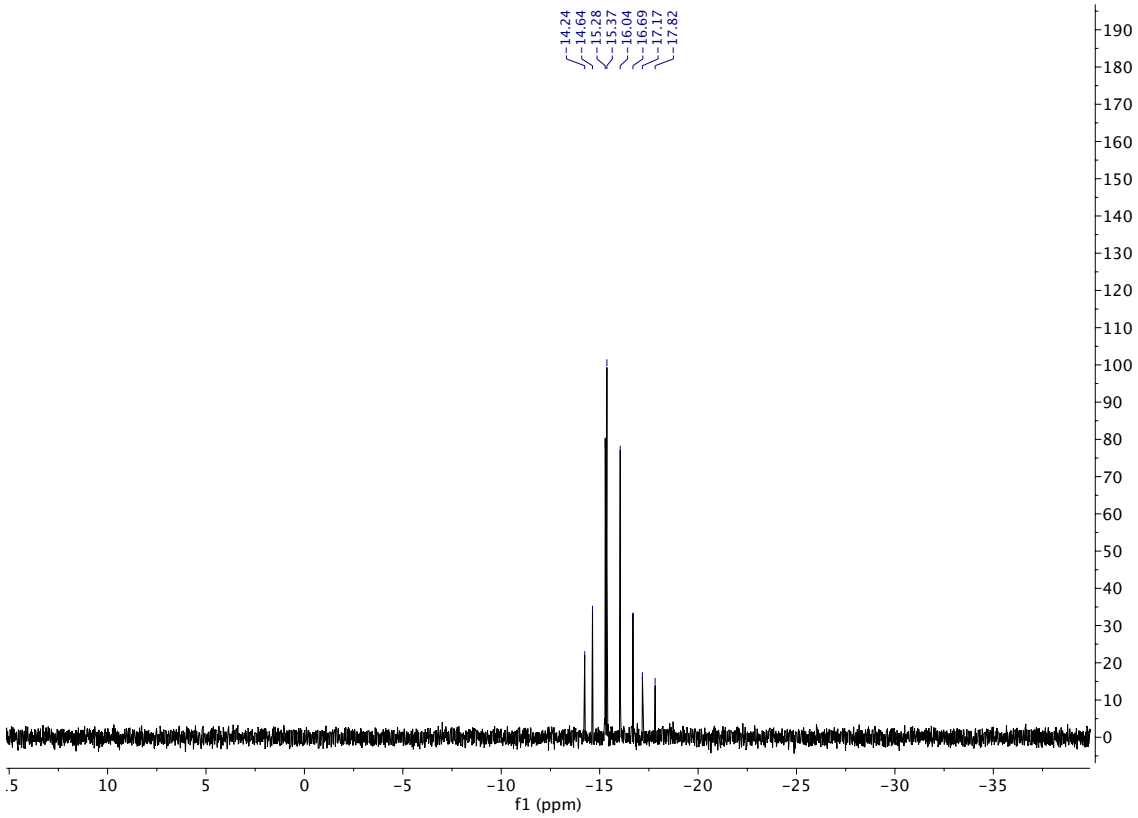


Figure S36. ^{31}P NMR (C_6D_6) of bis(2-di(*para*-tolyl)phosphinophenyl) phenylphosphine (**$^{p\text{-tol}}$L2**).

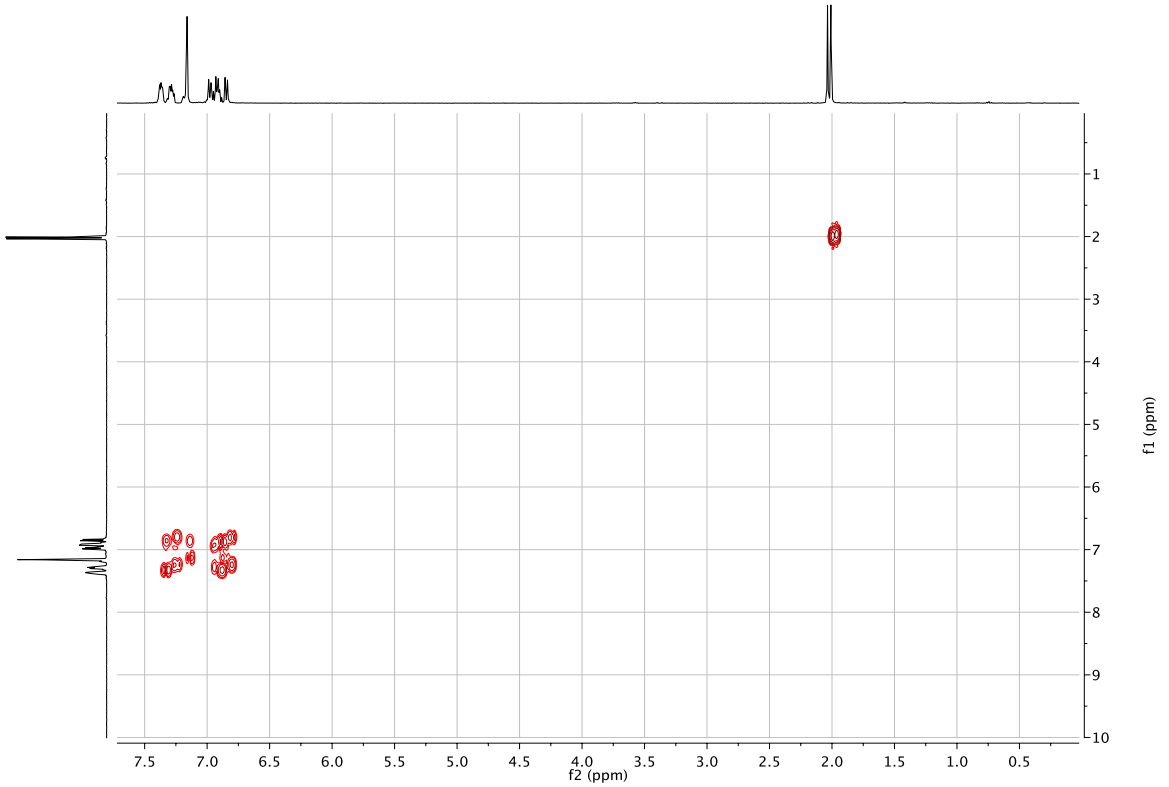


Figure S37. COSY (^{1}H-^{1}H) 2D NMR (C_6D_6) of bis(2-di(*para*-tolyl)phosphinophenyl) phenylphosphine (**$^{p\text{-tol}}$L2**).

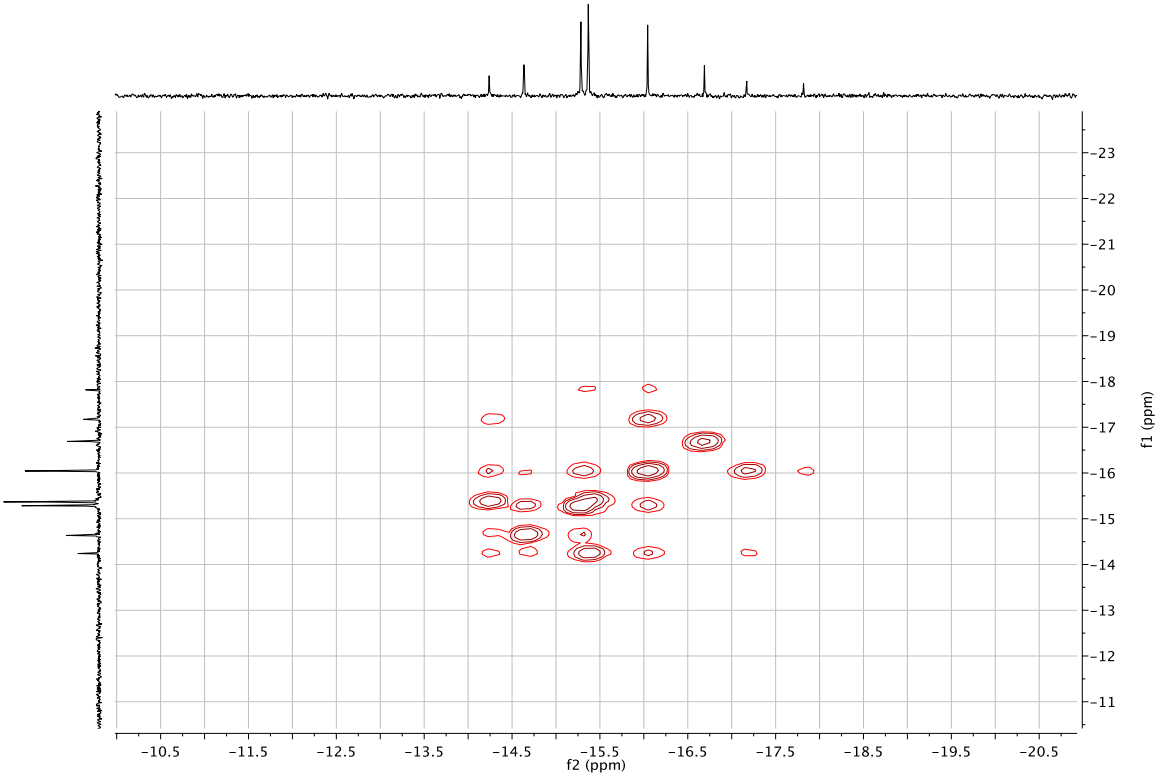


Figure S38. COSY (^{31}P-^{31}P) 2D NMR (C_6D_6) of bis(2-di(*para*-tolyl)phosphinophenyl) phenylphosphine ($^{p\text{-tol}}$**L2**).

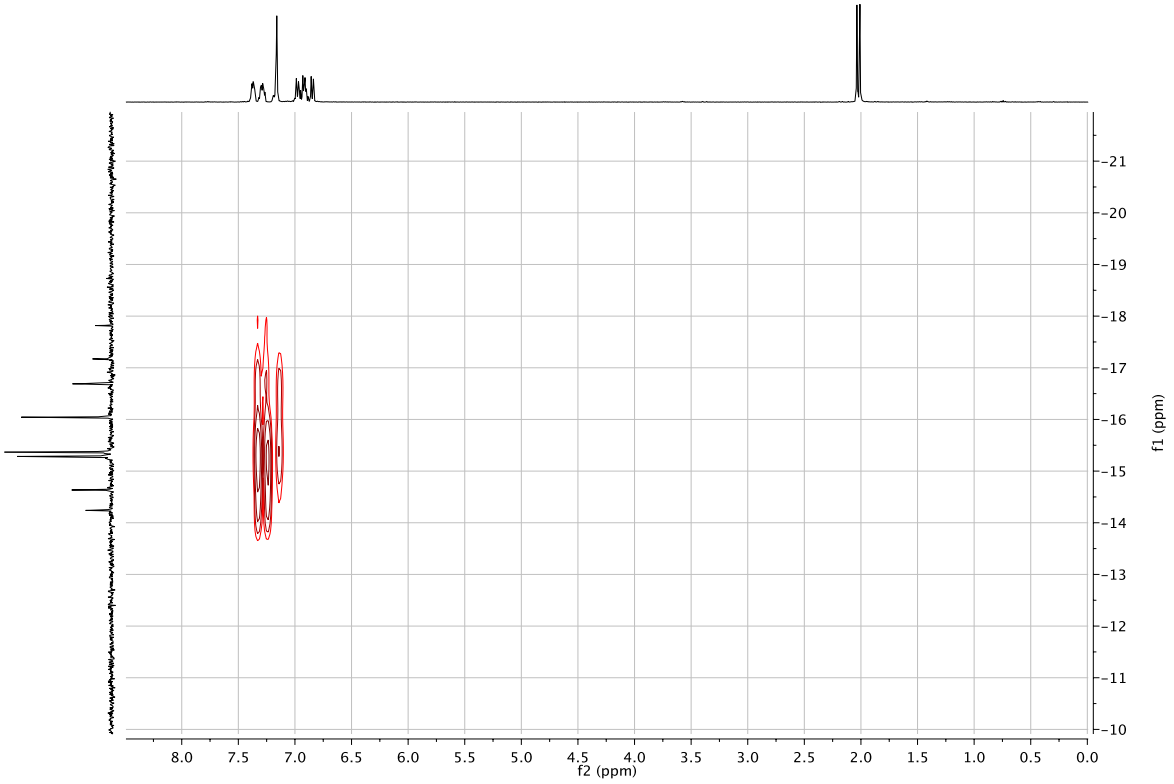


Figure S39. HMBC (^{1}H-^{31}P) 2D NMR (C_6D_6) of bis(2-di(*para*-tolyl)phosphinophenyl) phenylphosphine ($^{p\text{-tol}}$**L2**).

[(*p*-tolL1)Ni(BPI)] (*p*-tol1).

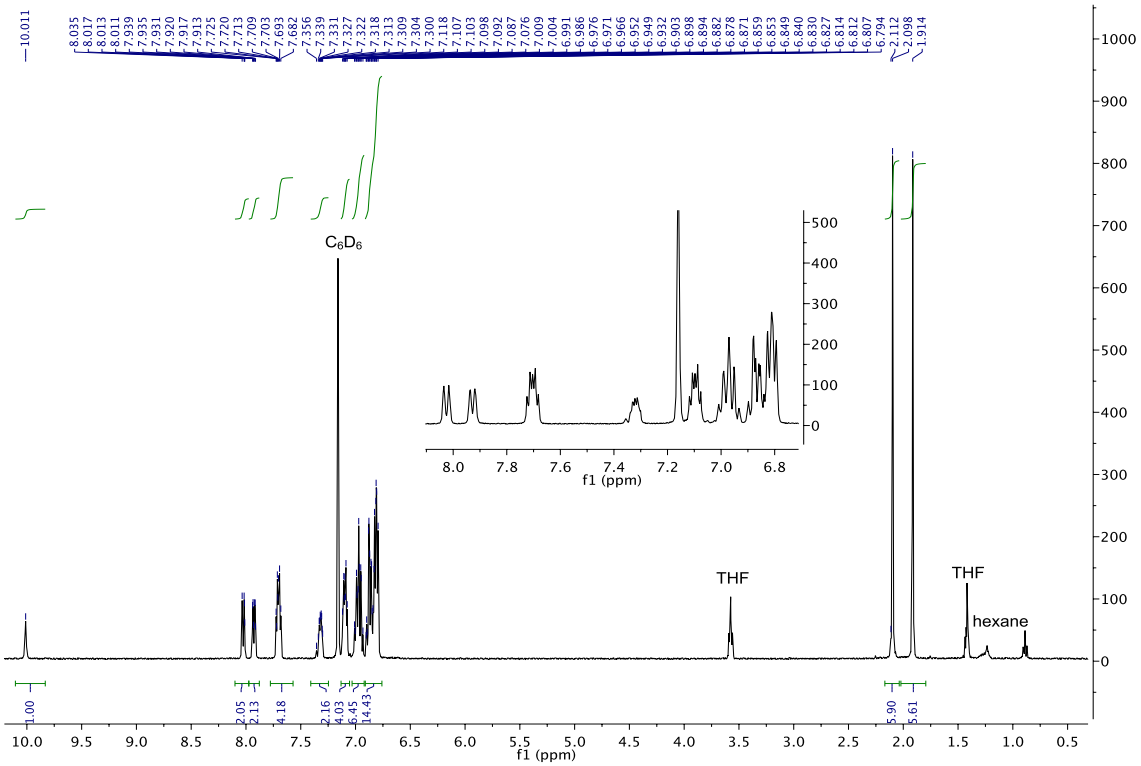


Figure S40. ^{1}H NMR (C_6D_6) of [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**). BPI = benzophenone imine.

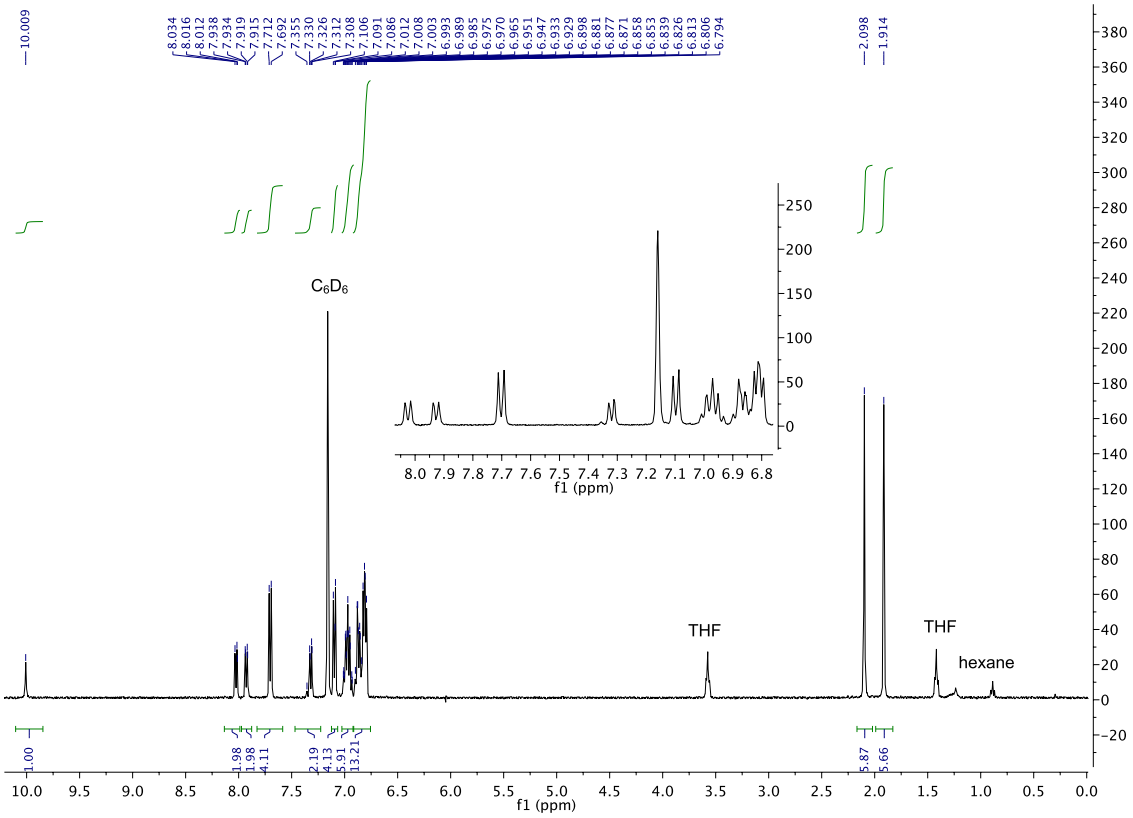


Figure S41. ^{1}H{^{31}P} NMR (C_6D_6) of [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**). BPI = benzophenone imine.

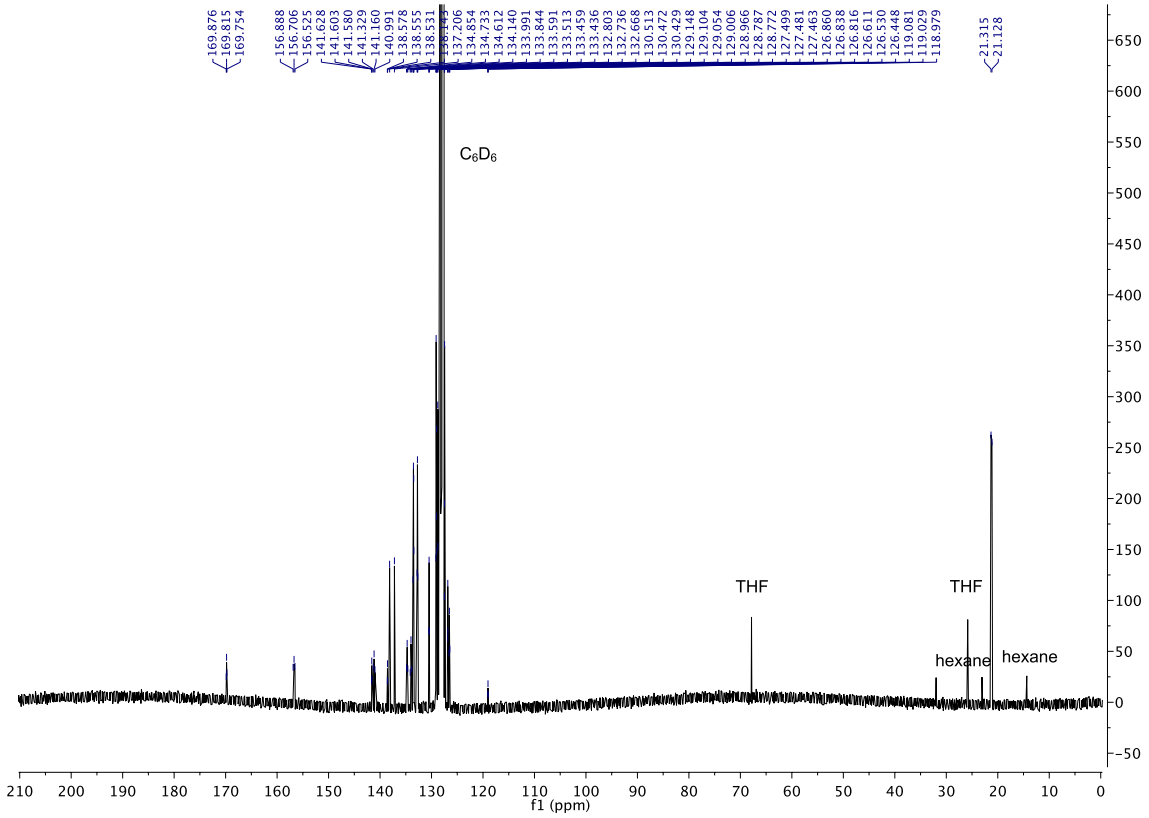


Figure S42. ^{13}C NMR (C_6D_6) of [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**). BPI = benzophenone imine.

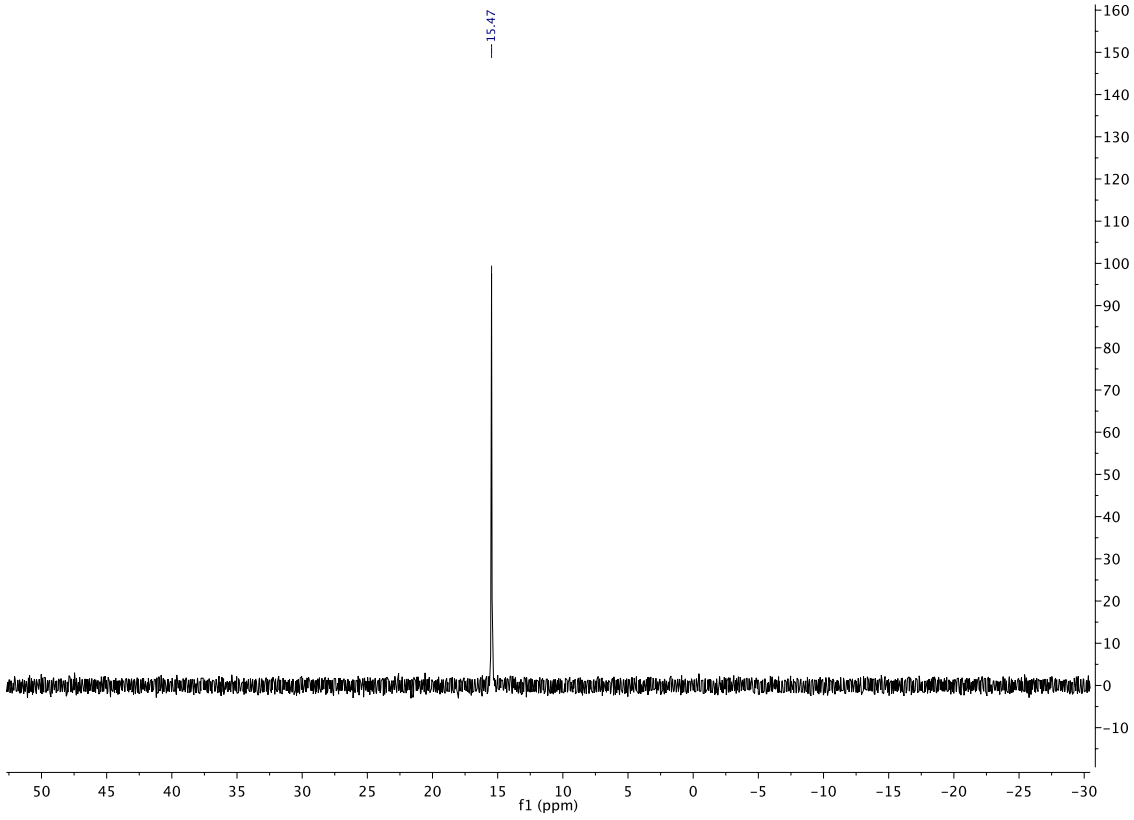


Figure S43. ^{31}P NMR (C_6D_6) of [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**). BPI = benzophenone imine.

[(^{Ph}L1)Ni(BPI)] (^{Ph}1)

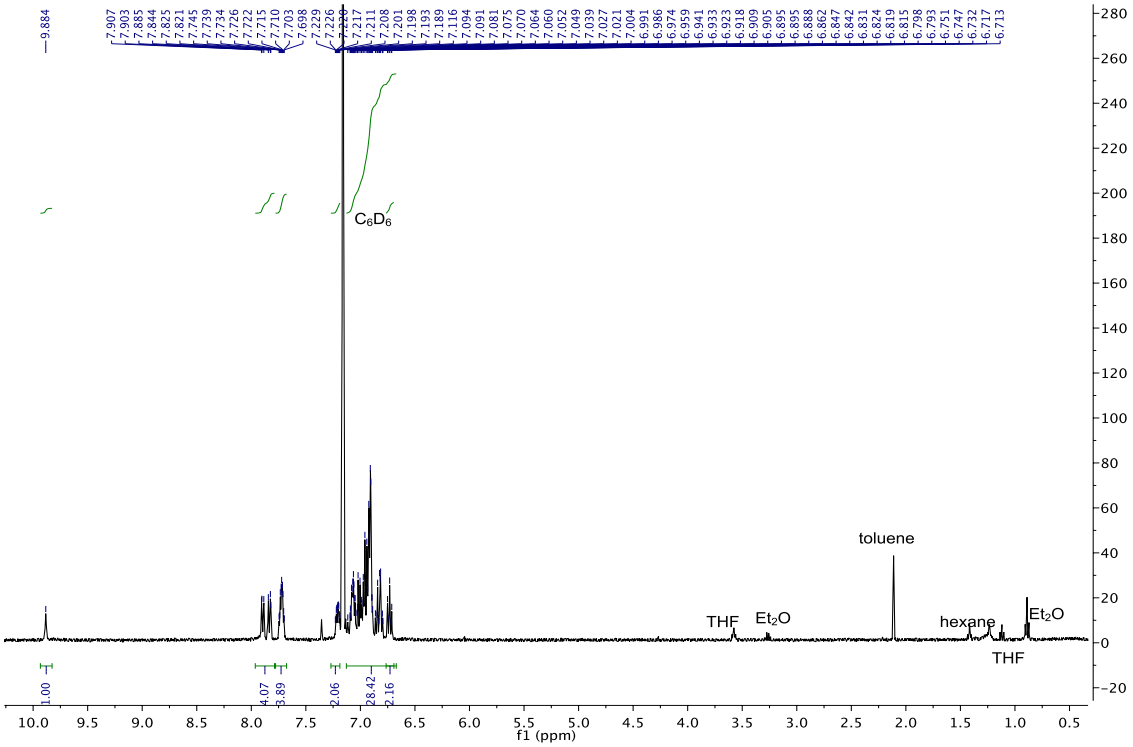


Figure S44. ^{1}H NMR (C_6D_6) of [(^{Ph}**L1**)Ni(BPI)] (^{Ph}**1**). BPI = benzophenone imine.

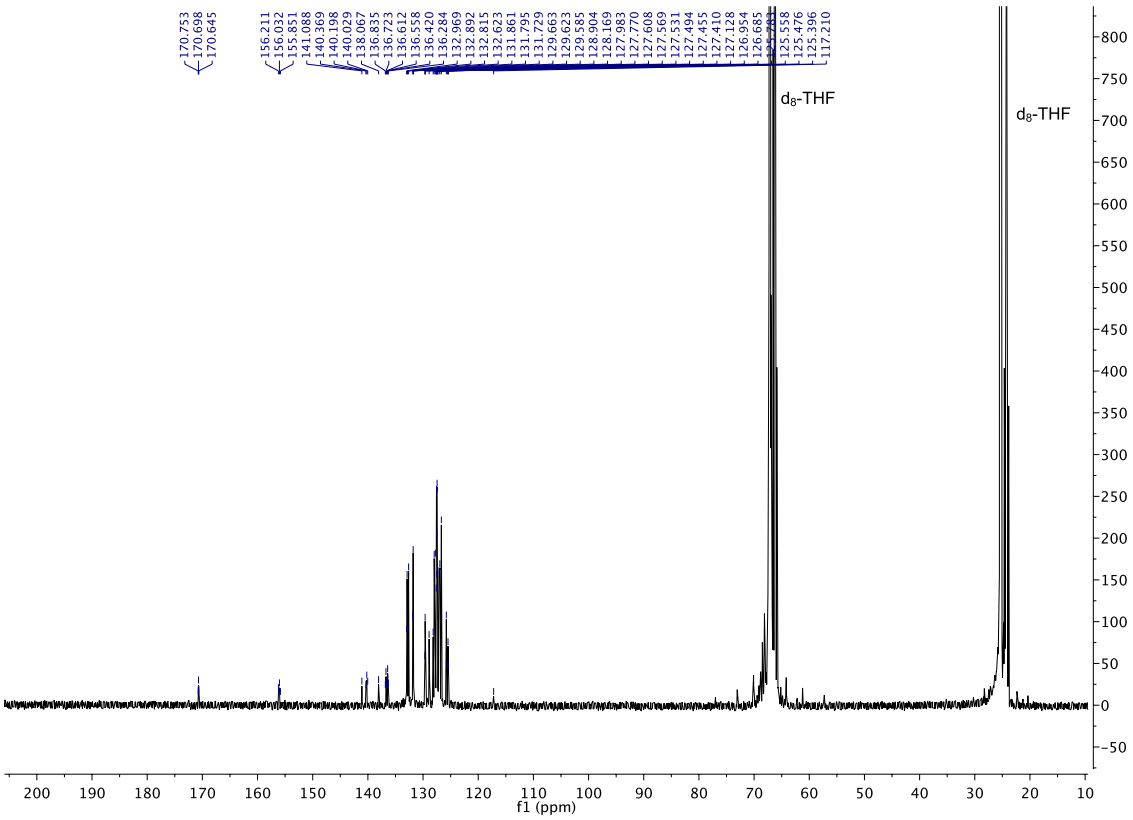


Figure S45. ^{13}C NMR (d_8-THF) of [($^{p\text{-tol}}$**L1**)Ni(BPI)] ($^{p\text{-tol}}$**1**). BPI = benzophenone imine.

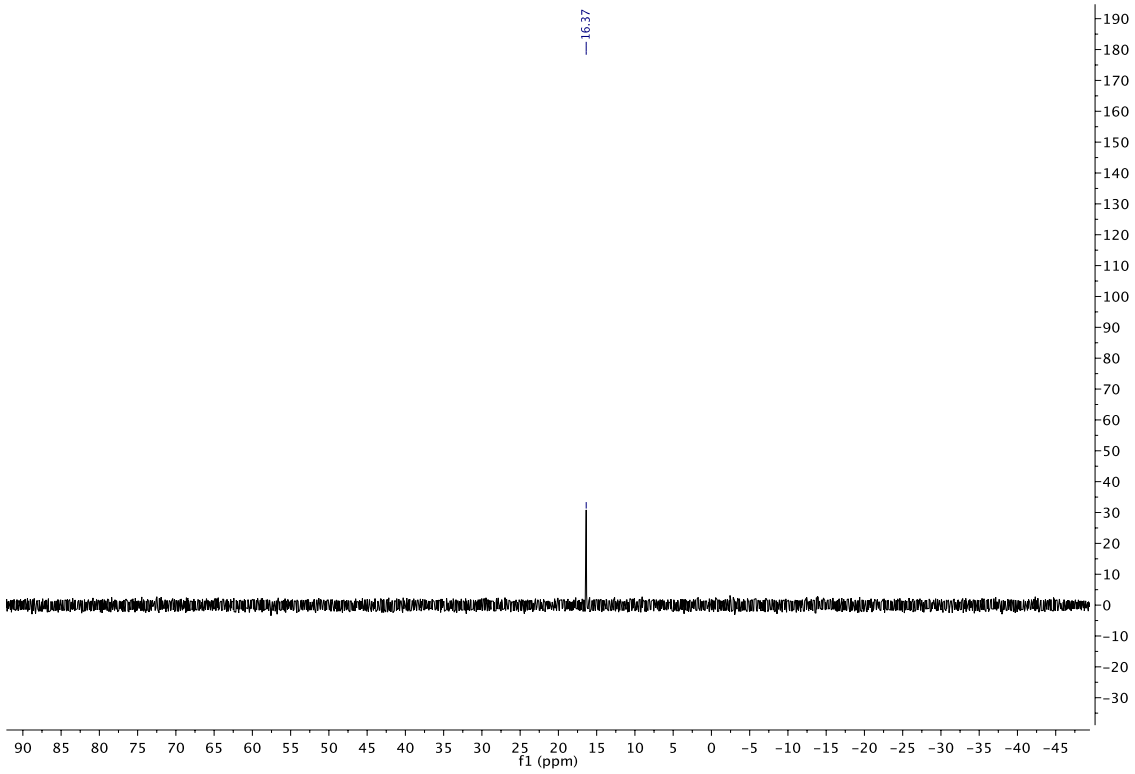


Figure S46. ^{31}P NMR (C_6D_6) of [(*p*-tol**L1**)Ni(BPI)] (*p*-tol**1**). BPI = benzophenone imine.

[(*p*-tolL2**)Ni(BPI)] (*p*-tol**2**)].**

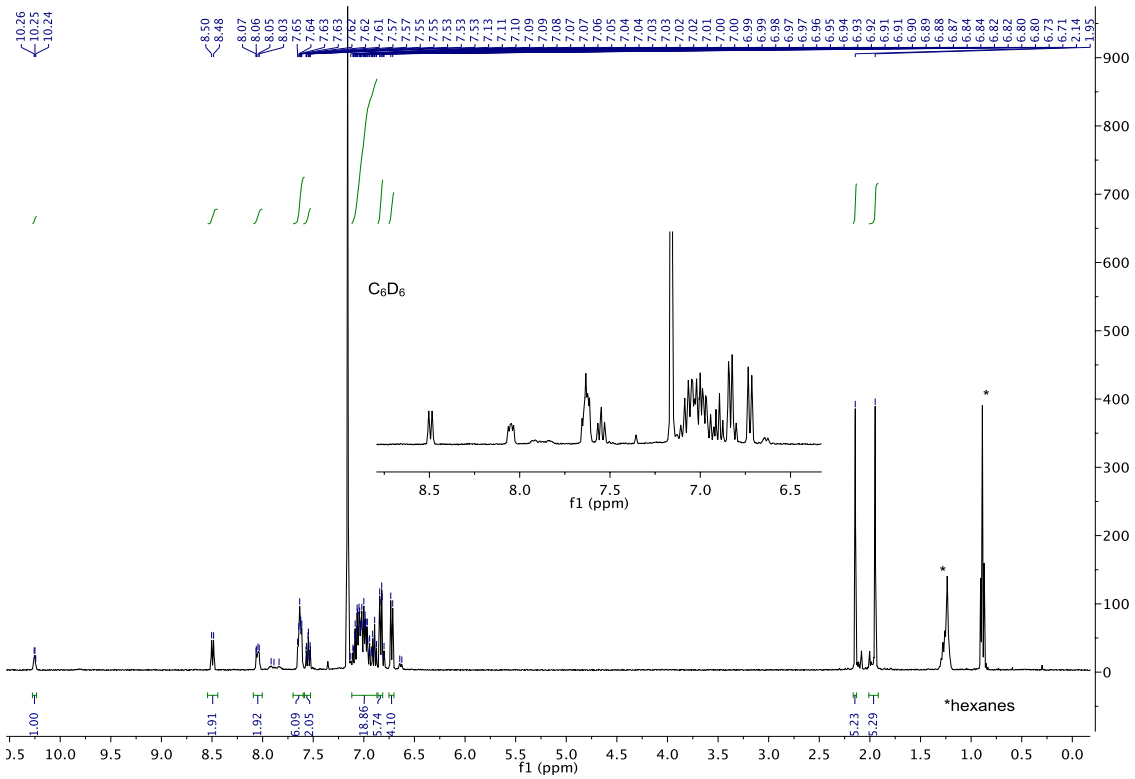


Figure S47. ^{1}H NMR (C_6D_6) of [(*p*-tol**L2**)Ni(BPI)] (*p*-tol**L2**). BPI = benzophenone imine.

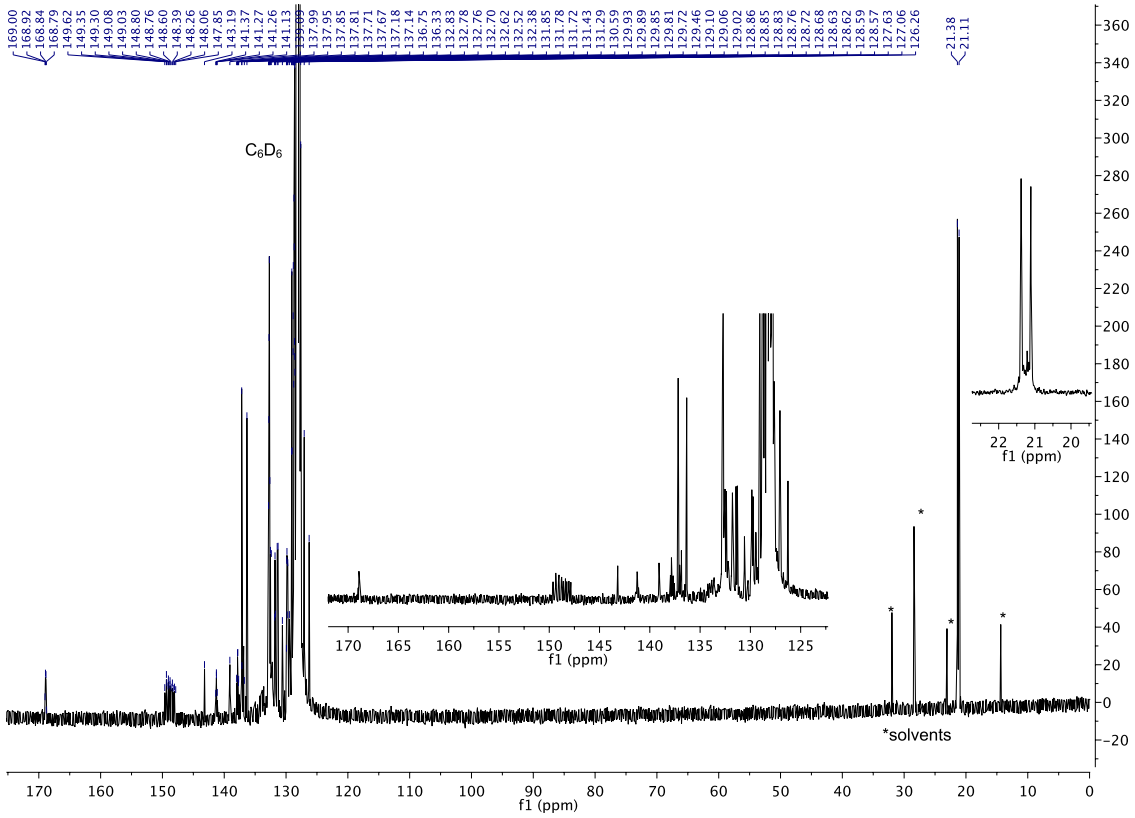


Figure S48. ^{13}C NMR (C_6D_6) of [(*p*-tol**L2**)Ni(BPI)] (*p*-tol**2**). BPI = benzophenone imine.

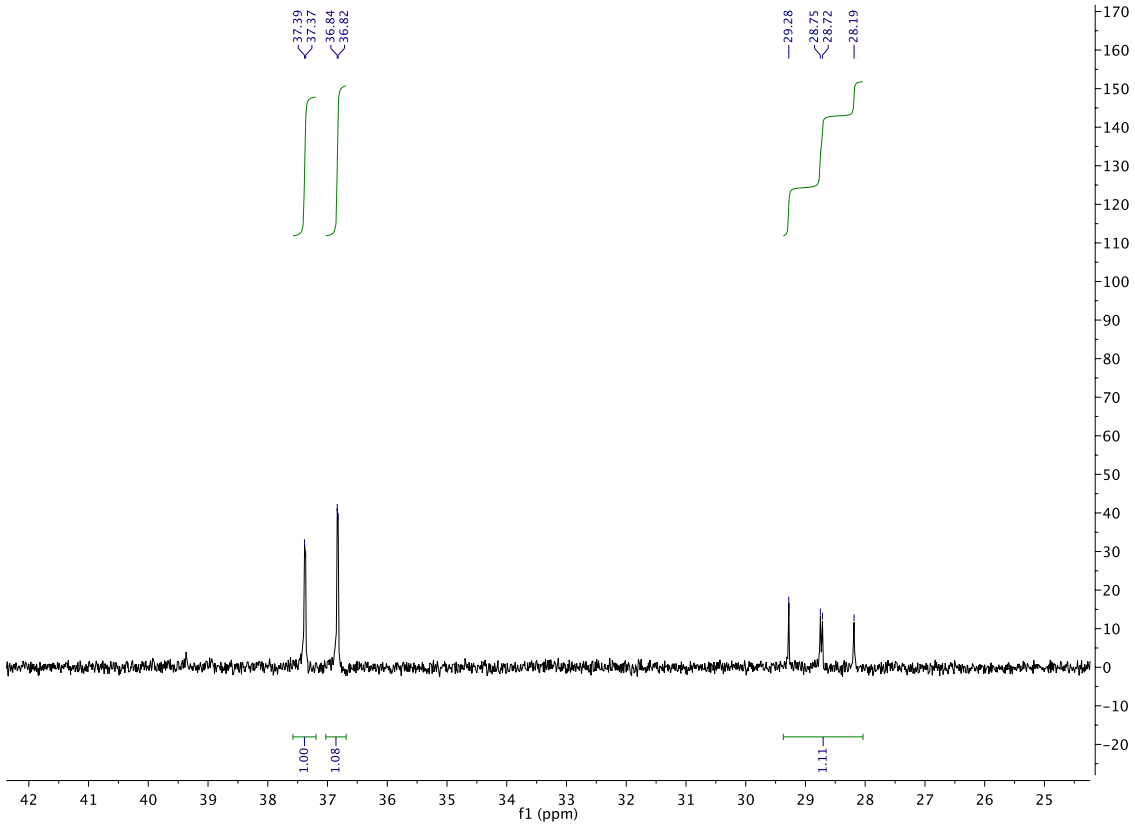


Figure S49. ^{31}P NMR (C_6D_6) of [(*p*-tol**L2**)Ni(BPI)] (*p*-tol**2**). BPI = benzophenone imine.

[(^{Ph}L3)Ni(BPI)] (^{Ph}3)

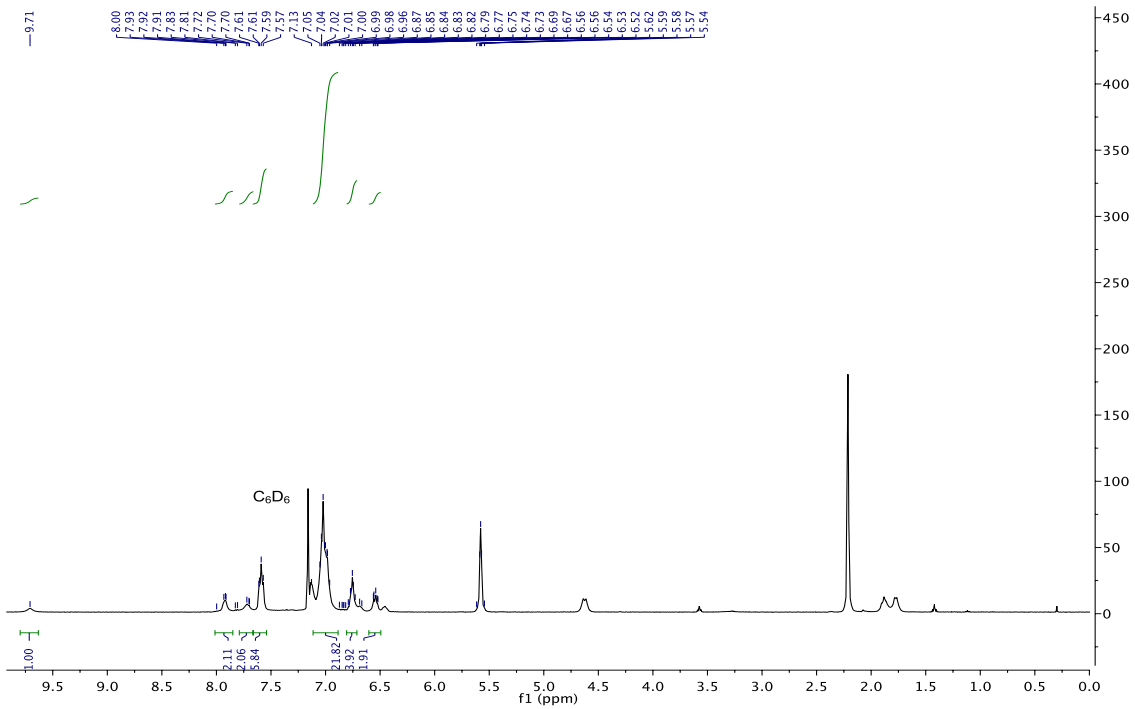


Figure S50. ^{31}H NMR (C_6D_6) of [(^{Ph}**L3**)Ni(BPI)] (^{Ph}**3**). The NMR have been recorded just after its formation and still contains cod at 5.5 and 2.1 ppm in addition to some unreacted $Ni(cod)_2$at 4.6 and 1.9 ppm. BPI = benzophenone imine.

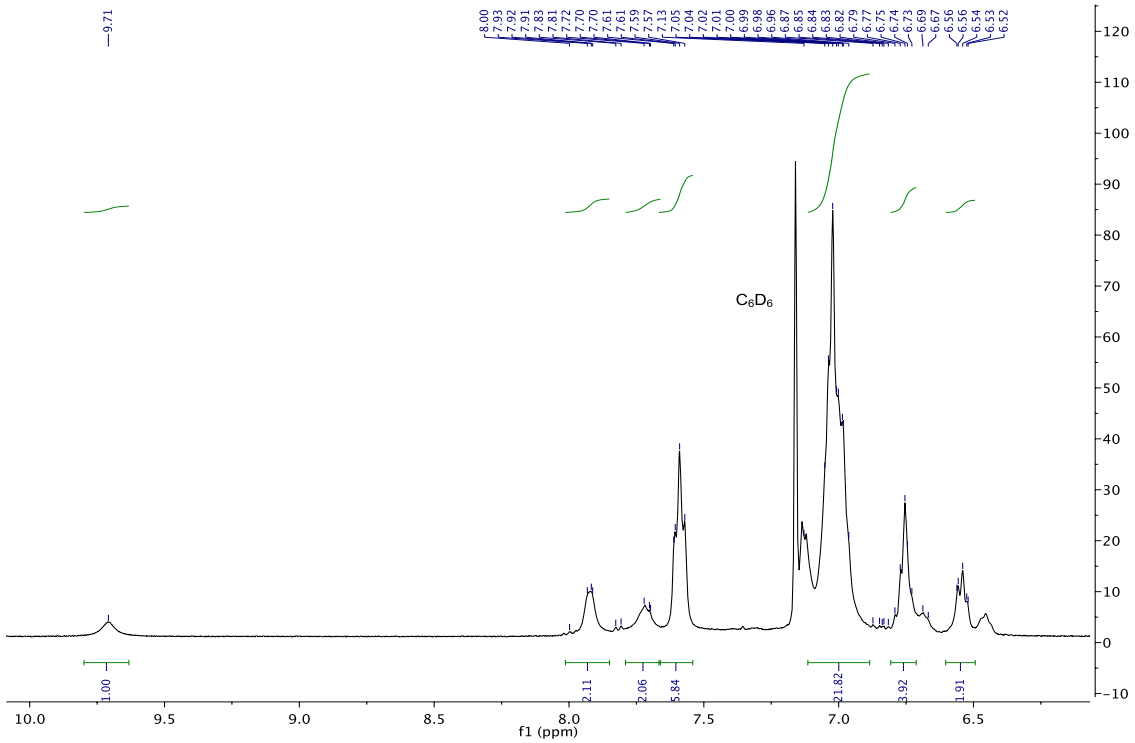


Figure S51. ^{31}H NMR (C_6D_6) of [(^{Ph}**L3**)Ni(BPI)] (^{Ph}**3**).Zoom in the aromatic and imine region. BPI = benzophenone imine.

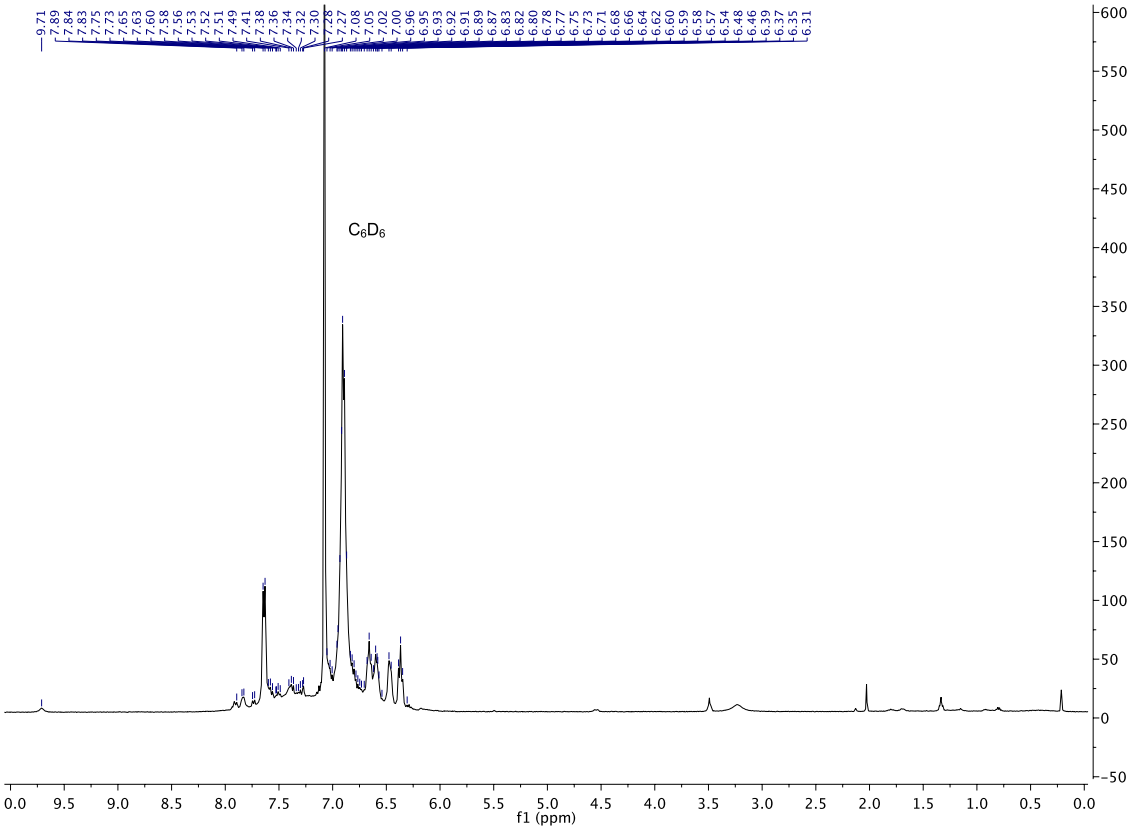


Figure S52. ^{31}H NMR (C_6D_6) of [(**^{Ph}L3**)Ni(BPI)] **^{Ph}3** when the compound start to decompose. BPI = benzophenone imine.

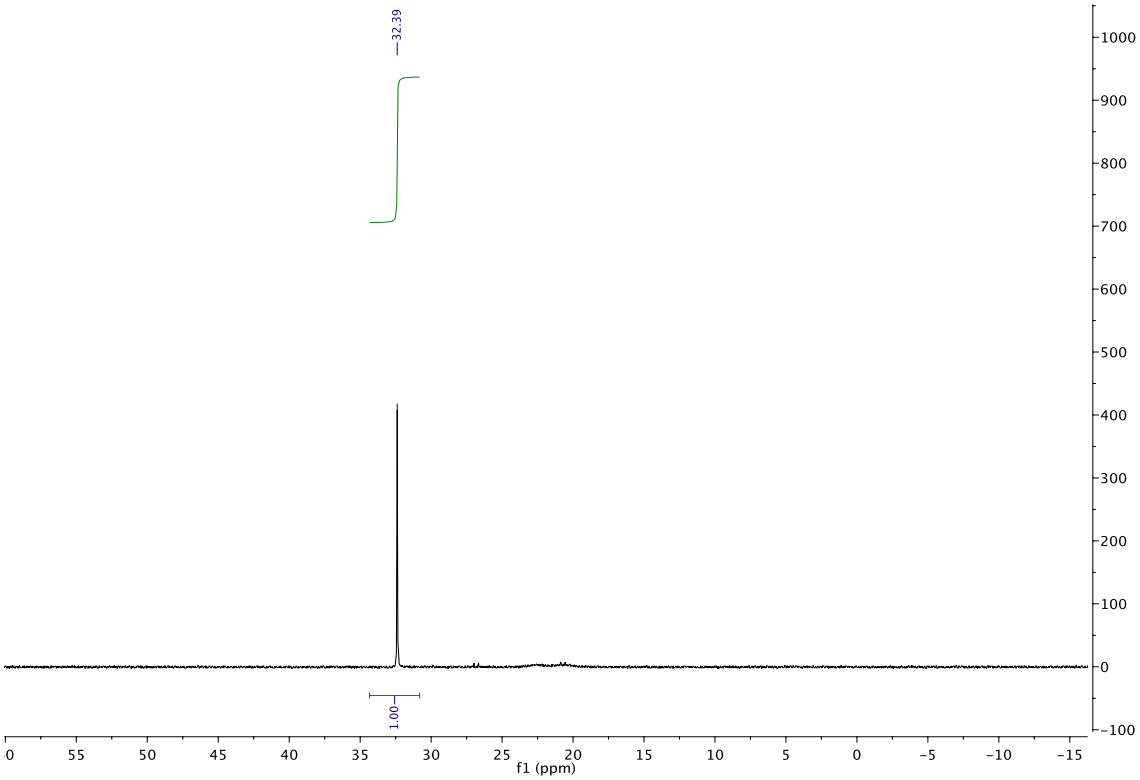


Figure S53. ^{31}P NMR (C_6D_6) of [(**^{Ph}L3**)Ni(BPI)] (**^{Ph}3**). BPI = benzophenone imine.

In-situ characterization of [($^{p\text{-tol}}$L2)Ni(HC≡CPh)] ($^{p\text{-tol}}$4-Ph)

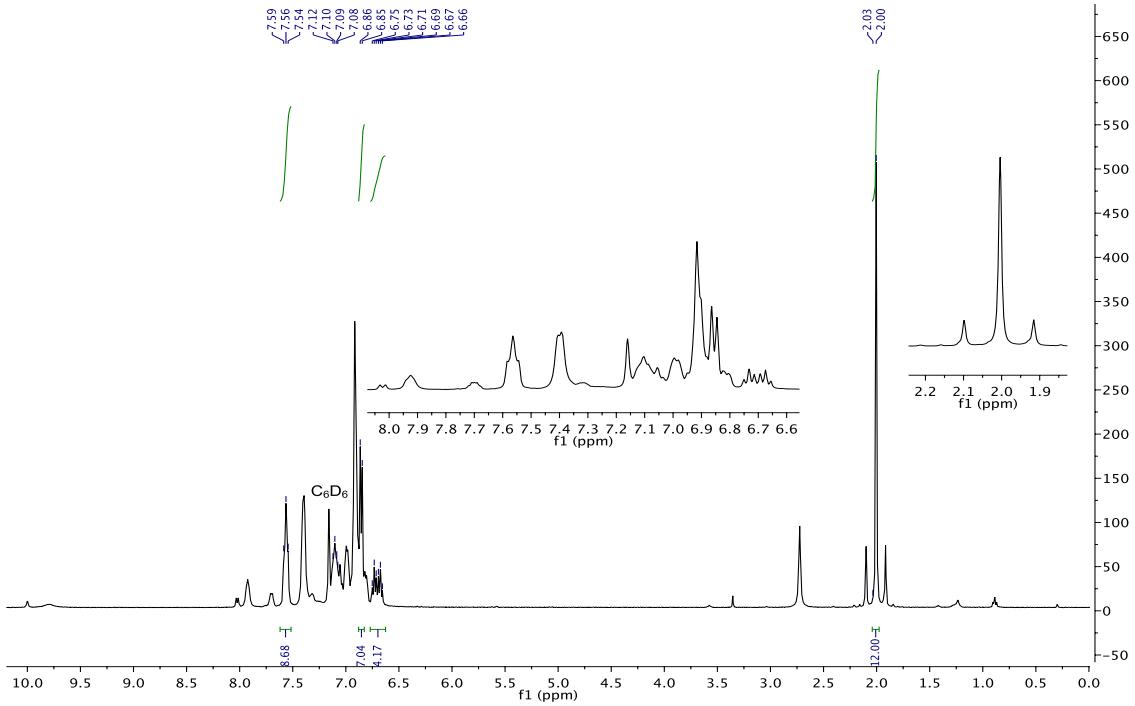


Figure S54. *In-situ* ^{1}H NMR (C_6D_6) characterization of [($^{p\text{-tol}}$**L1**)Ni(HC≡CPh ($^{p\text{-tol}}$**4-Ph**) from the reaction of $^{p\text{-tol}}$**1** with phenylacetylene. Integrated values are attributed to compound $^{p\text{-tol}}$**4-Ph**. The rest of the spectrum contains mainly a mixture of $^{p\text{-tol}}$**1**, phenylacetylene and BPI.

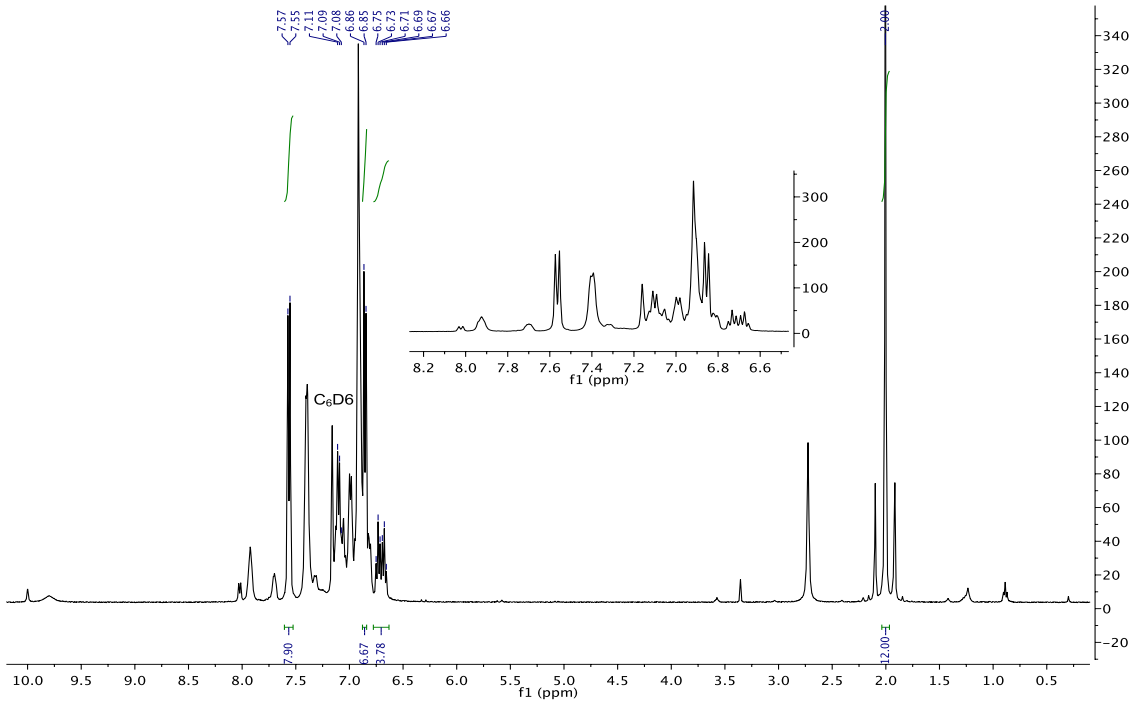


Figure S55. *In-situ* ^{1}H{^{31}P} NMR (C_6D_6) characterization of [($^{p\text{-tol}}$**L1**)Ni(HC≡CPh ($^{p\text{-tol}}$**4-Ph**) from the reaction of $^{p\text{-tol}}$**1** with phenylacetylene. Integrated values are attributed to compound $^{p\text{-tol}}$**4-Ph**. The rest of the spectrum contains mainly a mixture of $^{p\text{-tol}}$**1**, phenylacetylene and BPI.

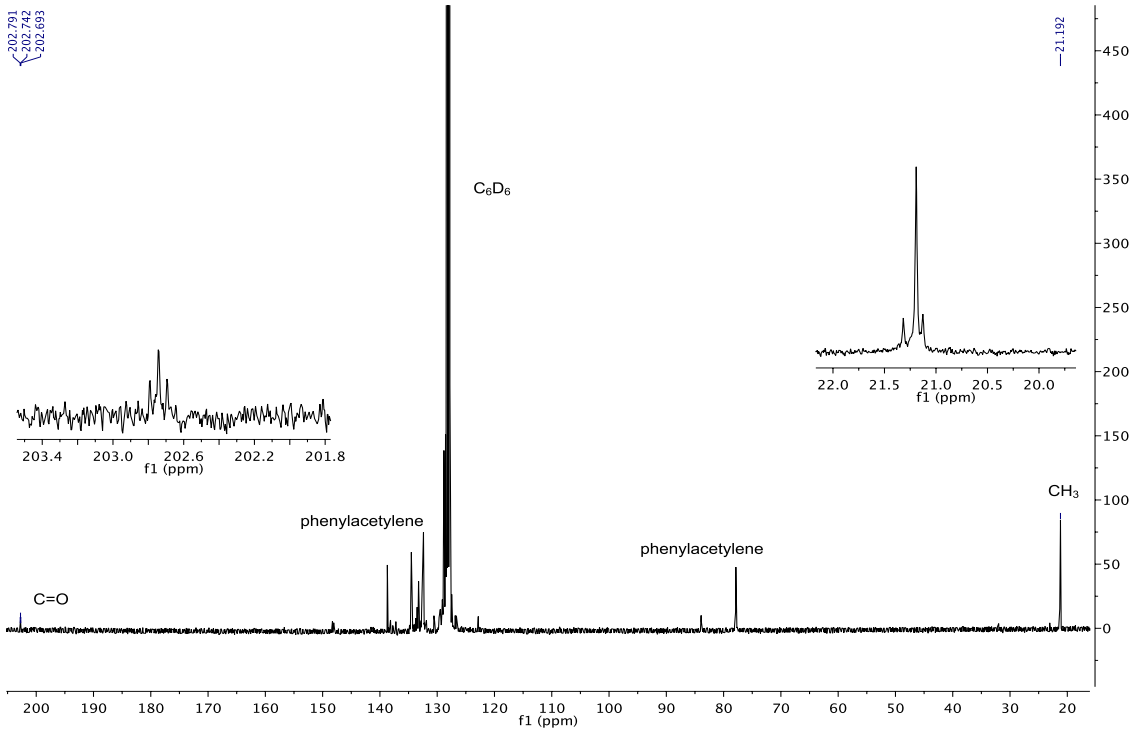


Figure S56. *In-situ* ^{13}C NMR (C_6D_6) characterization of [(*p*-tol**L1**)Ni(HCPh)] (*p*-tol**4-Ph**) from the reaction of *p*-tol**1** with phenylacetylene. This spectrum shows the unbound ketone from the ligand at 202.7 ppm, and the methyl groups from the *para*-tolyl substituents as a singlet at 21.2 ppm, characteristic of the bidentate state of the ligand.

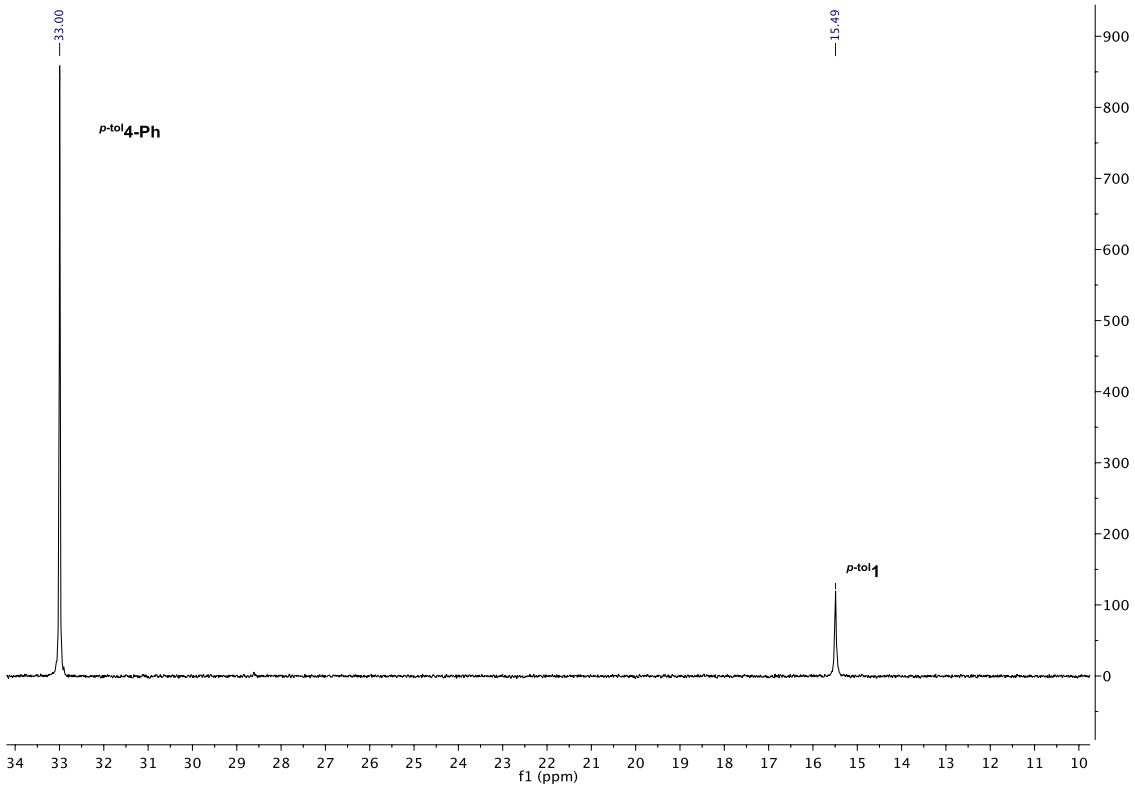


Figure S57. *In-situ* ^{31}P NMR (C_6D_6) characterization of [(*p*-tol**L1**)Ni(HC≡CPh)] (*p*-tol**4-Ph**) from the reaction of *p*-tol**1** with phenylacetylene.

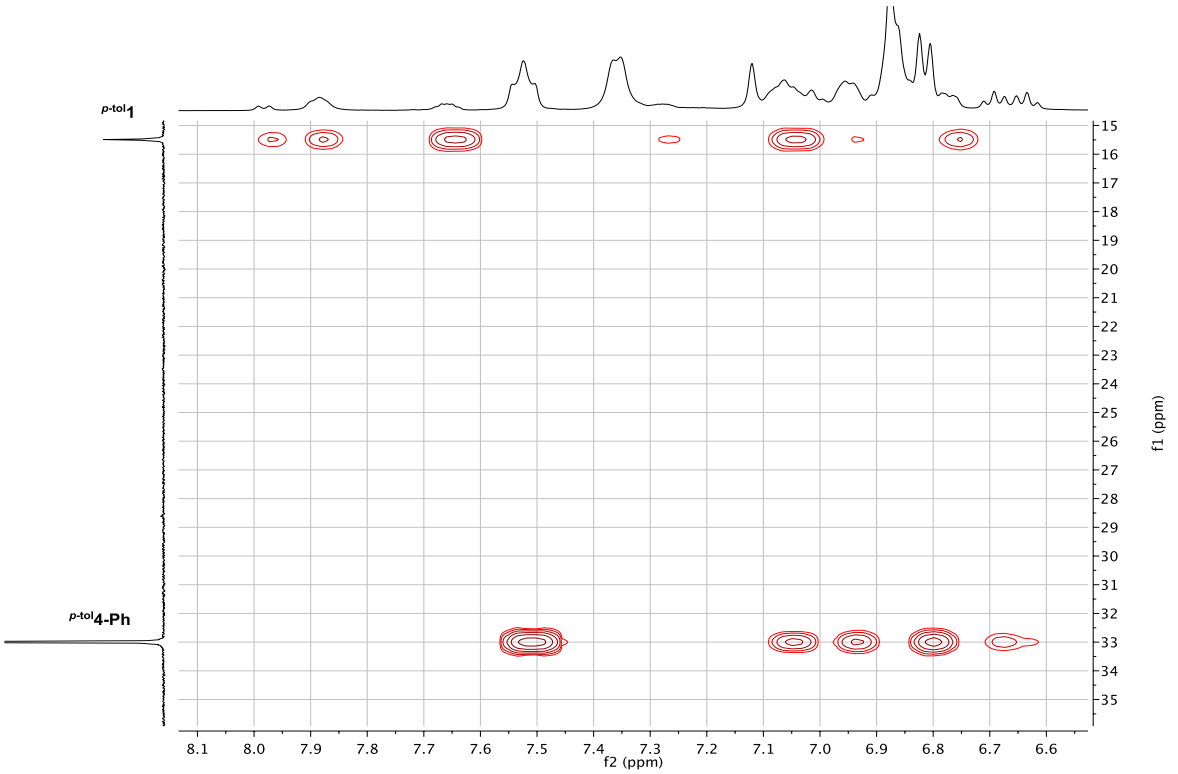


Figure S58. *In-situ* HMBC (^{1}H-^{31}P) 2D NMR (C_6D_6) characterization of [(*p*-tol**L1**)Ni(HC≡CPh)] (*p*-tol**4-Ph**) from the reaction of *p*-tol**1** with phenylacetylene. Zoom in the aromatic region.

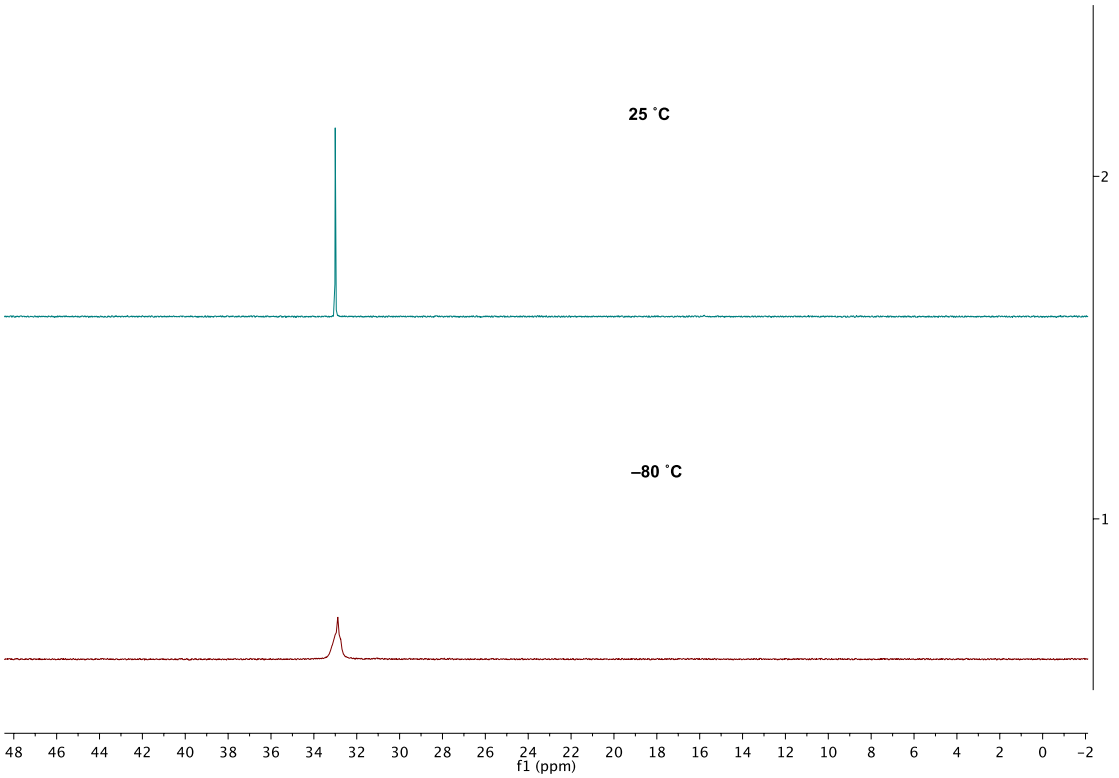


Figure S59. Variable temperature (VT) ^{31}P NMR (*d*-toluene) of [(*p*-tol**L1**)Ni(HC≡CPh)] (*p*-tol**4-Ph**) at 25 ˚C (top) and –80 ˚C (bottom).

In-situ characterization of [($^{p\text{-tol}}$L2)Ni(HC≡CCH$_2$OMe)] ($^{p\text{-tol}}$4-CH$_2$OMe)

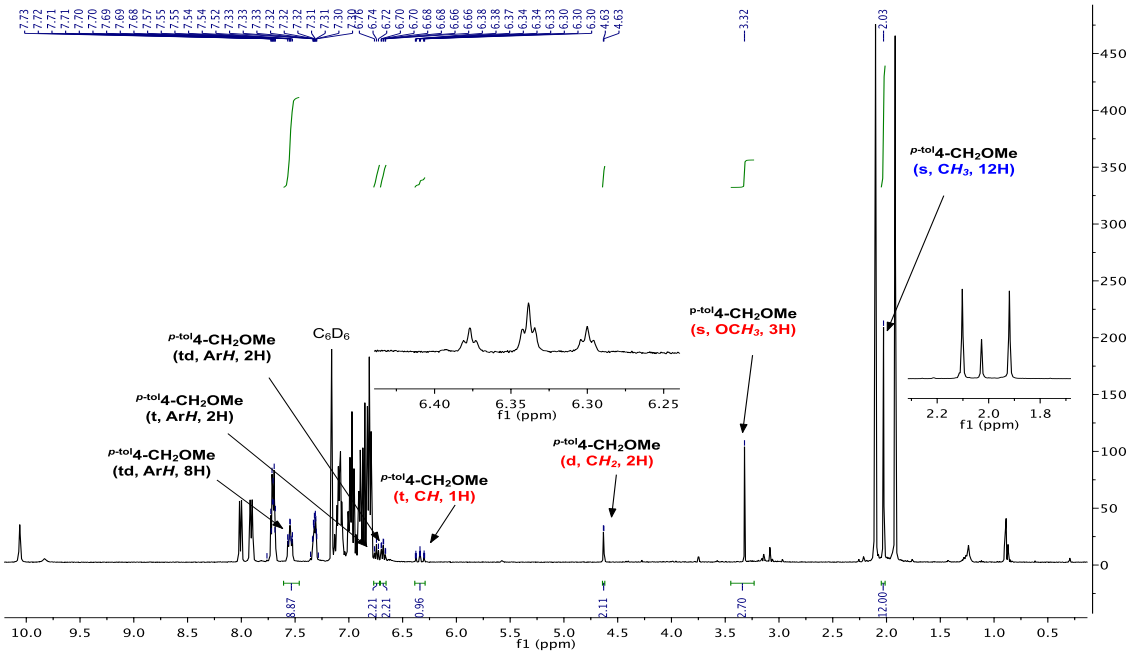


Figure S60. *In-situ* ^{1}H NMR (C_6D_6) characterization of [($^{p\text{-tol}}$**L1**)Ni(HC≡CCH$_2$OMe)] ($^{p\text{-tol}}$**4-CH$_2$OMe**) from the reaction of $^{p\text{-tol}}$**1** with methyl propargyl ether. Integrated values are attributed to compound $^{p\text{-tol}}$**4-CH$_2$OMe**. The rest of the spectrum contains mainly a mixture of $^{p\text{-tol}}$**1**, methyl propargyl ether and BPI.

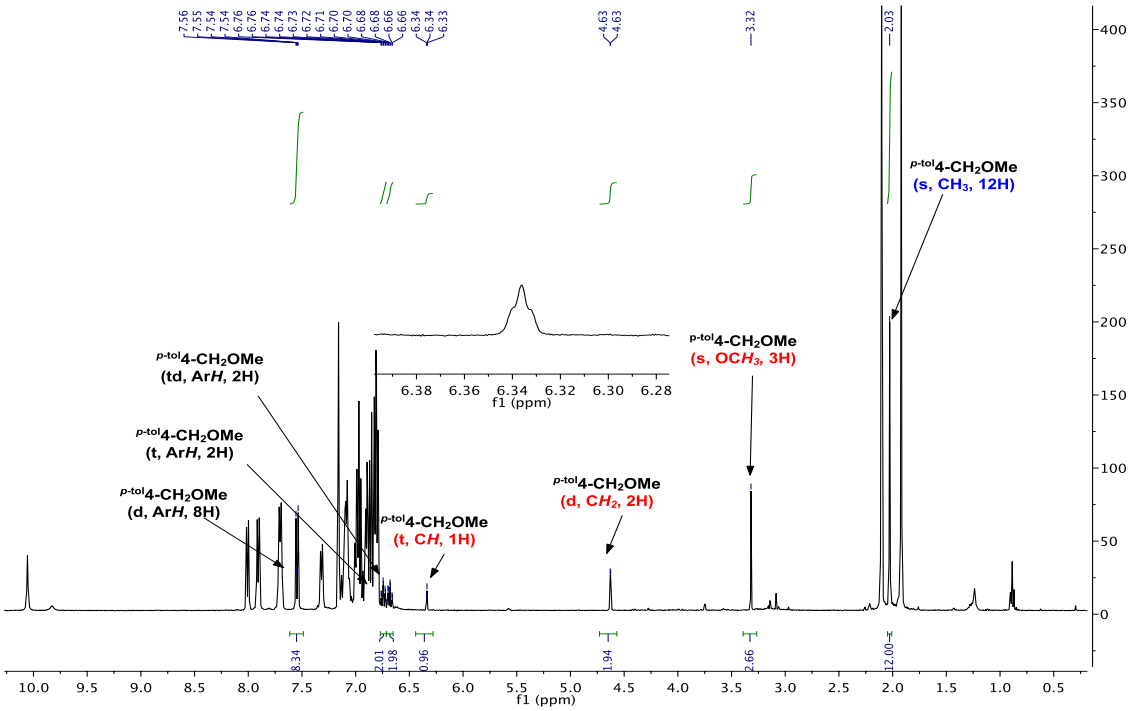


Figure S61. *In-situ* ^{1}H{^{31}P} NMR (C_6D_6) characterization of [($^{p\text{-tol}}$**L1**)Ni(HC≡CCH$_2$OMe)] ($^{p\text{-tol}}$**4-CH$_2$OMe**) from the reaction of $^{p\text{-tol}}$**1** with methyl propargyl ether. Integrated values are attributed to compound $^{p\text{-tol}}$**4-CH$_2$OMe**. The rest of the spectrum contains mainly a mixture of $^{p\text{-tol}}$**1**, methyl propargyl ether and BPI.

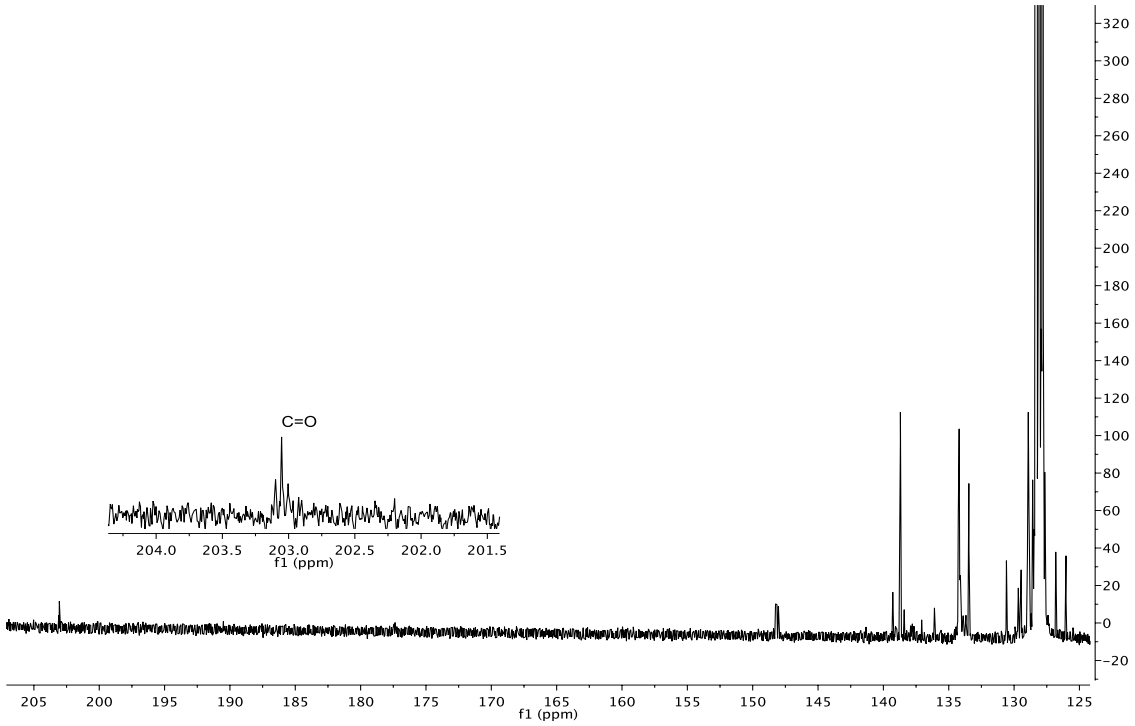


Figure S62. *In-situ* ^{13}C NMR (C_6D_6) characterization of [(**$^{p\text{-tol}}$L1**)Ni(HC≡CCH_2OMe)] (**$^{p\text{-tol}}$4-CH_2OMe**) from the reaction of **$^{p\text{-tol}}$1** with methyl propargyl ether. This spectrum shows the unbound ketone from the ligand at 203 ppm.

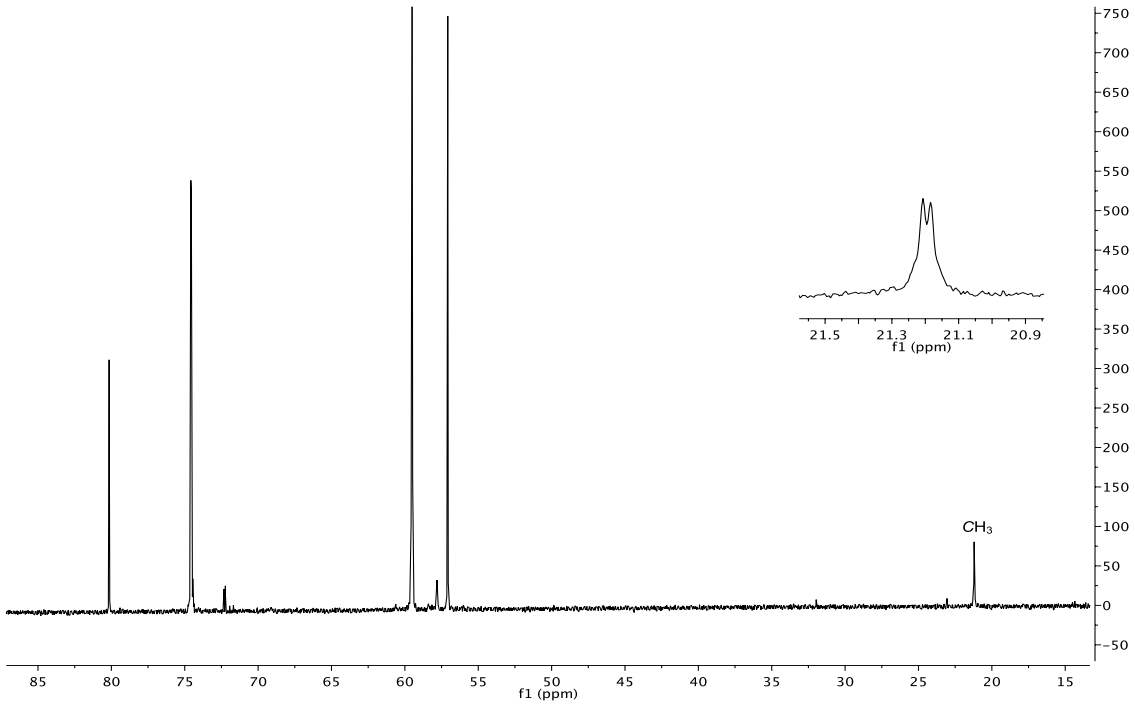


Figure S63. *In-situ* ^{13}C NMR (C_6D_6) characterization of [(**$^{p\text{-tol}}$L1**)Ni(HC≡CCH_2OMe)] (**$^{p\text{-tol}}$4-CH_2OMe**) from the reaction of **$^{p\text{-tol}}$1** with methyl propargyl ether. This spectrum shows the methyl group from the *para*-tolyl substituents as one doublet, characteristic of the bidentate state of the ligand.

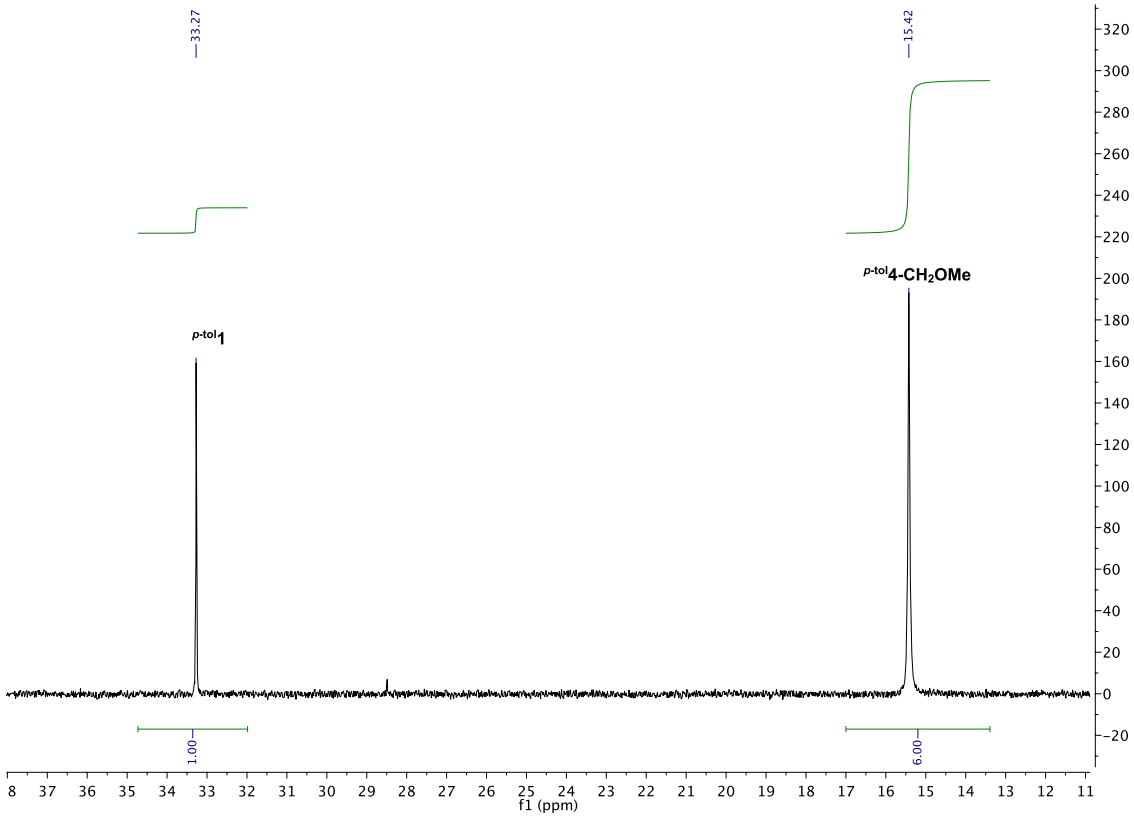


Figure S64. *In-situ* ^{31}P NMR (C_6D_6) characterization of [(**$^{p\text{-tol}}$L1**)Ni(HC≡CCH$_2$OMe)] (**$^{p\text{-tol}}$4-CH$_2$OMe**) from the reaction of **$^{p\text{-tol}}$1** with methyl propargyl ether.

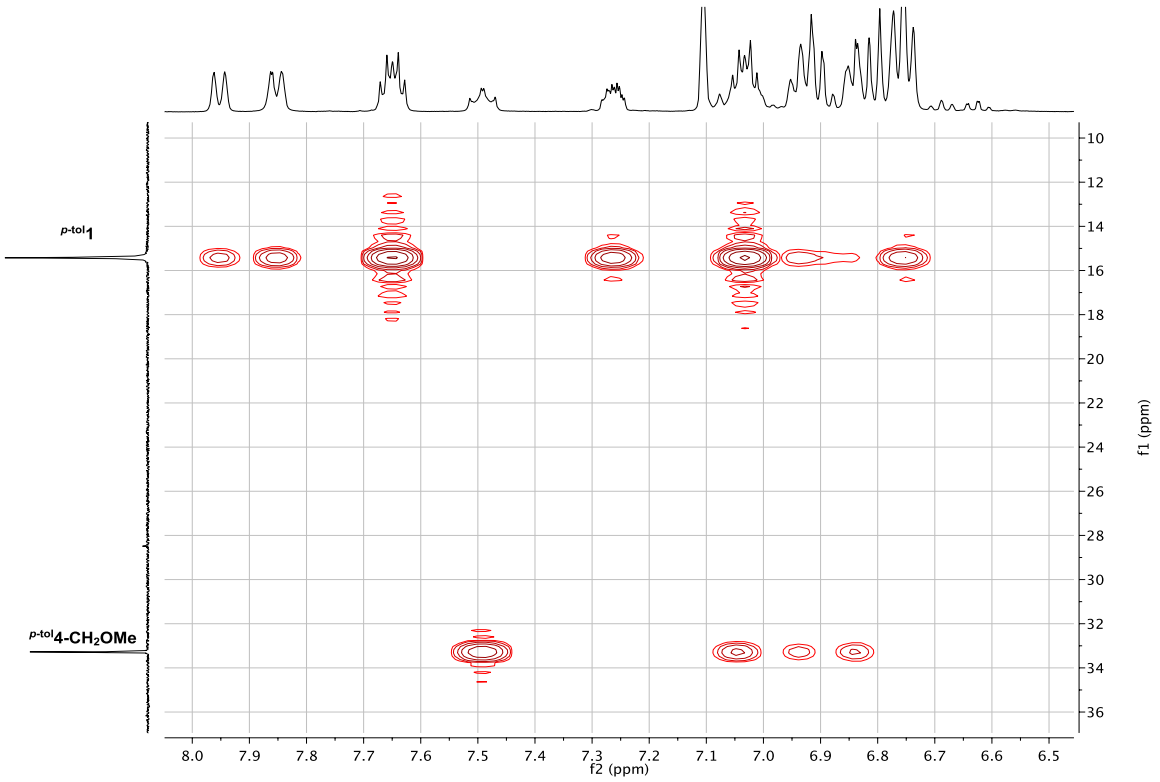


Figure S65. *In-situ* HMBC (^{1}H-^{31}P) 2D NMR (C_6D_6) characterization of [(**$^{p\text{-tol}}$L1**)Ni(HC≡CCH$_2$OMe)] (**$^{p\text{-tol}}$4-CH$_2$OMe**) from the reaction of **$^{p\text{-tol}}$1** with methyl propargyl ether. Zoom in the aromatic region.

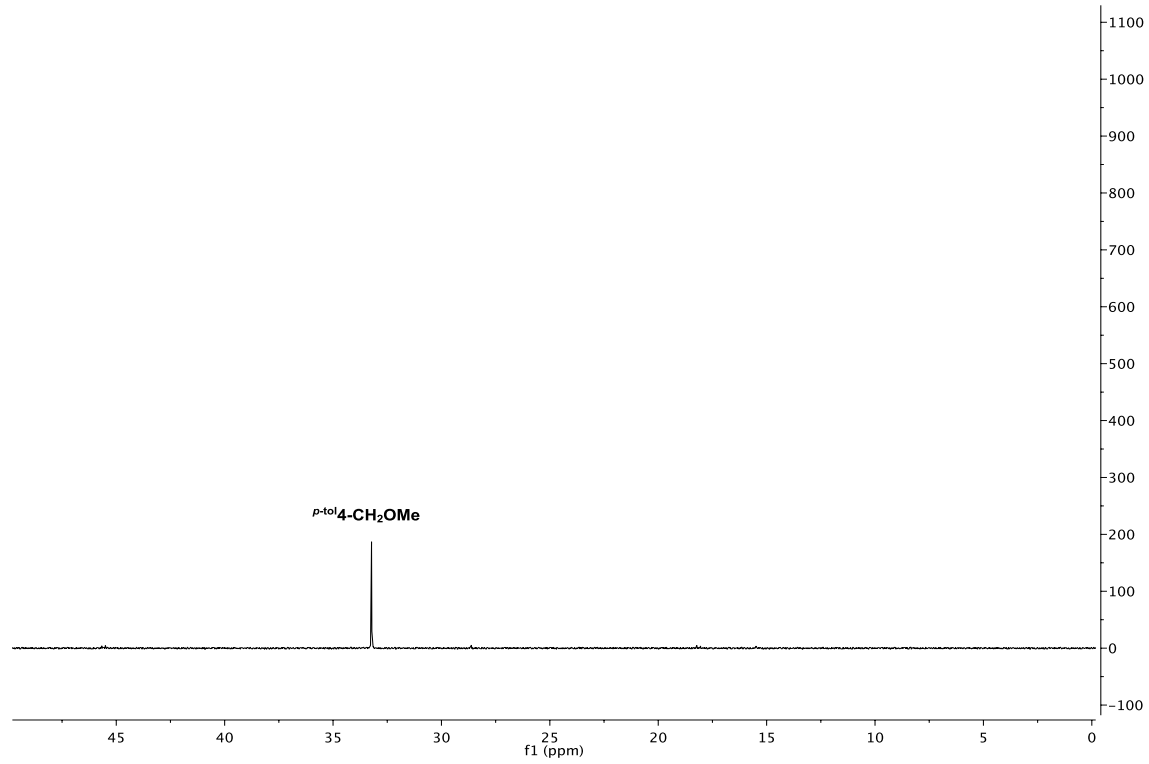


Figure S66. *In-situ* ^{31}P NMR (C_6D_6) characterization of [(**$^{p\text{-tol}}$L1**)Ni(HC≡CCH$_2$OMe)] (**$^{p\text{-tol}}$4-CH$_2$OMe**) from the reaction of **$^{p\text{-tol}}$1** with an excess of methyl propargyl ether.

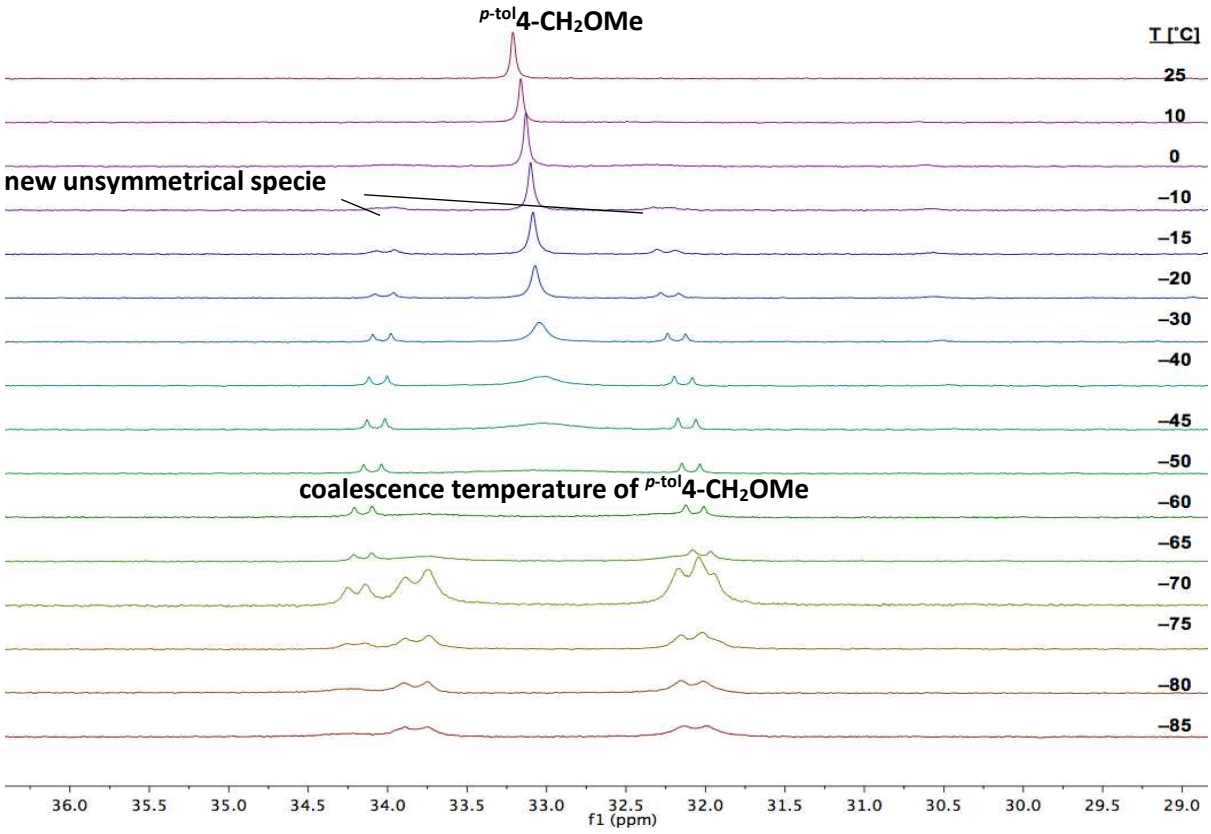


Figure S67 Variable temperature (VT) ^{31}P NMR (*d*-toluene) of [(**$^{p\text{-tol}}$L1**)Ni(HC≡CCH$_2$OMe)] (**$^{p\text{-tol}}$4-CH$_2$OMe**) from 25 ˚C (top) to –85 ˚C (bottom).

[(*p*-tolL2)Ni(HC≡CPh)] (*p*-tol5-Ph)

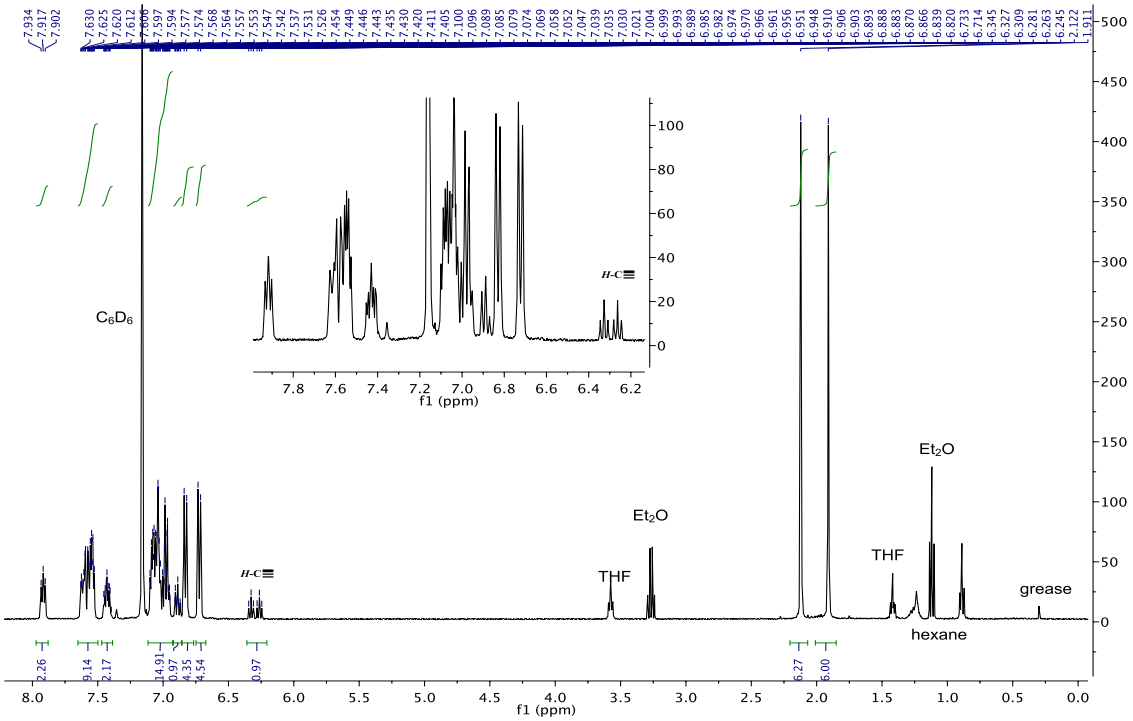


Figure S68. ^{1}H NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**).

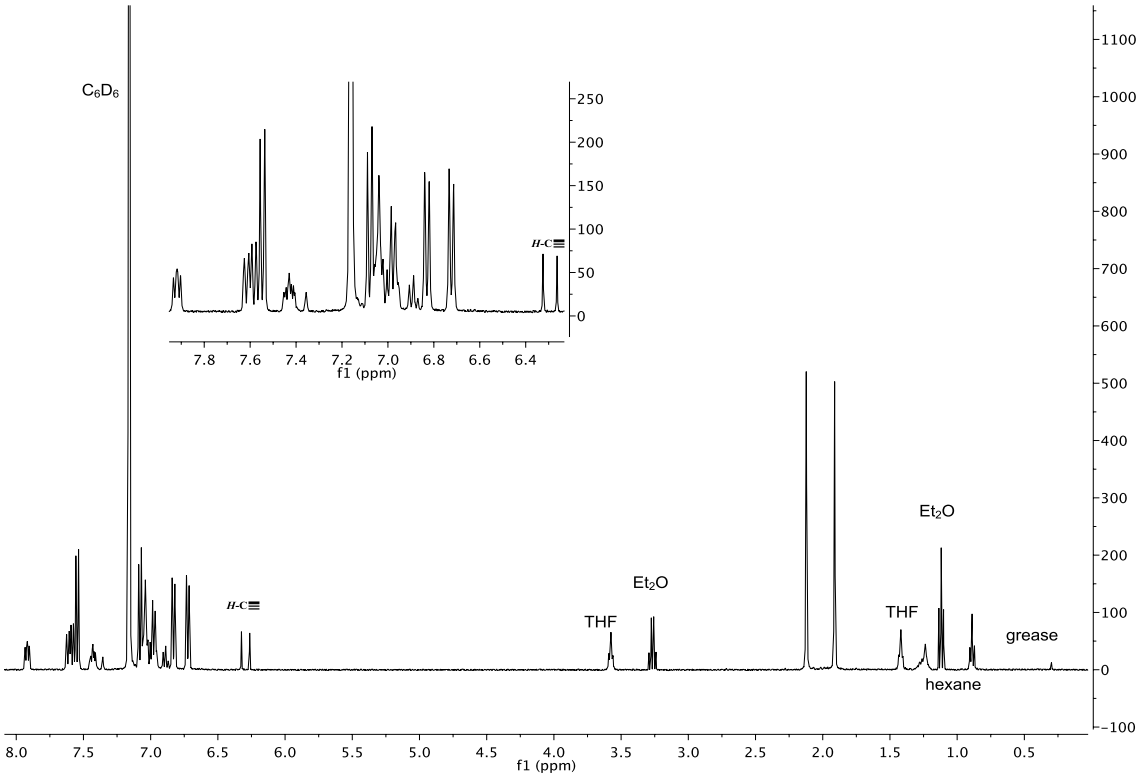


Figure S69. Selective ^{1}H{^{31}P} NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**). The ^{31}P-decoupling NMR is performed with the phosphorus atoms appearing at 28.1 ppm as a doublet in ^{31}P NMR.

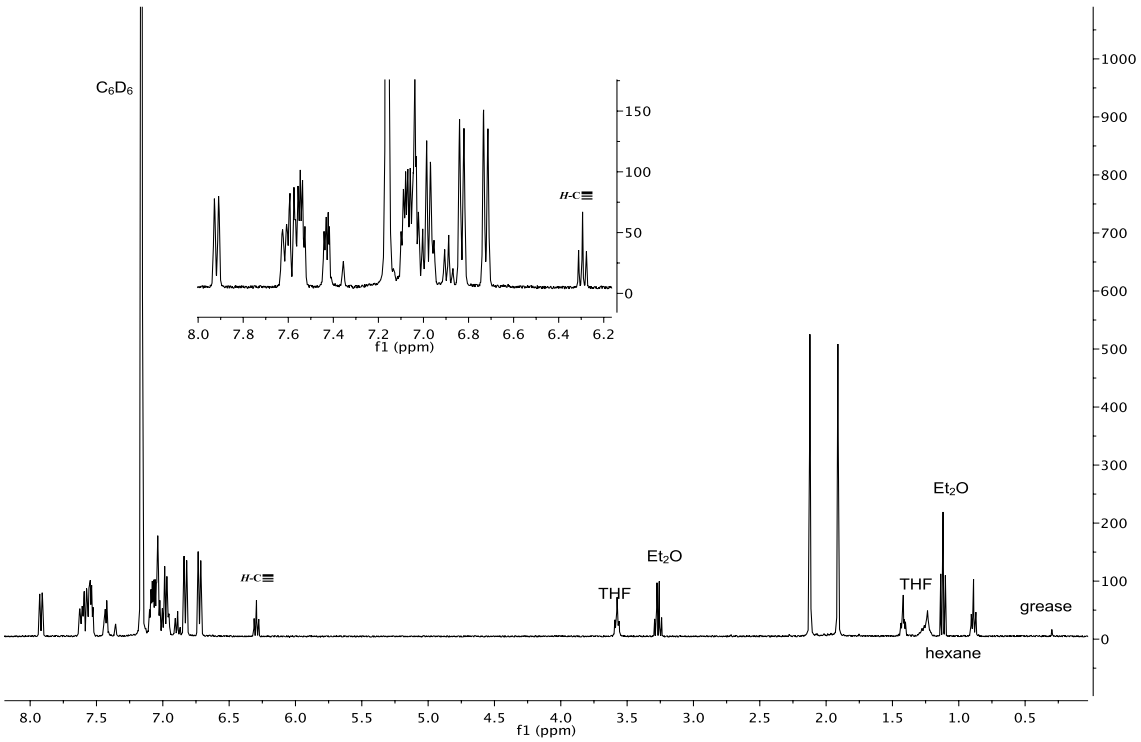


Figure S70. Selective $^{1}H\{^{31}P\}$ NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**). The ^{31}P-decoupling NMR is performed with the phosphorus atom appearing at 78.7 ppm as a triplet in ^{31}P NMR.

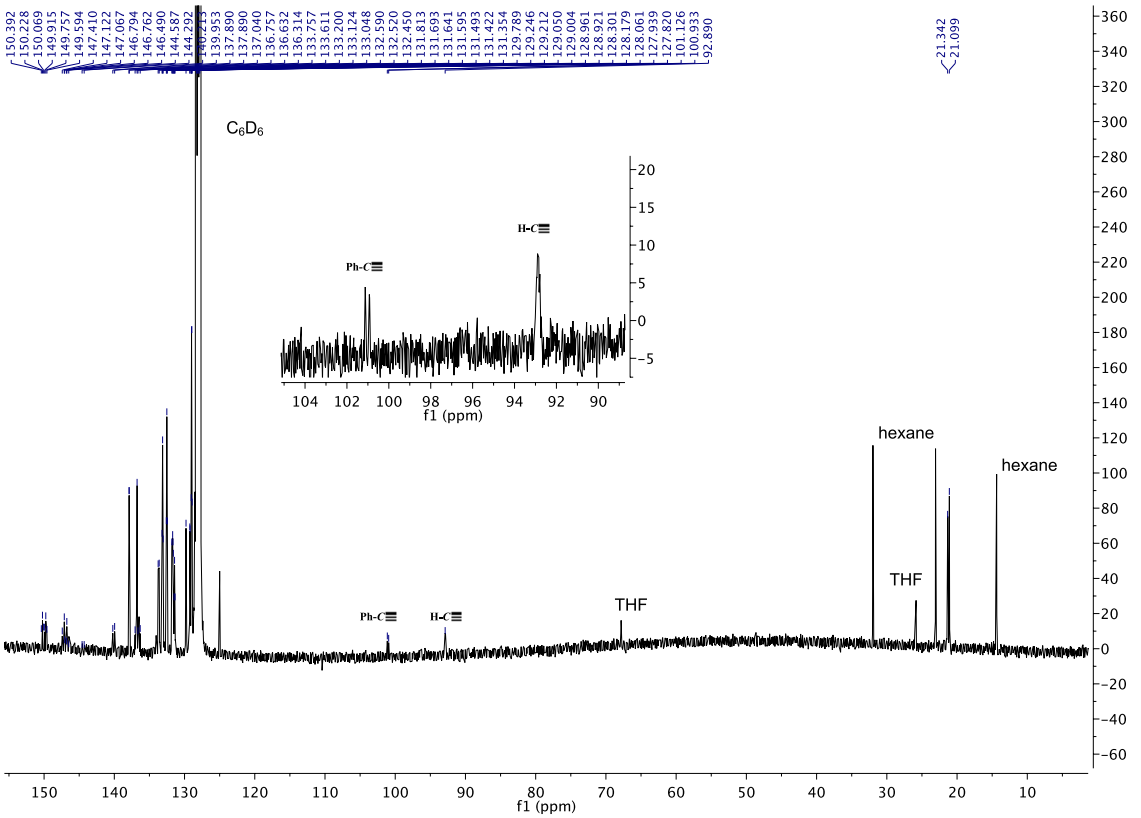


Figure S71. ^{13}C NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**).

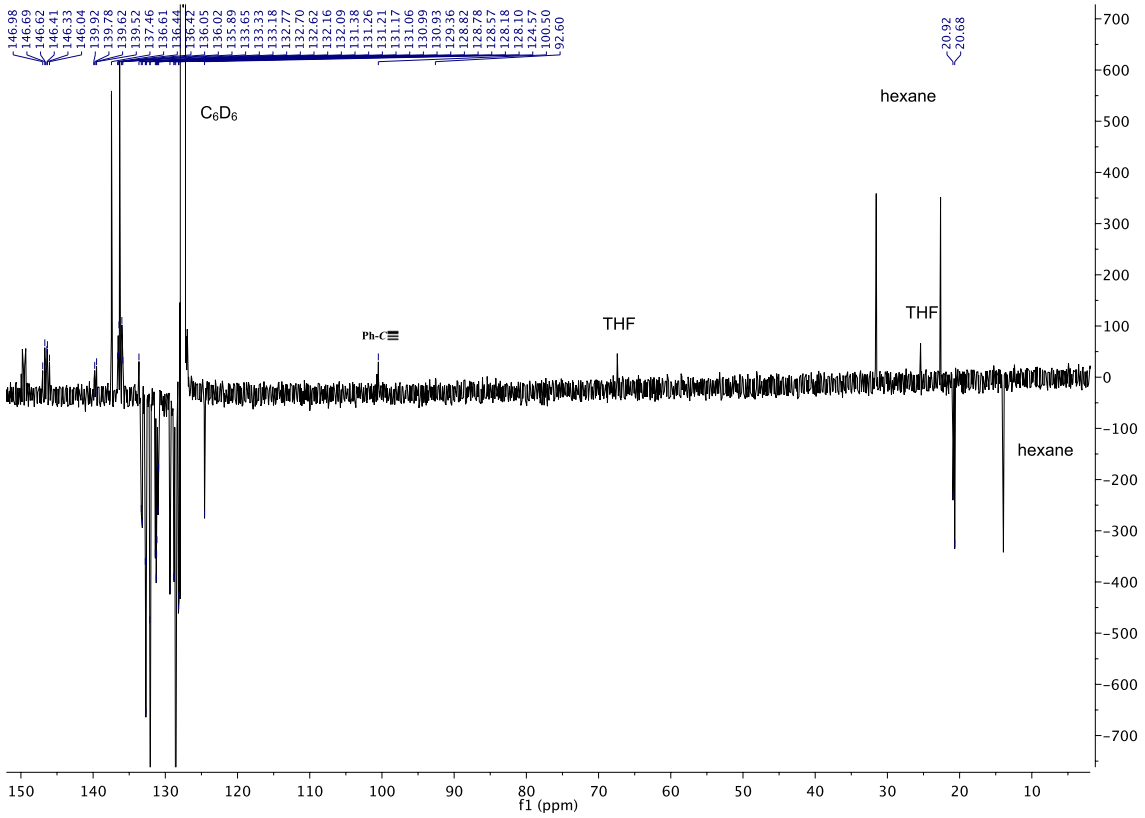


Figure S72. APT ^{13}C NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**).

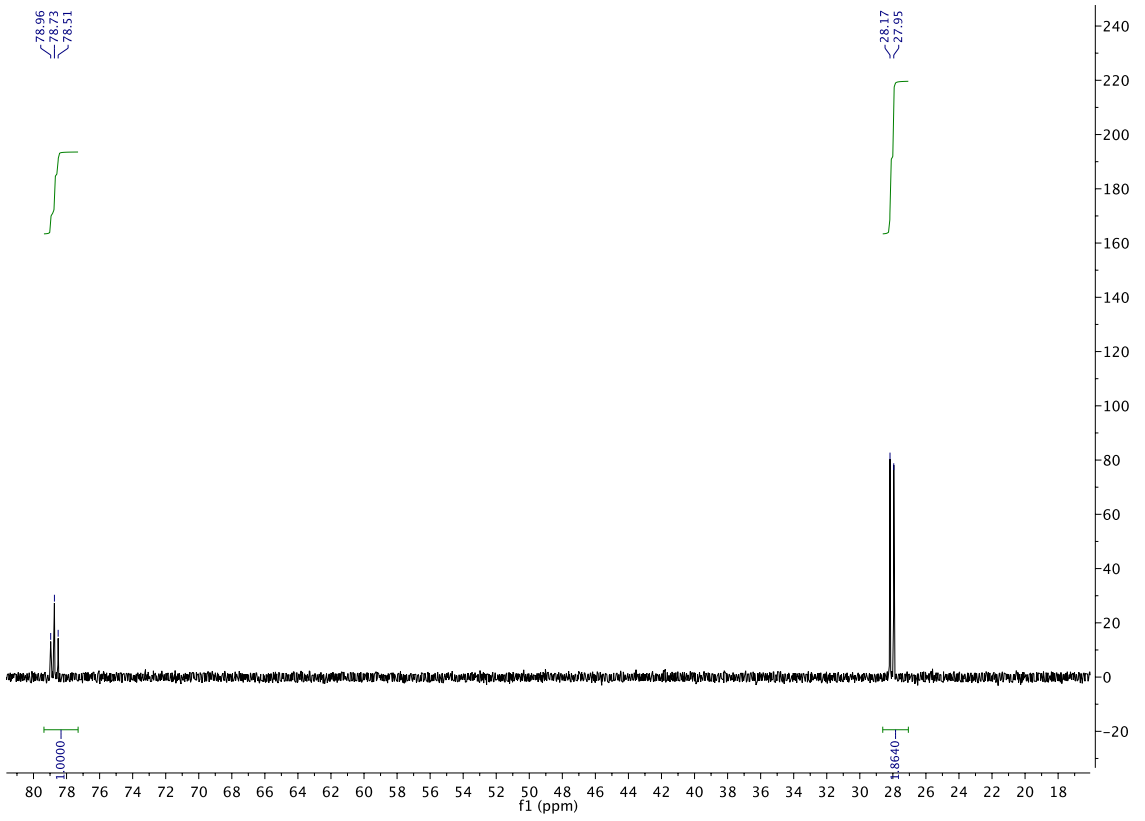


Figure S73. ^{31}P NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**).

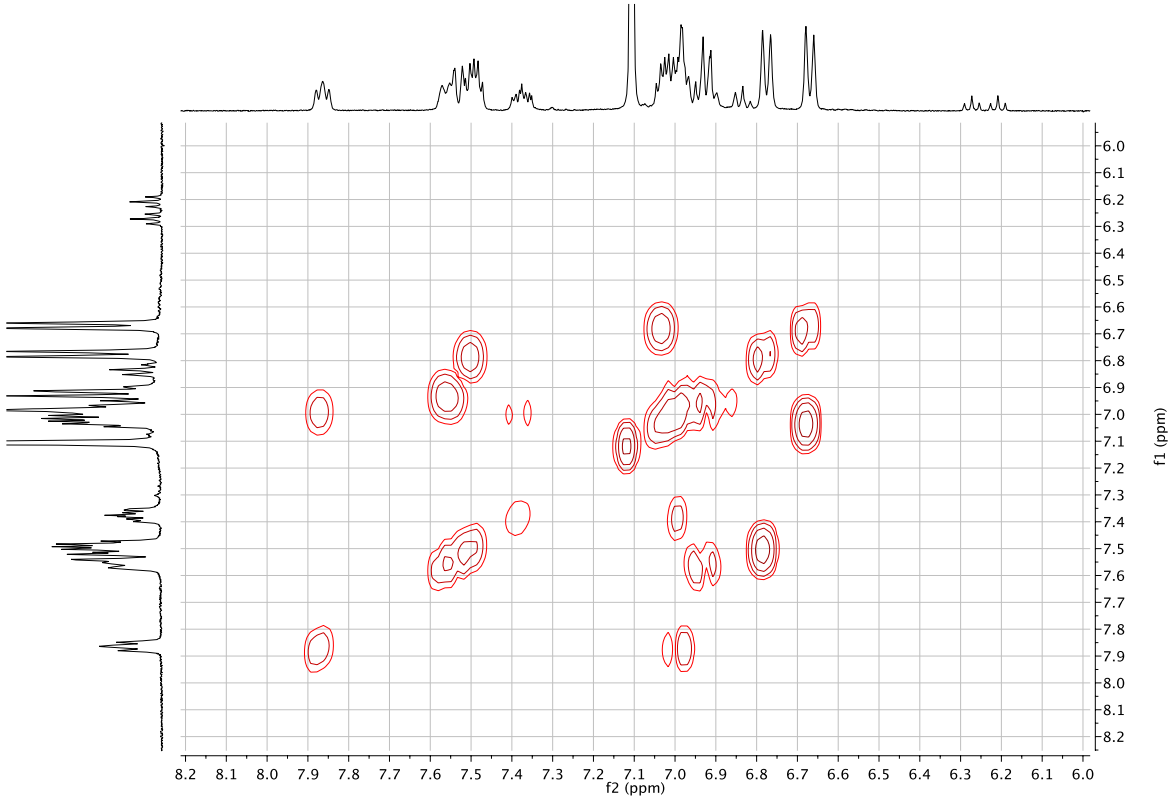


Figure S74. COSY (^{1}H-^{1}H) 2D NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**). Zoom in the region of interest, showing that ≡C*H* at 6.29 (dt) does not couple with any other protons.

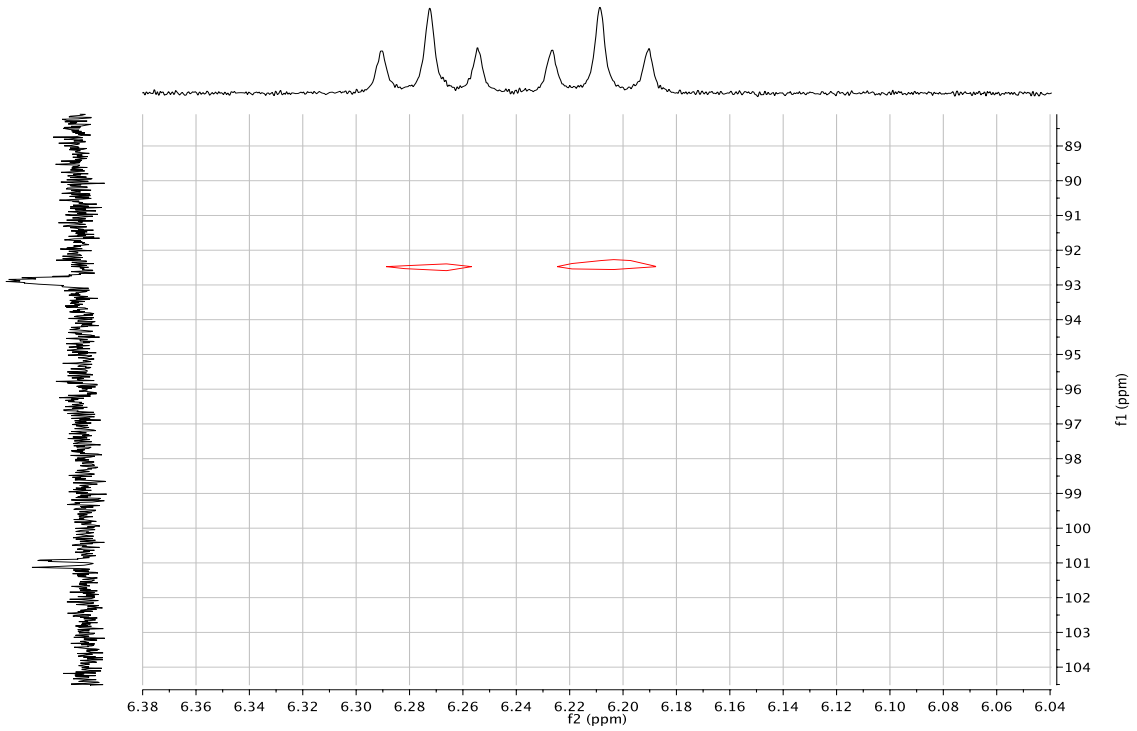


Figure S75. HMBC (^{1}H-^{13}C) 2D NMR (C_6D_6) of [(*p*-tol**L2**)Ni(HC≡CPh)] (*p*-tol**5-Ph**). Zoom in the region of interest, showing the ^{1}H-^{13}C weak coupling between the proton and carbon of the terminal alkyne.

[(p-tolL2)Ni(DC≡CPh)]**

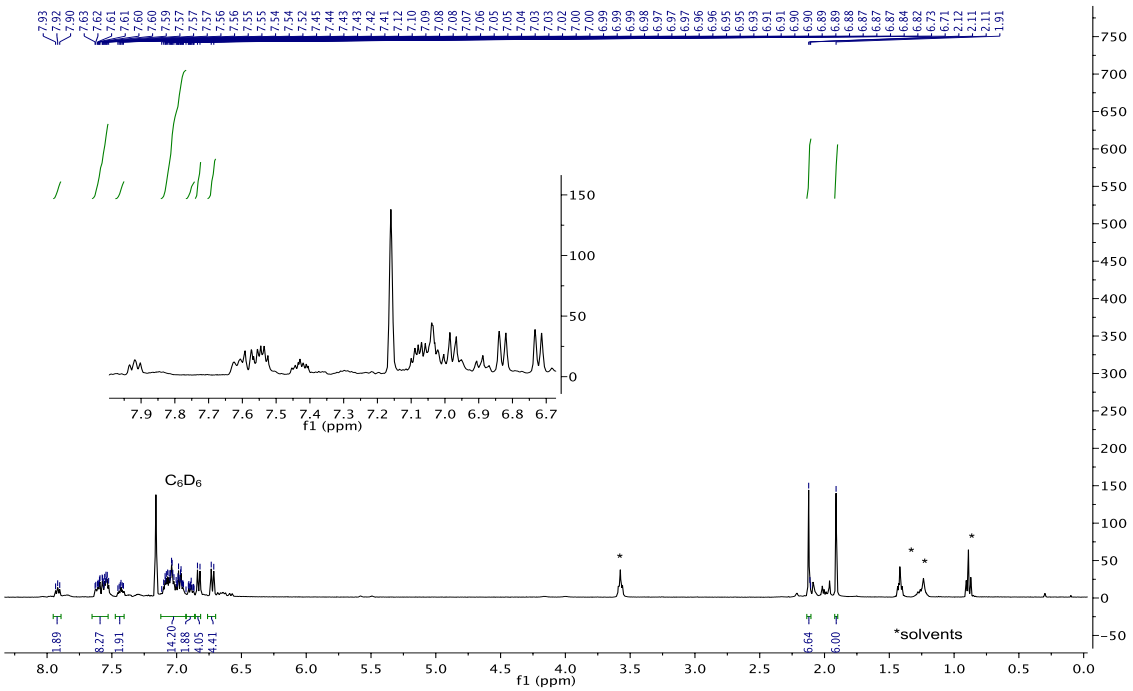


Figure S76. ^{1}H NMR (C_6D_6) of [(p-tol**L2**)Ni(DC≡CPh)], showing the disappearance of the doublet of triplet a 6.30 ppm.

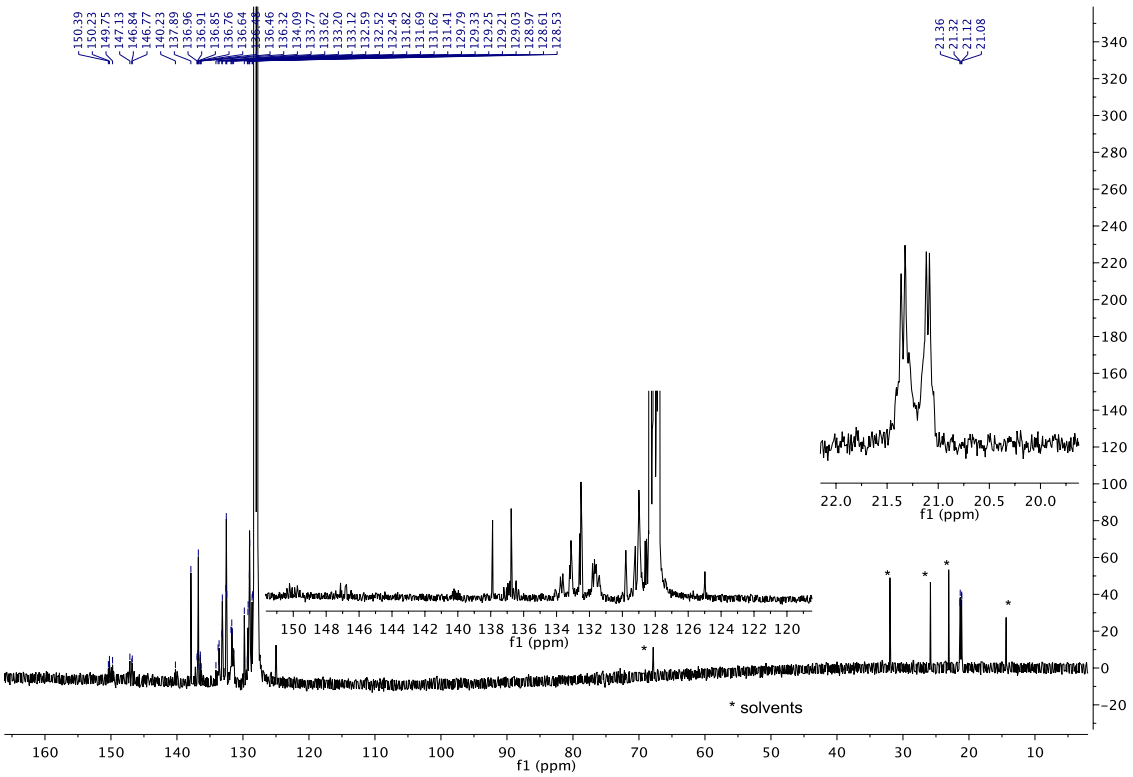


Figure S77. ^{13}C NMR (C_6D_6) of [(p-tol**L2**)Ni(DC≡CPh).

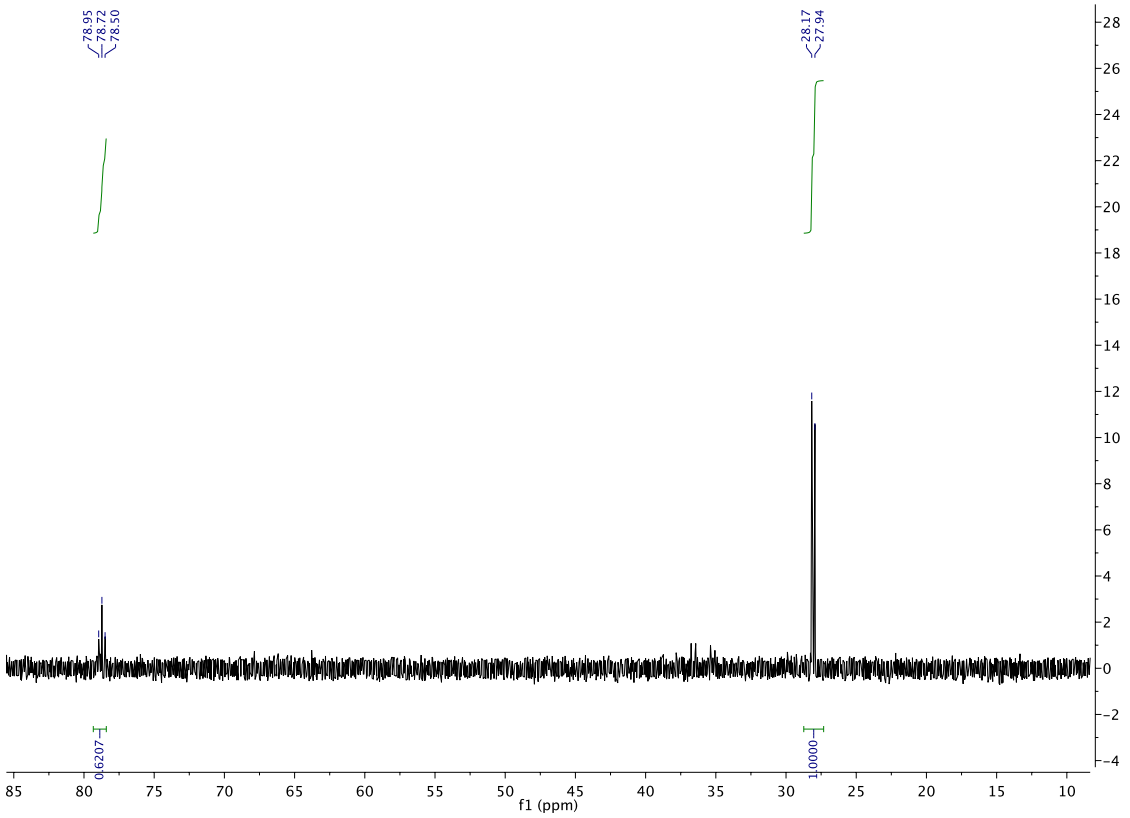


Figure S78. ^{31}P NMR (C_6D_6) of [($^{p\text{-tol}}$**L2**)Ni(DC≡CPh).

[(^{Ph}L3)Ni(HC≡CPh)] (^{Ph}6-Ph)

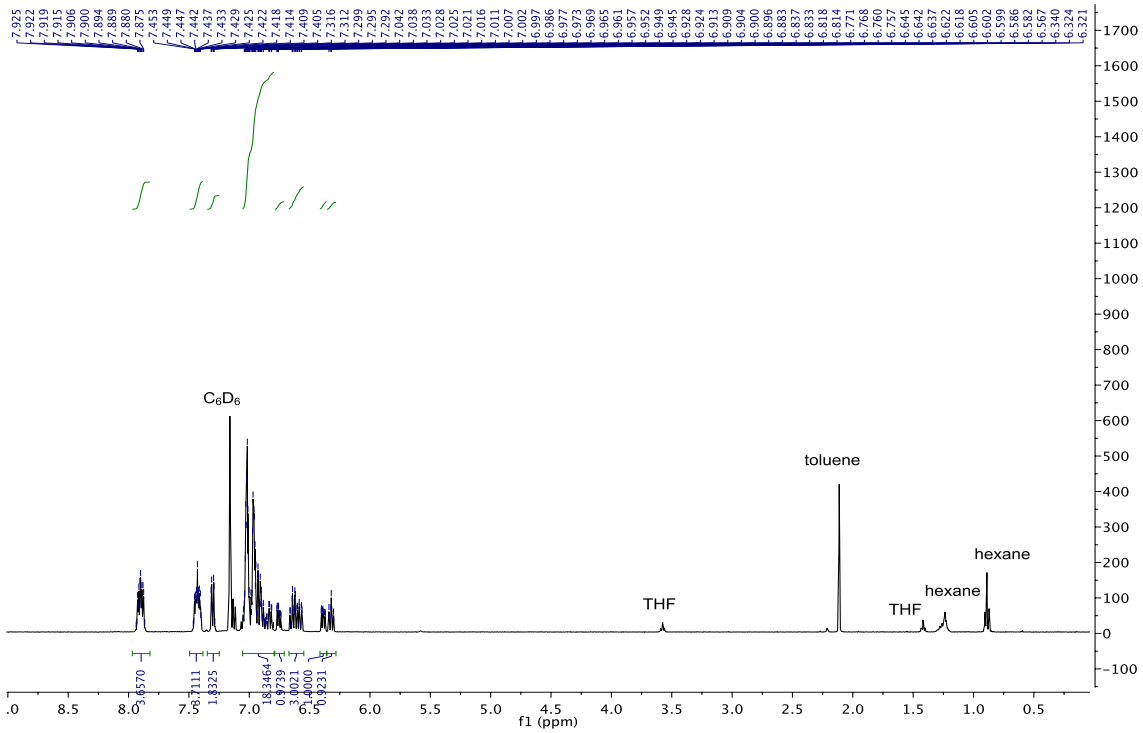


Figure S79. ^{1}H NMR (C_6D_6) of [(^{Ph}**L3**)Ni(HC≡CPh)] (^{Ph}**6-Ph**).

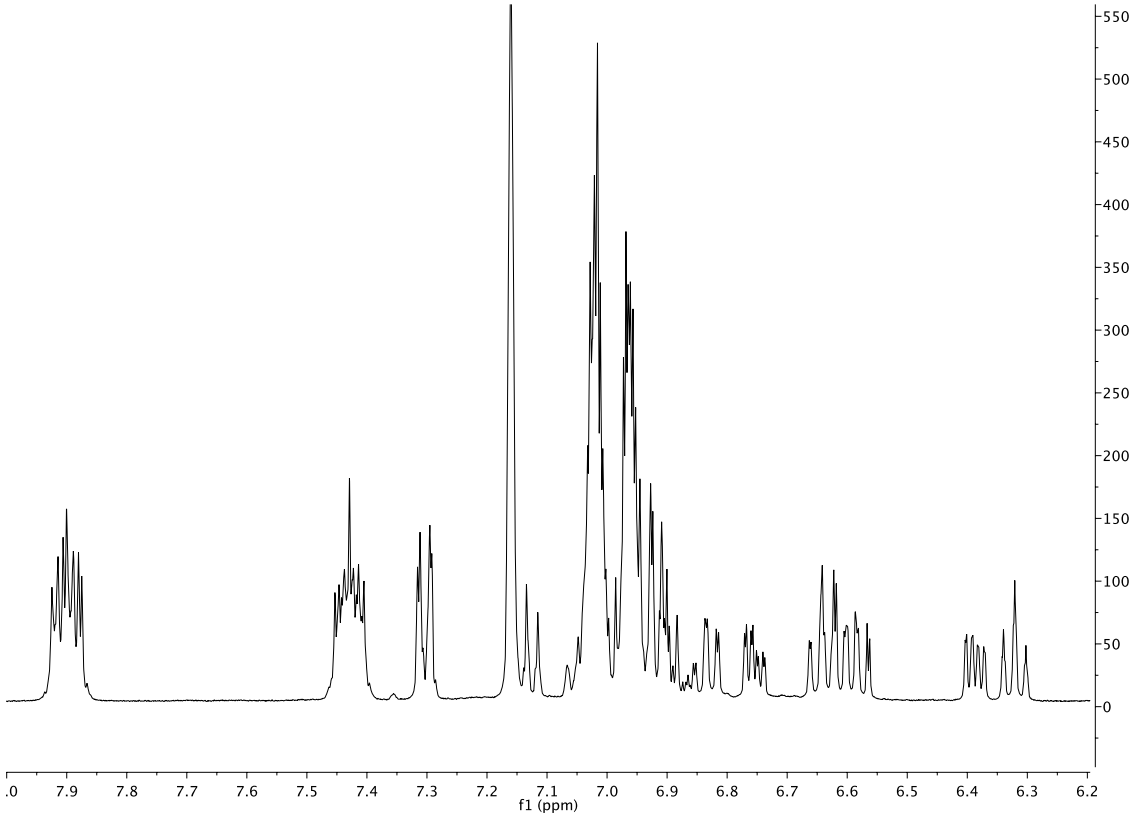


Figure S80. ^{1}H NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**). Zoom in the aromatic region.

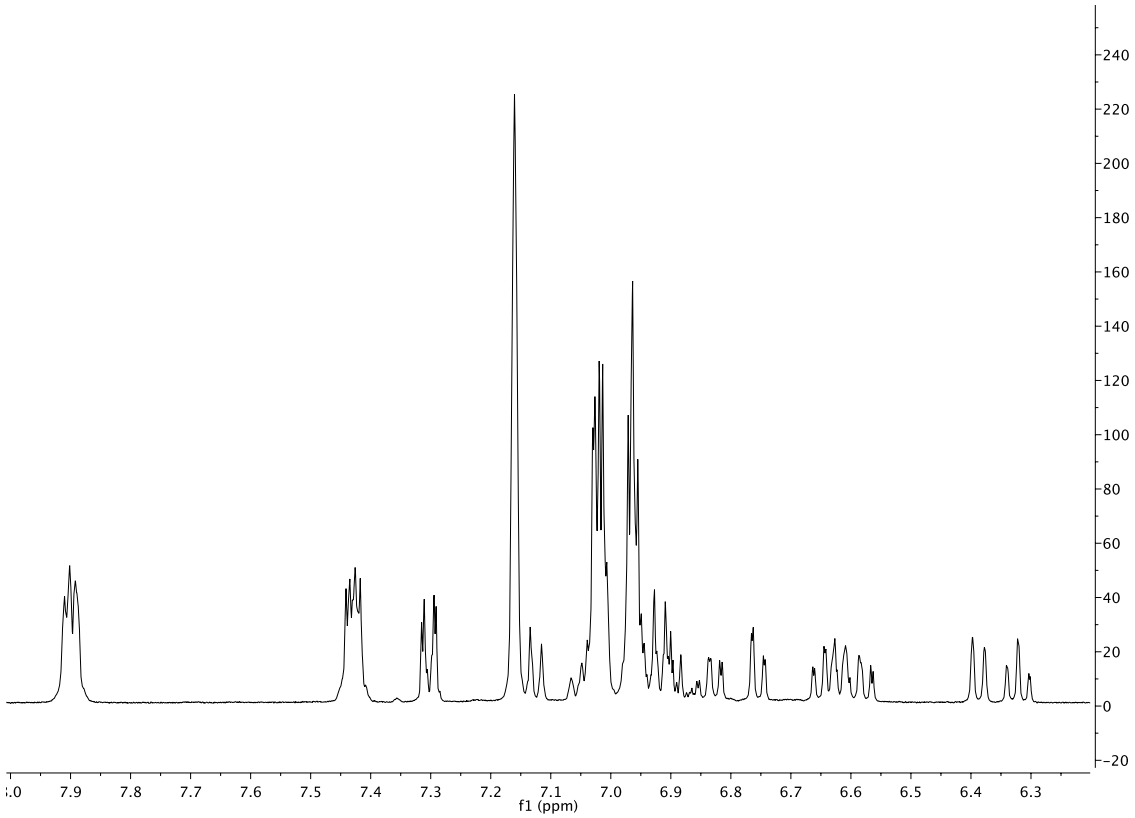


Figure S81. $^{1}H\{^{31}P\}$ NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**). Zoom in the aromatic region.

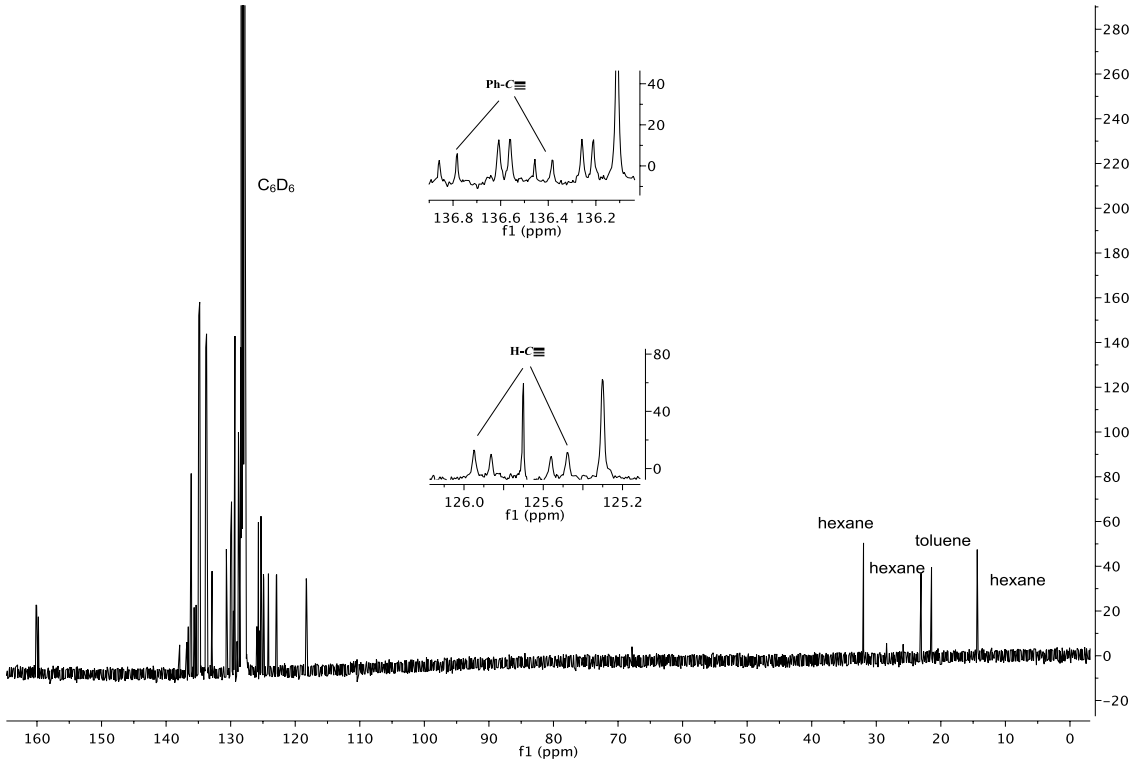


Figure S82. ^{13}C NMR (C_6D_6) of [(^{Ph}L3)Ni(HC≡CPh)] (**^{Ph}6-Ph**).

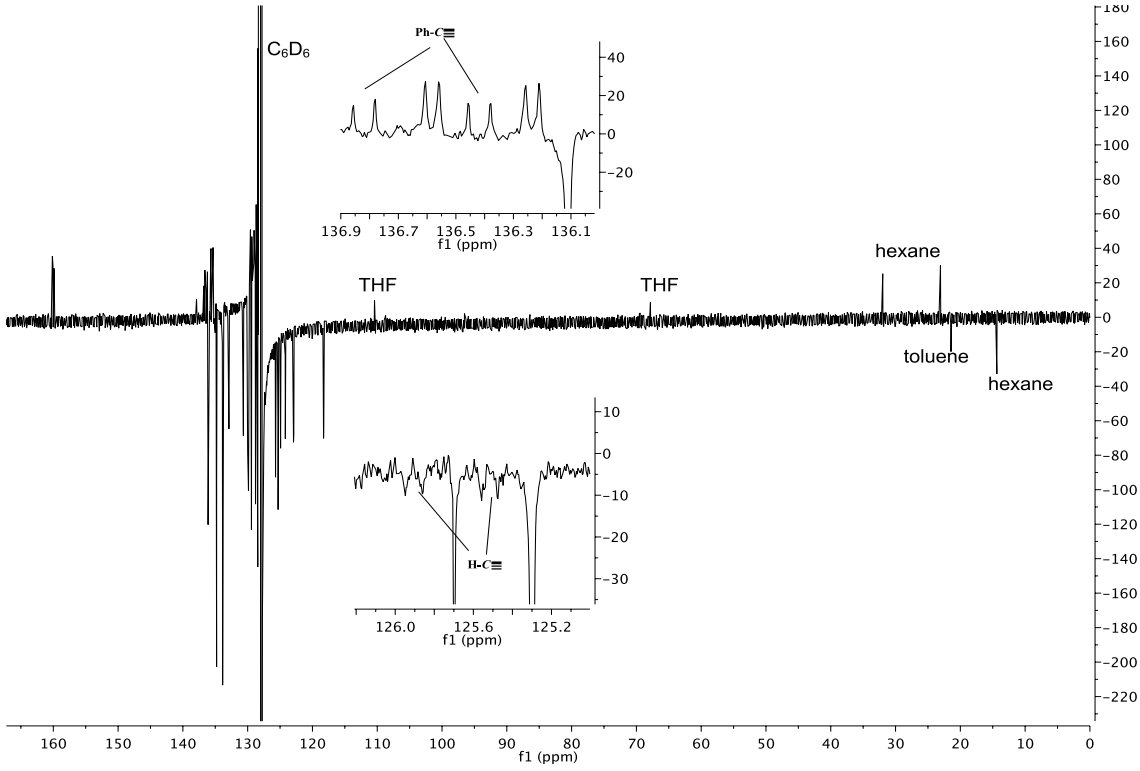


Figure S83. APT ^{13}C NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**).

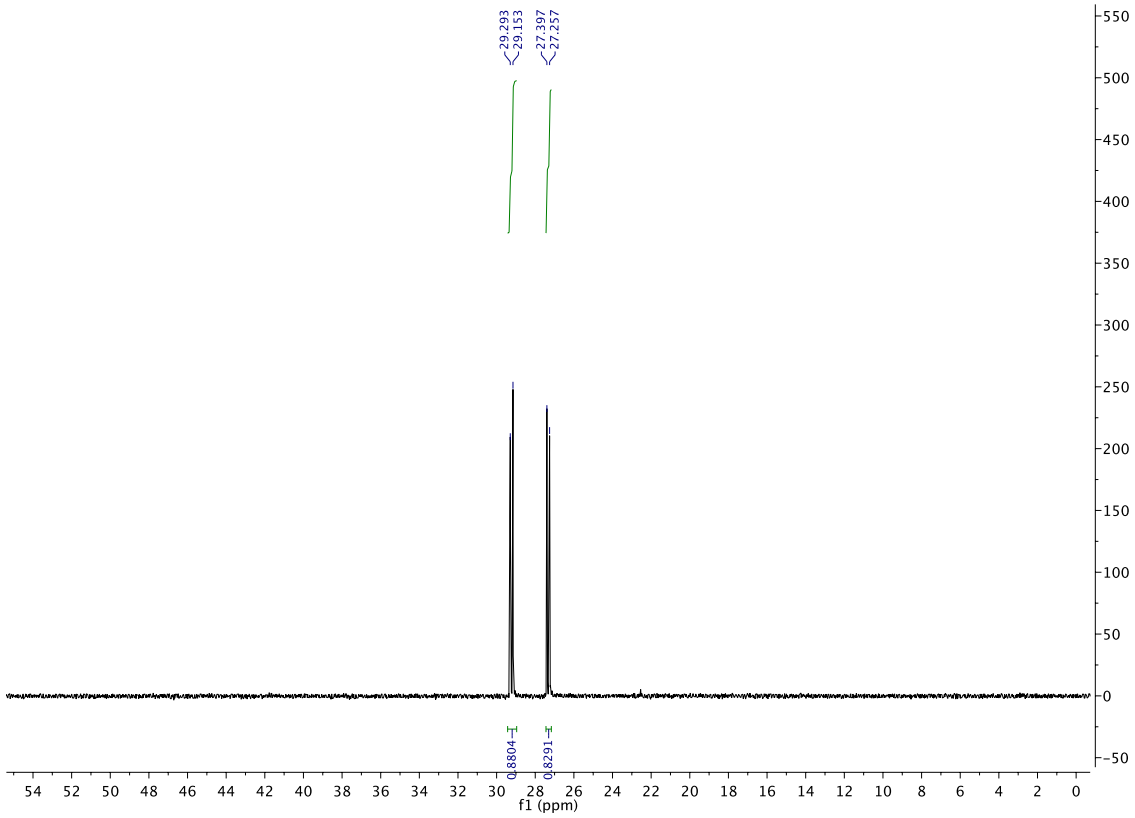


Figure S84. ^{31}P NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**).

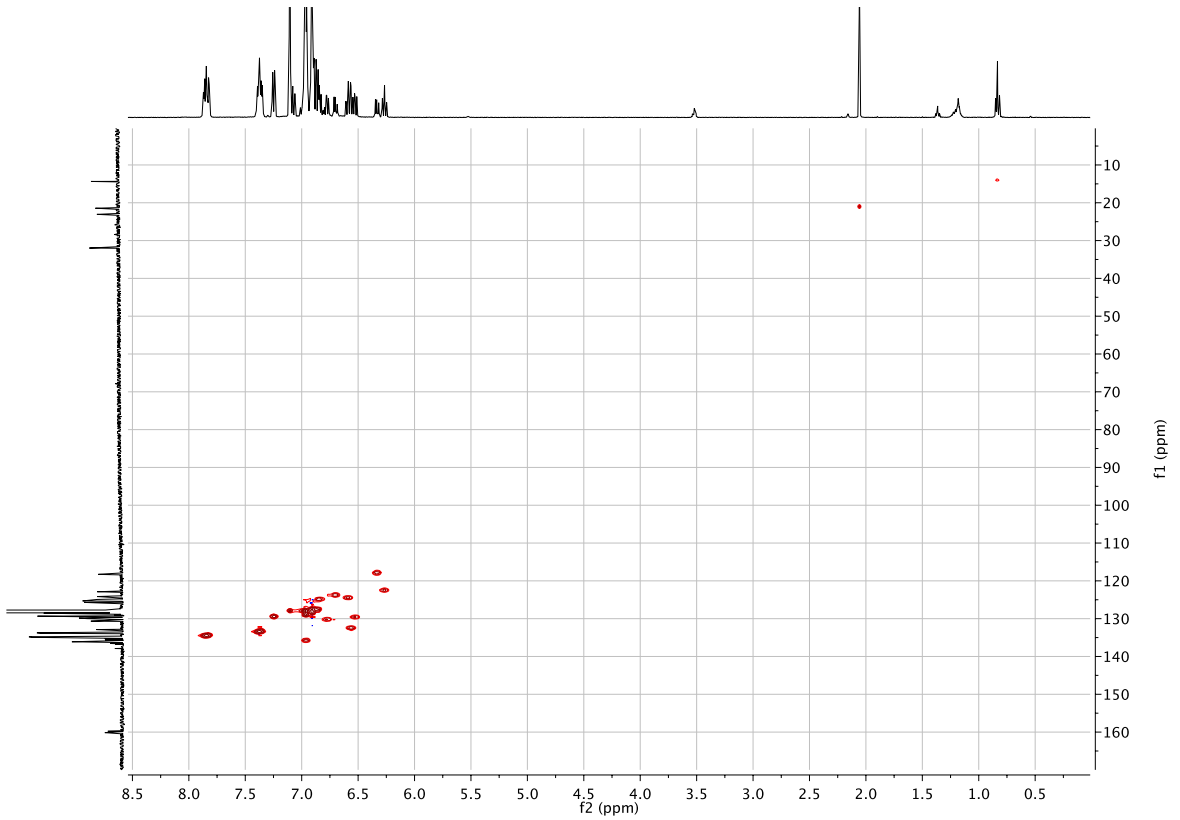


Figure S85. HMQC (^{1}H-^{13}C) 2D NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**).

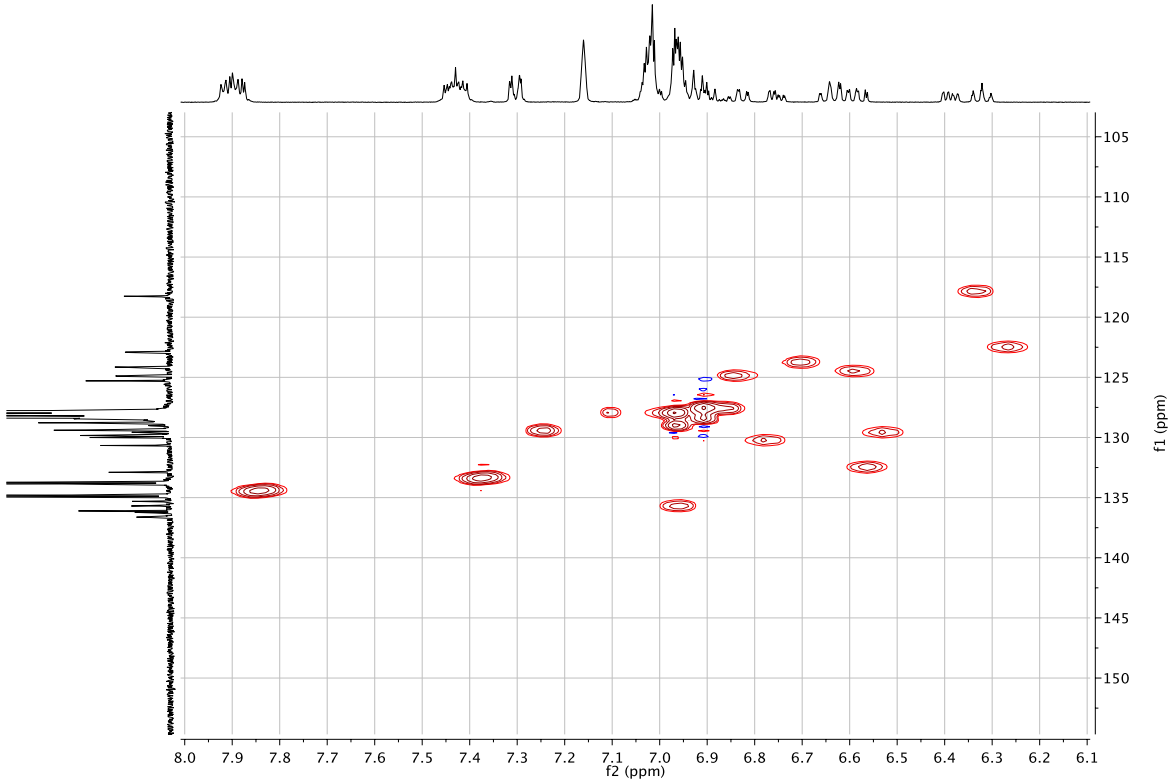


Figure S86. HMQC (^{1}H-^{13}C) 2D NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**). Zoom in the aromatic and alkyne region.

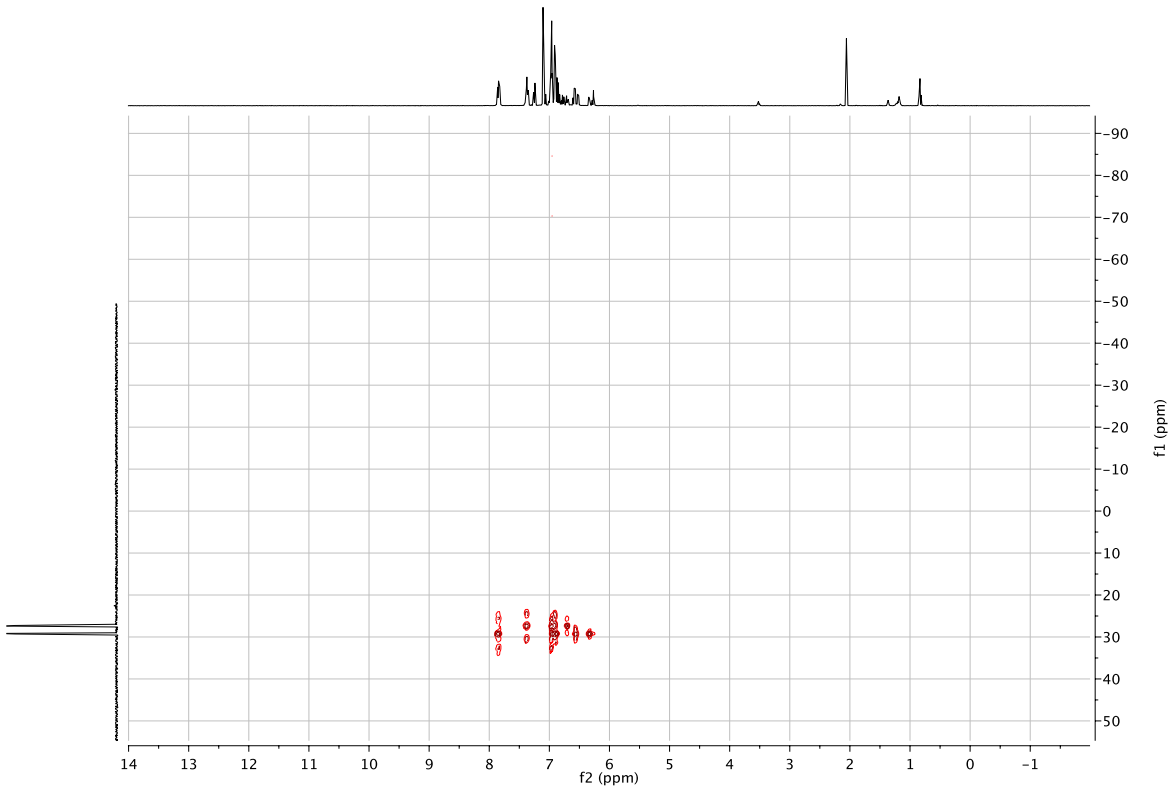


Figure S87. HMBC (^{1}H-^{31}P) 2D NMR (C_6D_6) of [(**^{Ph}L3**)Ni(HC≡CPh)] (**^{Ph}6-Ph**).

[(^{Ph}L3)Ni(DC≡CPh)]

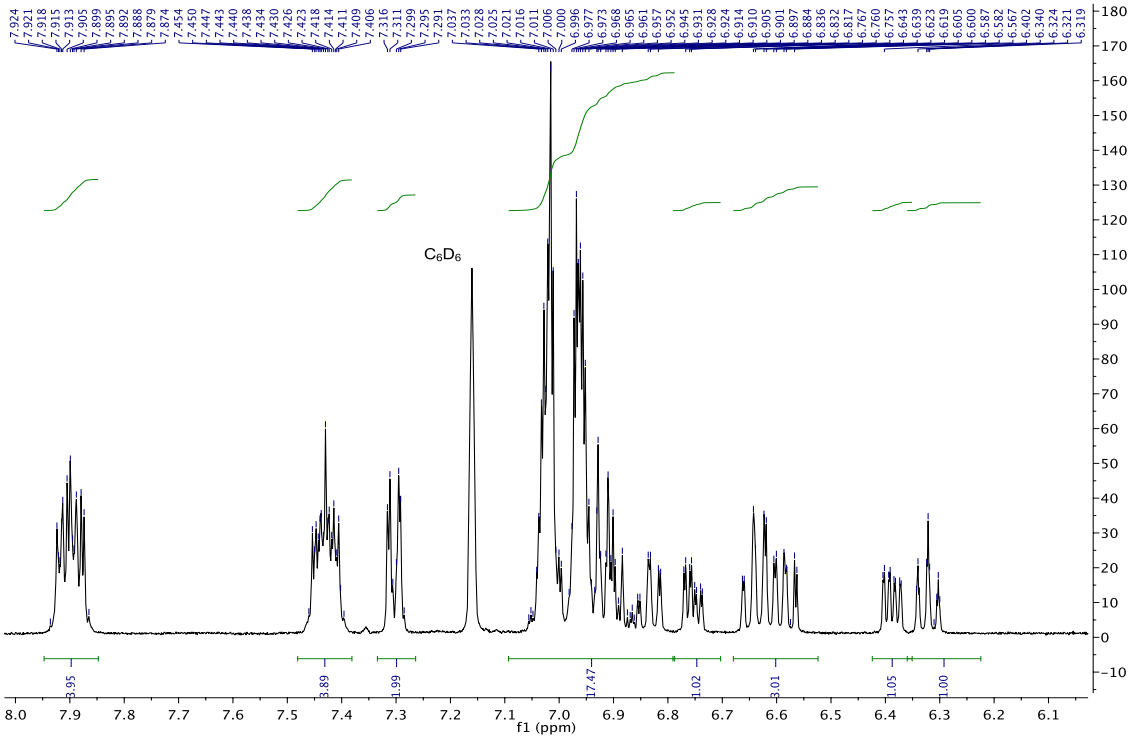


Figure S88. ^{1}H NMR (C_6D_6) of [(^{Ph}**L3**)Ni(DC≡CPh)]

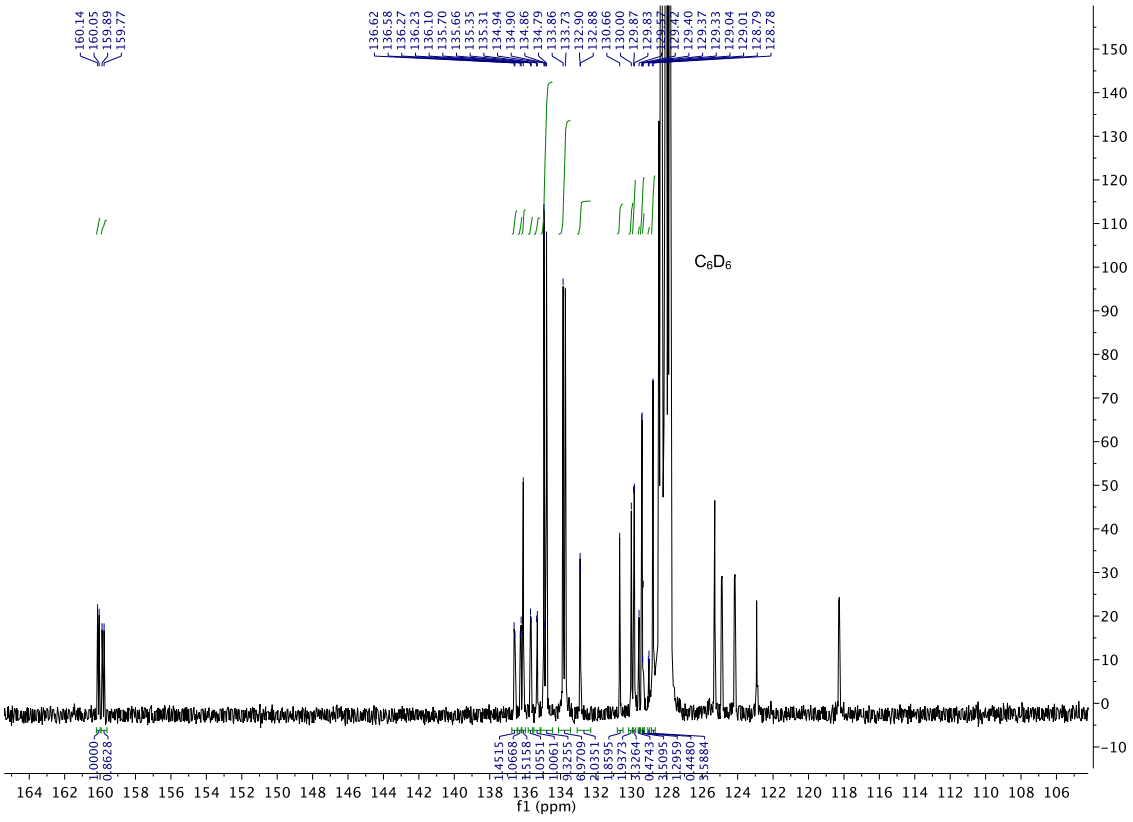


Figure S89. ^{13}C NMR (C_6D_6) of [(^{Ph}**L3**)Ni(DC≡CPh)].

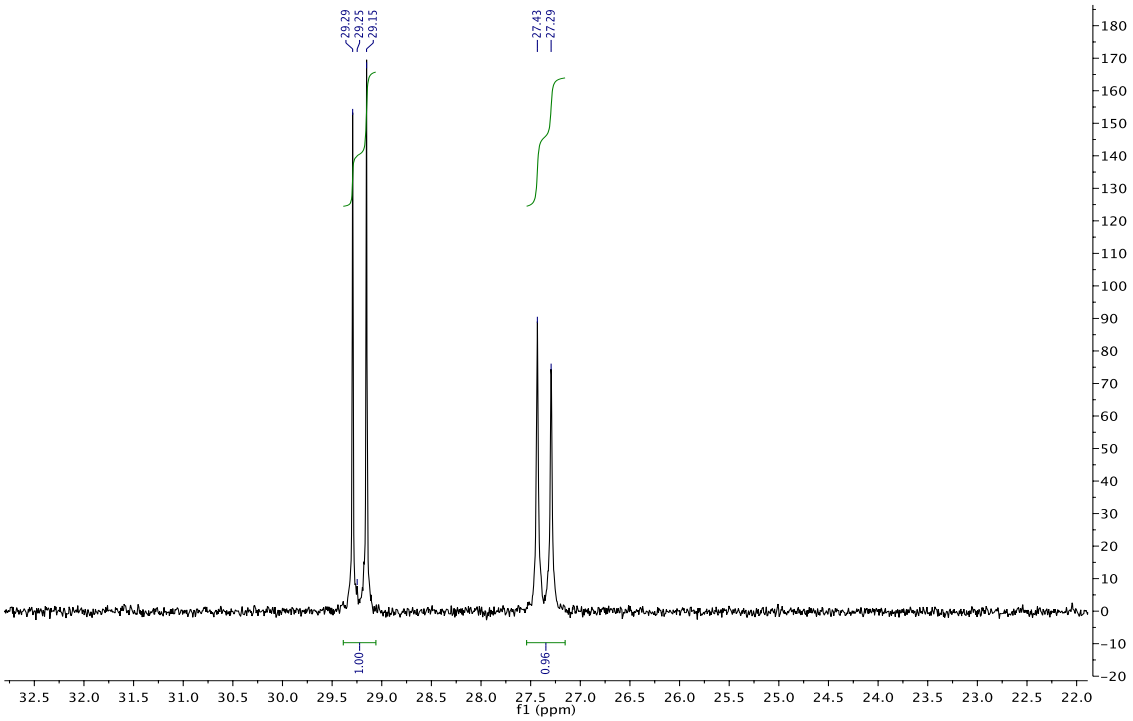


Figure S90. ^{31}P NMR (C_6D_6) of [(^{Ph}**L3**)Ni(DC≡CPh)].

In-situ **generation of [(^{Ph}L3)Ni(PhC≡CPh)] from the reaction of ^{Ph}L3 + Ni(cod)$_2$ + diphenylacetylene.**

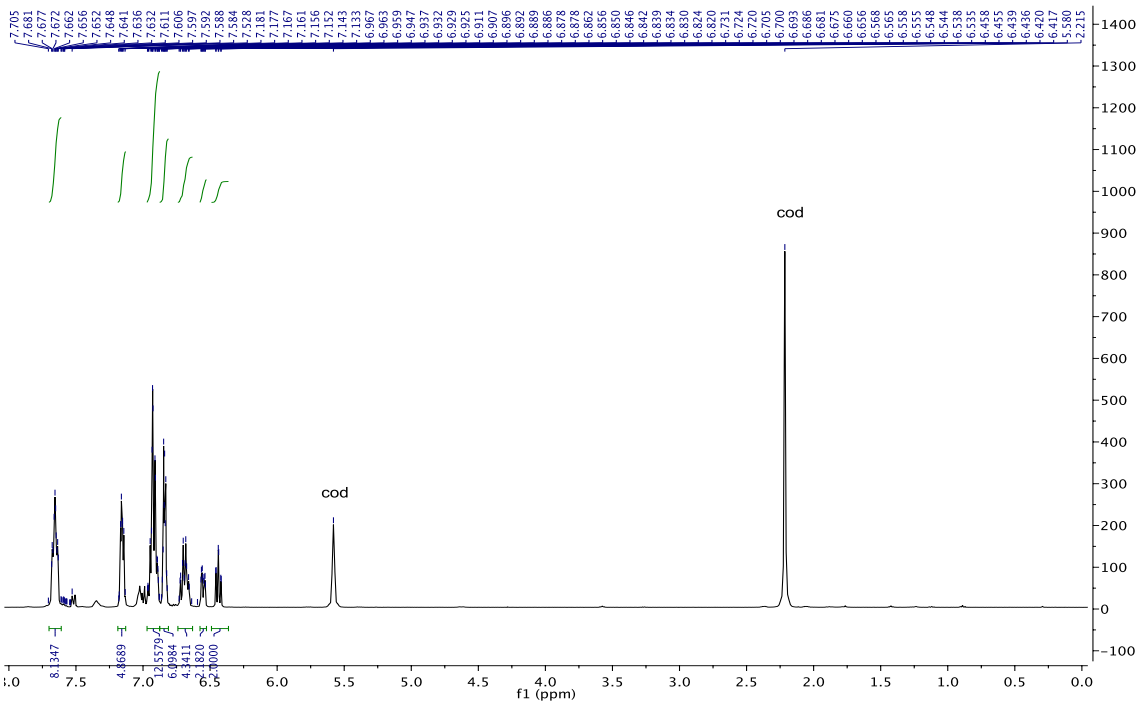


Figure S91. *In-situ* ^{1}H NMR (C_6D_6) of [(^{Ph}**L3**)Ni(PhC≡CPh)] from the reaction of ^{Ph}**L3** + Ni(cod)$_2$ + diphenylacetylene. The small peaks at 7.03 and 7.53 ppm correspond to an excess of free diphenylacetylene.

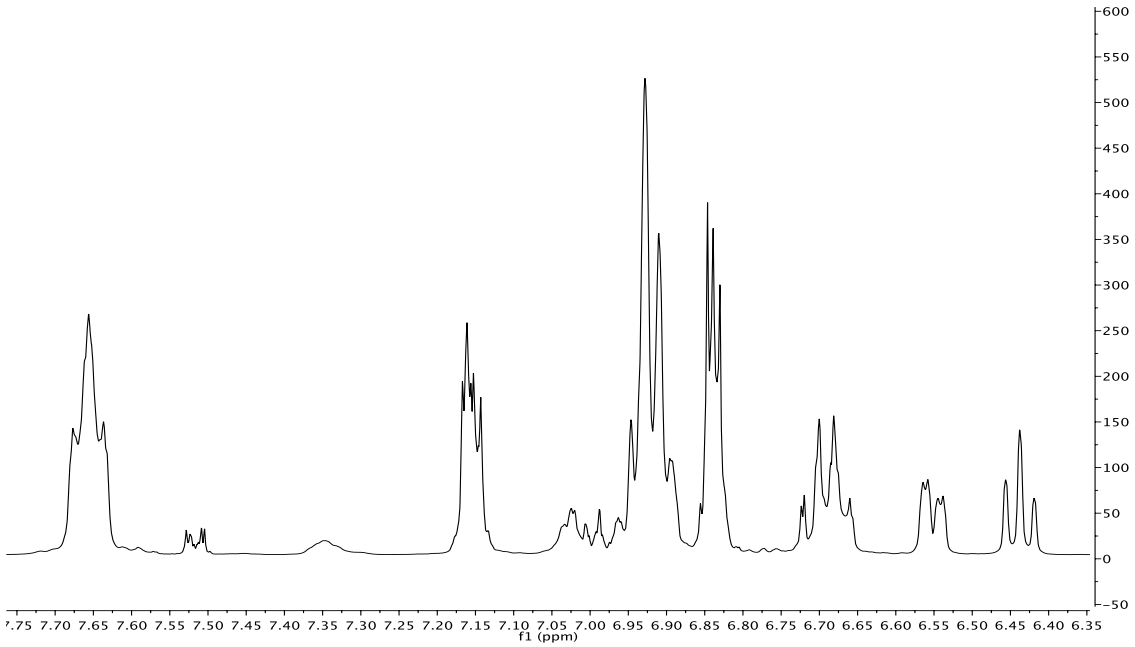


Figure S92. *In-situ* ^{1}H NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene. Zoom in the aromatic region. The small peaks at 7.03 and 7.53 ppm correspond to an excess of free diphenylacetylene.

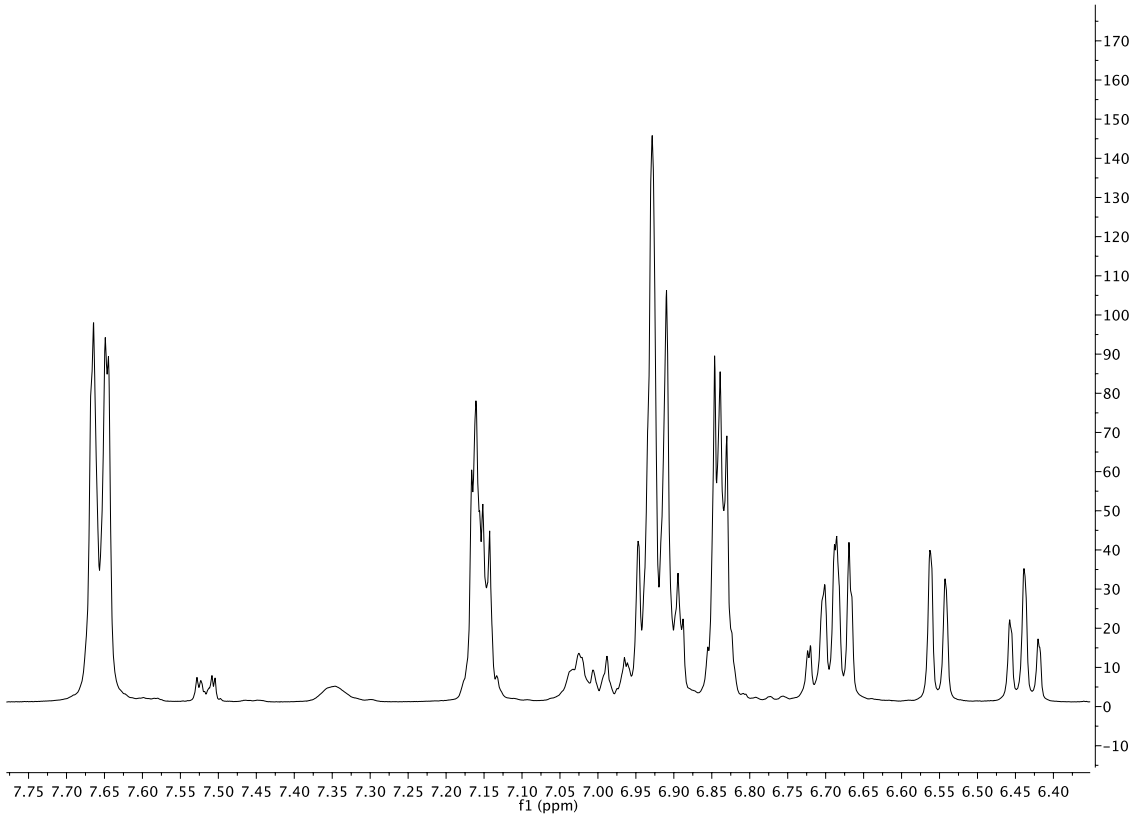


Figure S93. *In-situ* ^{1}H $\{^{31}P\}$ NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene. Zoom in the aromatic region. The small peaks at 7.03 and 7.53 ppm correspond to an excess of free diphenylacetylene.

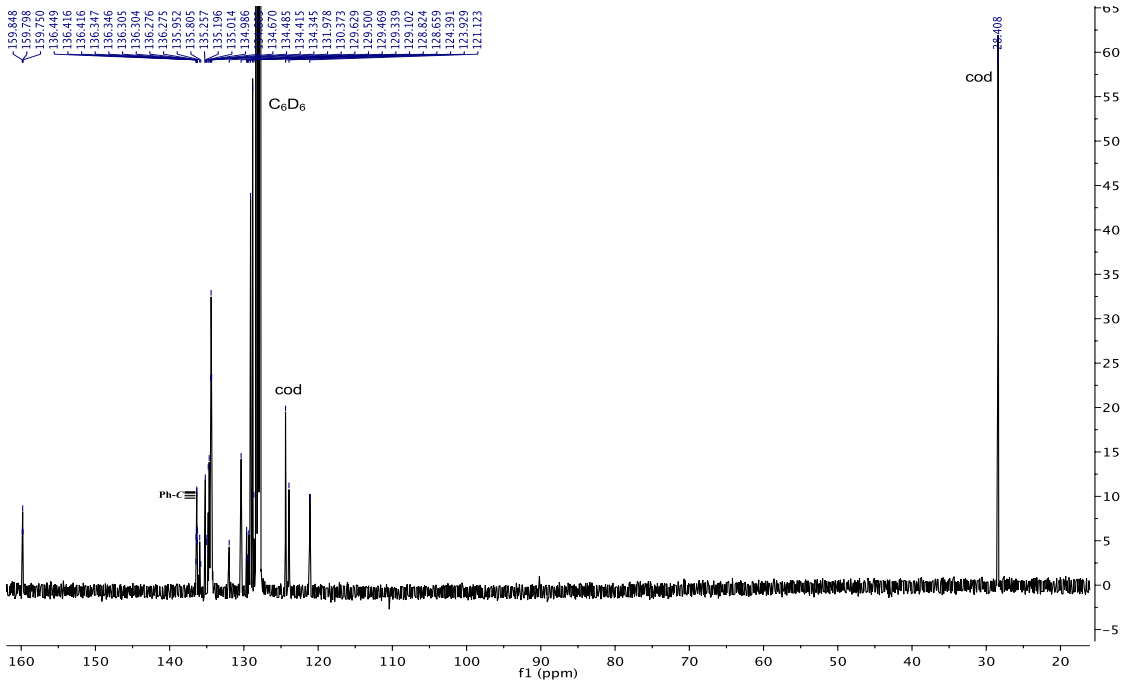


Figure S94. *In-situ* ^{13}C NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene.

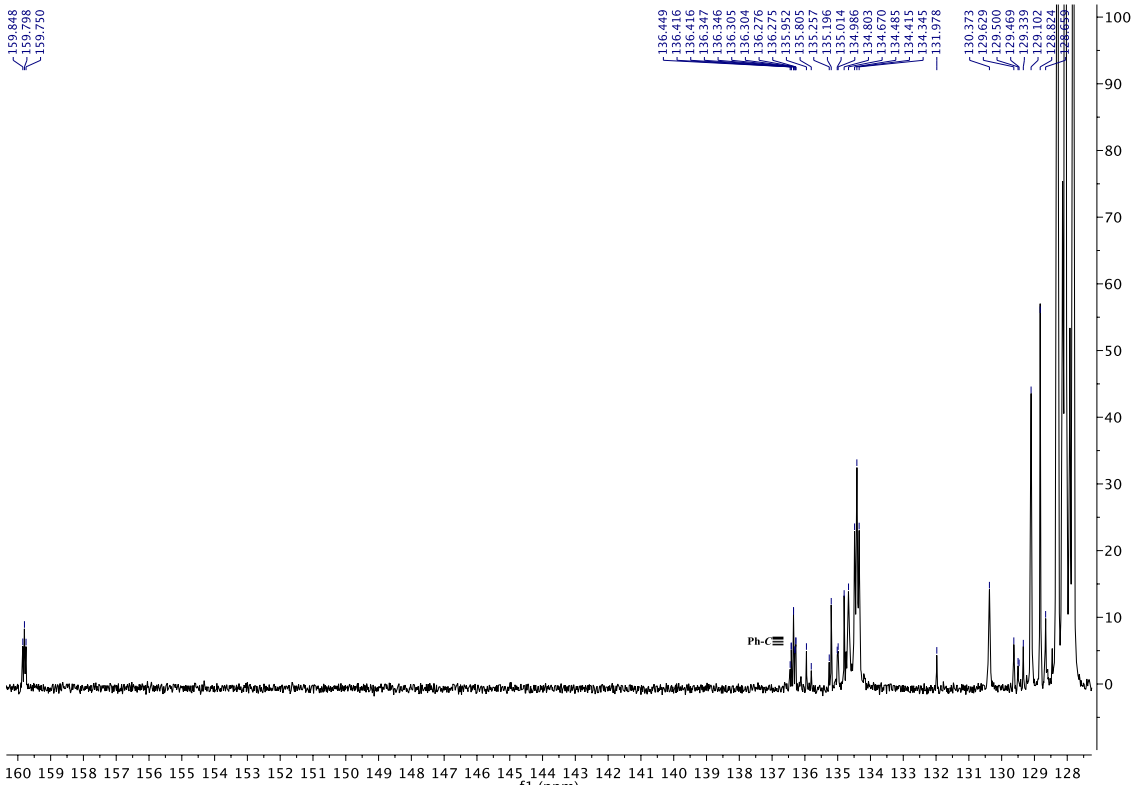


Figure S95. *In-situ* ^{13}C-NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene. Zoom in the aromatic and alkyne region.

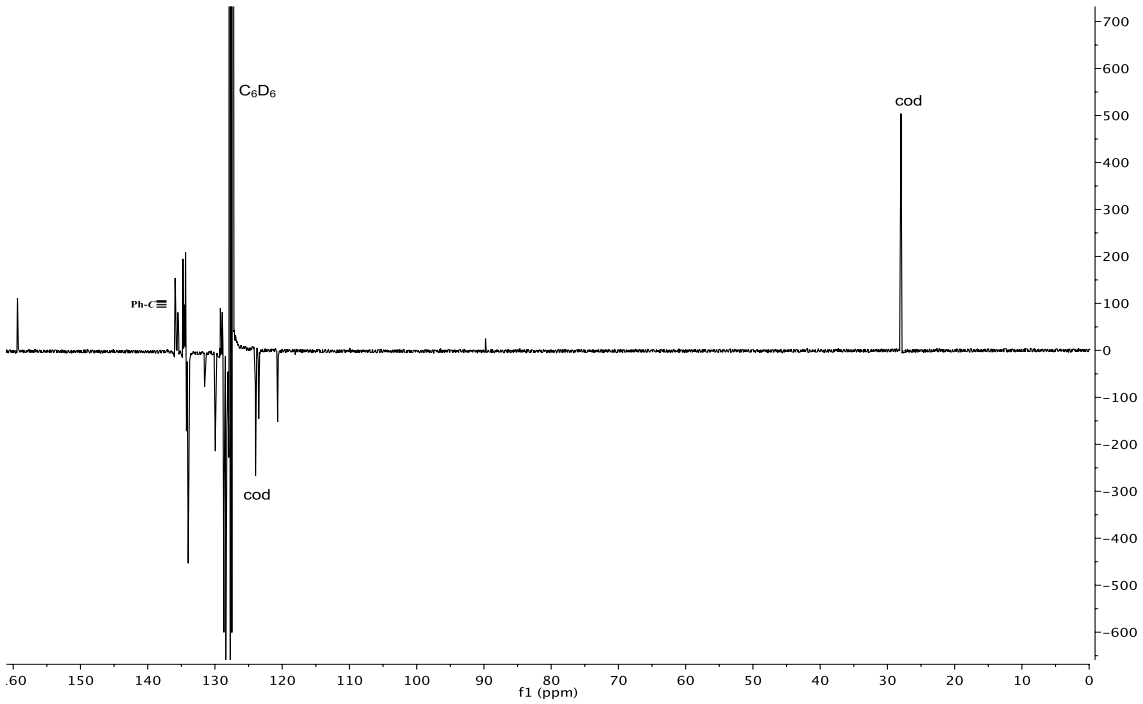


Figure S96. *In-situ* APT ^{13}C-NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene.

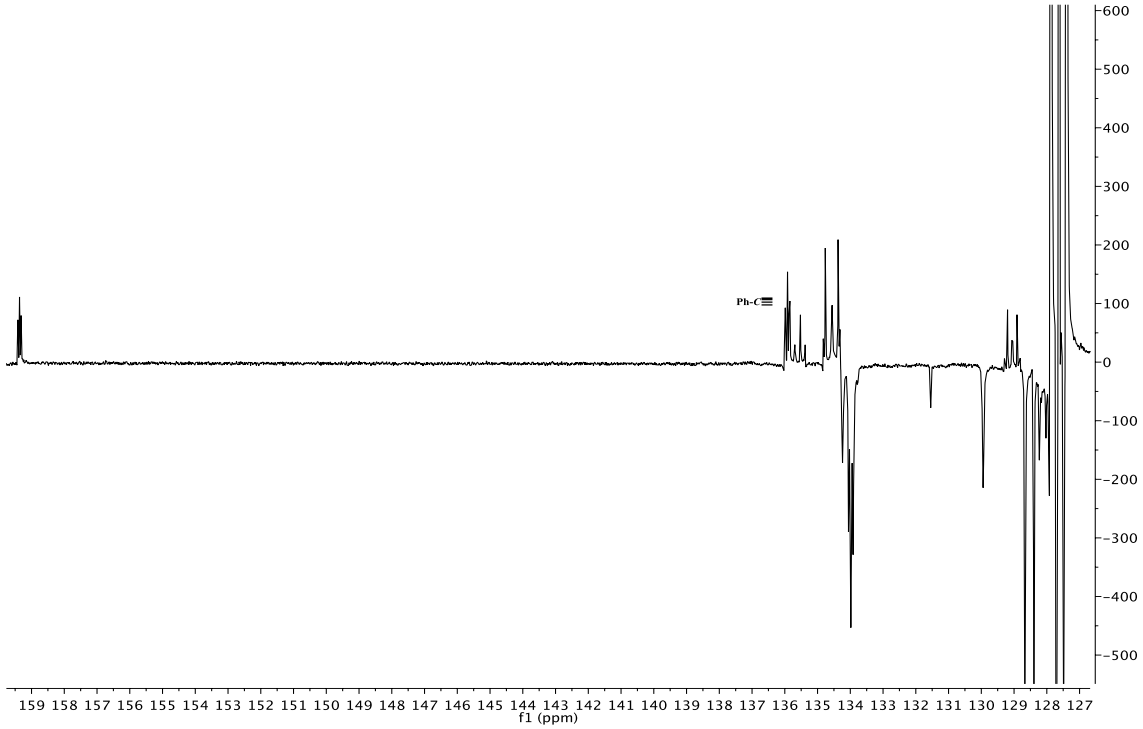


Figure S97. *In-situ* APT ^{13}C NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene. Zoom in the aromatic and alkyne region.

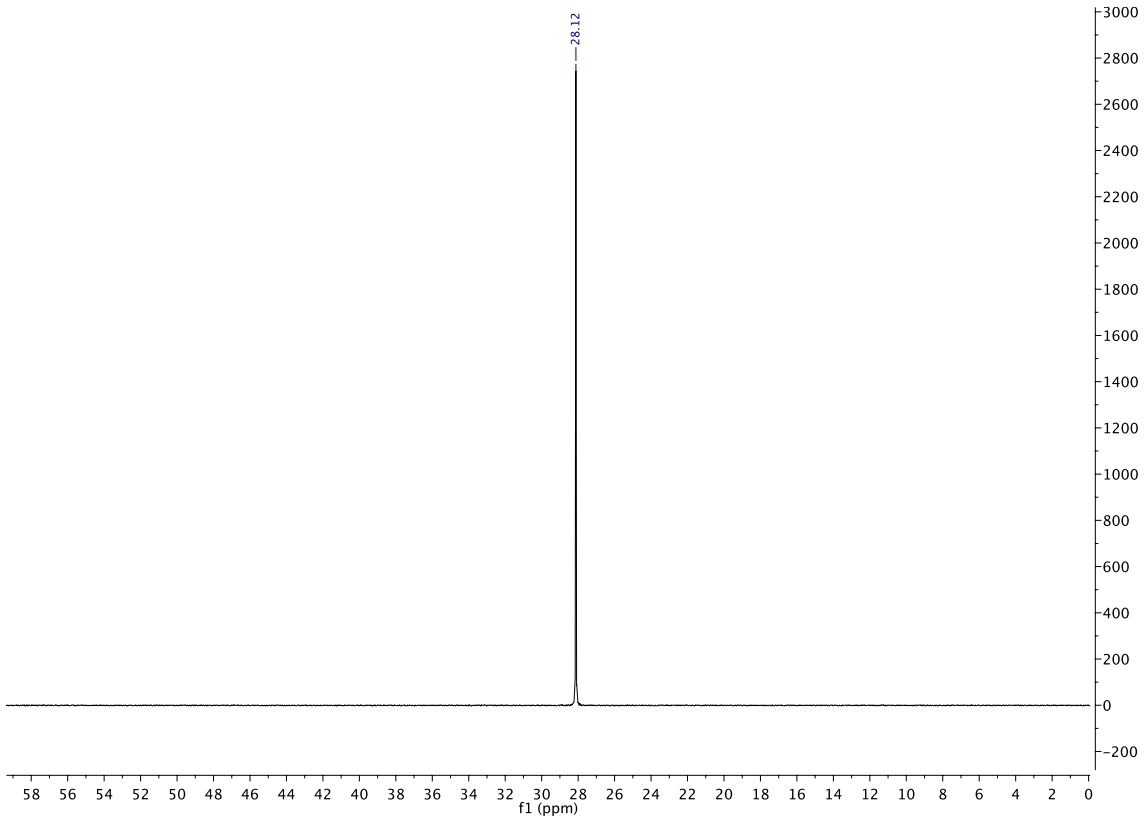


Figure S98. *In-situ* ^{31}P-NMR (C_6D_6) of [(**^{Ph}L3**)Ni(PhC≡CPh)] from the reaction of **^{Ph}L3** + $Ni(cod)_2$ + diphenylacetylene.

6. ATR-IR of isolated complexes

bis(2-di(*para*-tolyl)phosphinophenyl) phenylphosphine ($^{p\text{-tol}}$L2)

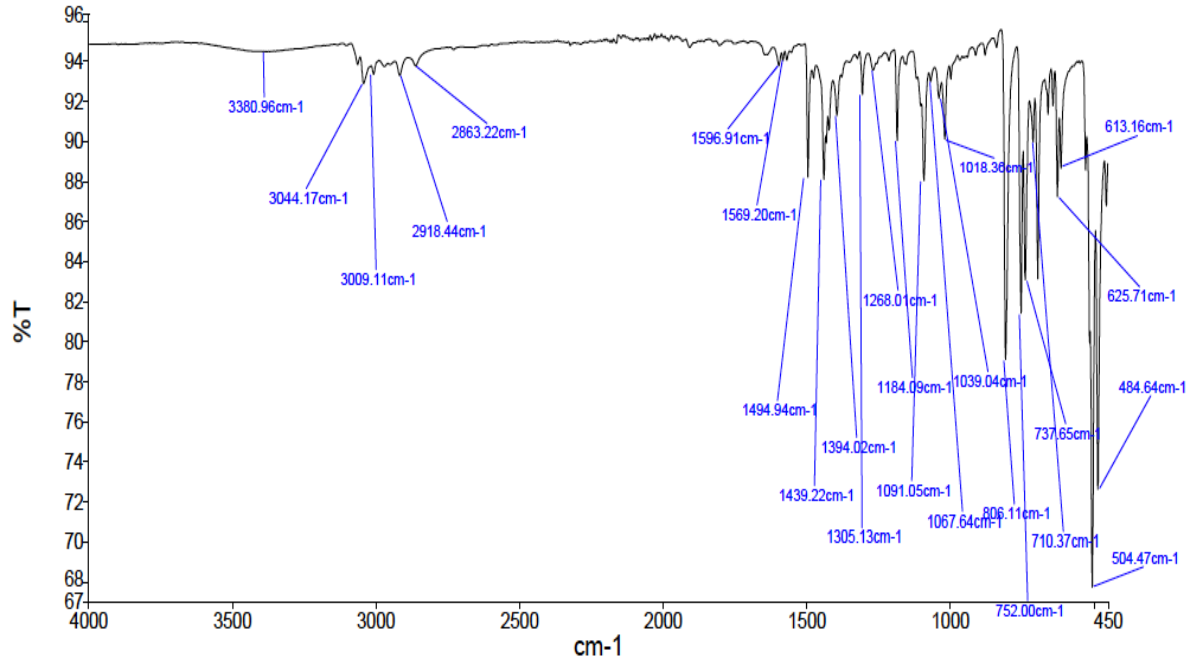


Figure S99. ATR-IR of bis(2-di(*para*-tolyl)phosphinophenyl) phenylphosphine ($^{p\text{-tol}}$**L2**).

[($^{p\text{-tol}}$L1)Ni(BPI)] ($^{p\text{-tol}}$1).

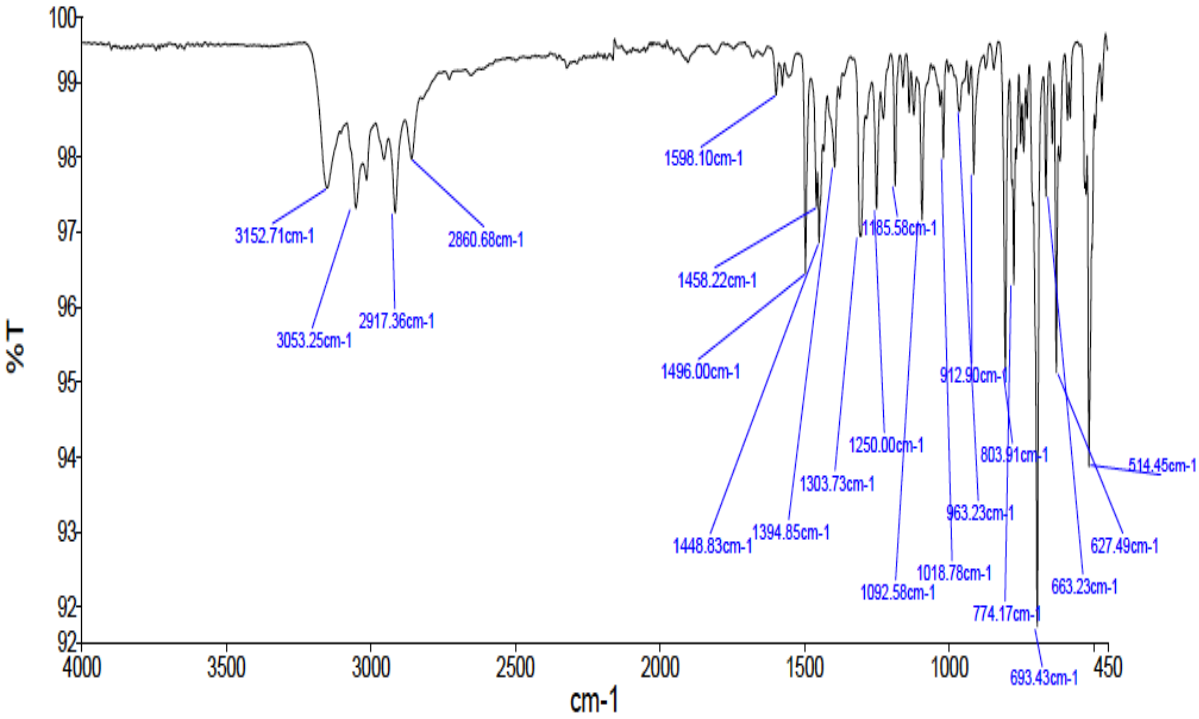


Figure S100. ATR-IR of [($^{p\text{-tol}}$**L1**)Ni(BPI)] ($^{p\text{-tol}}$**1**). BPI = benzophenone imine.

[(^{Ph}L1)Ni(BPI)] (^{Ph}1)

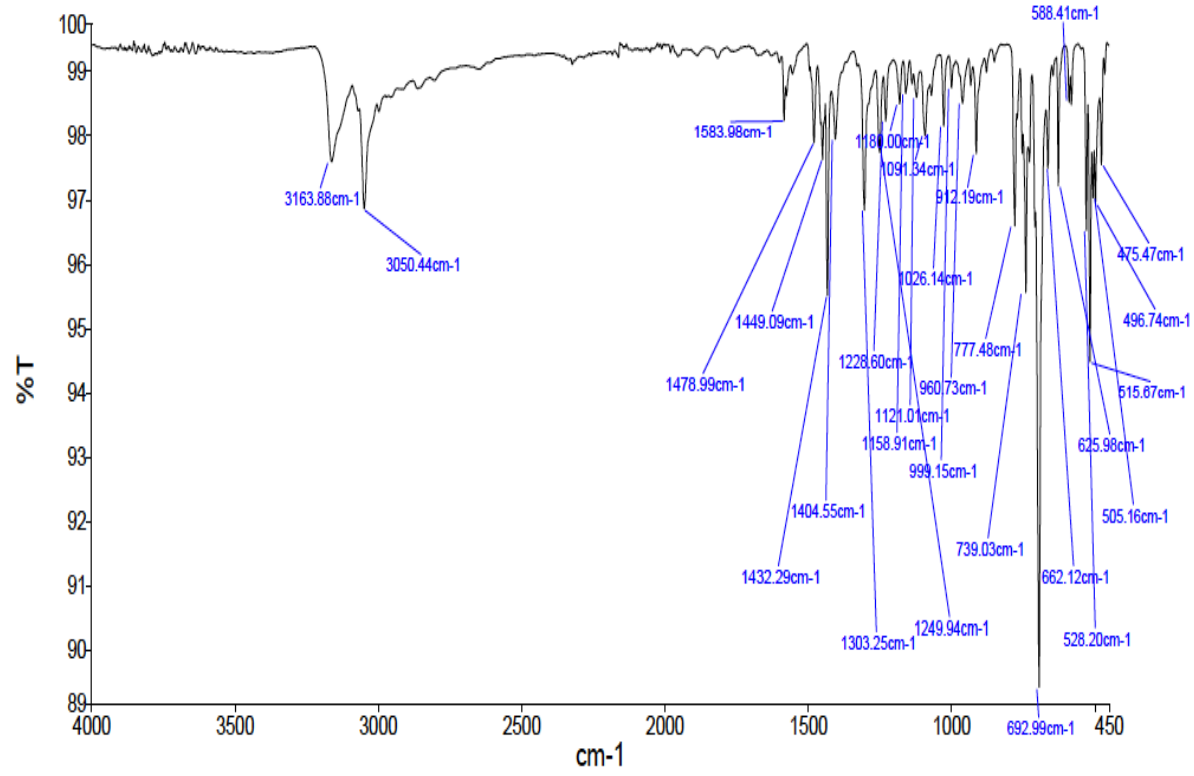


Figure S101. ATR-IR of [(^{Ph}**L1**)Ni(BPI)] (^{Ph}**1**). BPI = benzophenone imine.

[($^{p\text{-}tol}$L2)Ni(BPI)] ($^{p\text{-}tol}$2)

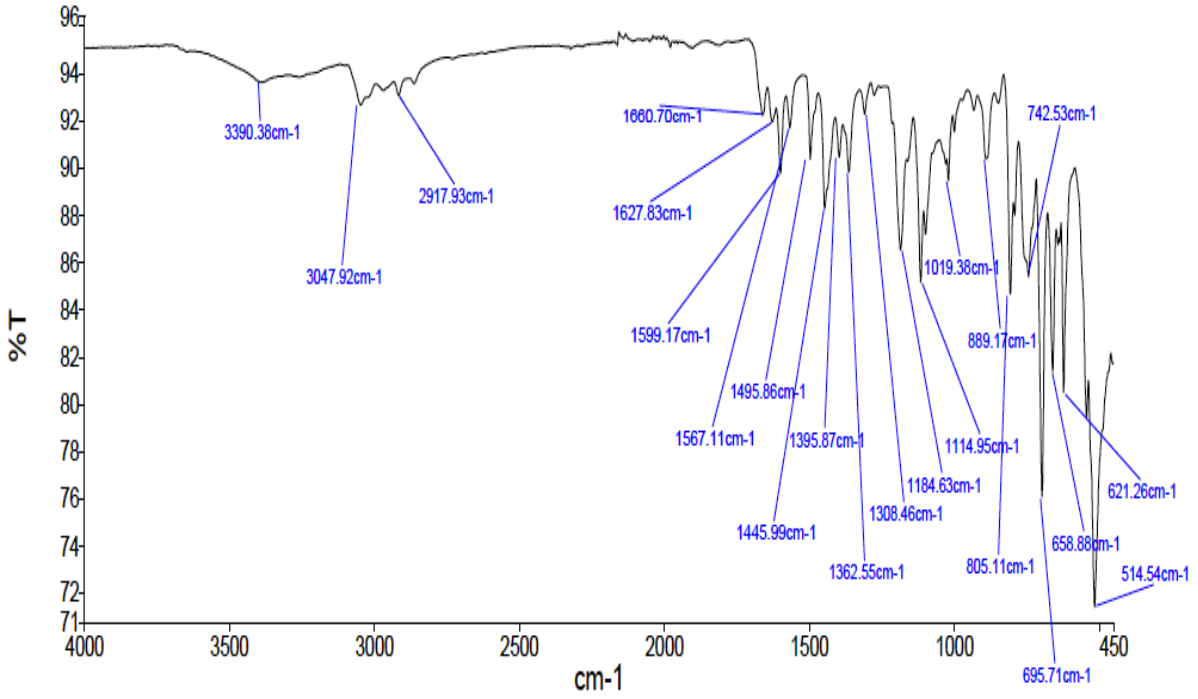


Figure S102. ATR-IR of [($^{p\text{-}tol}$**L2**)Ni(BPI)] ($^{p\text{-}tol}$**2**). BPI = benzophenone imine.

[(^{Ph}L3)Ni(BPI)] (^{Ph}3)

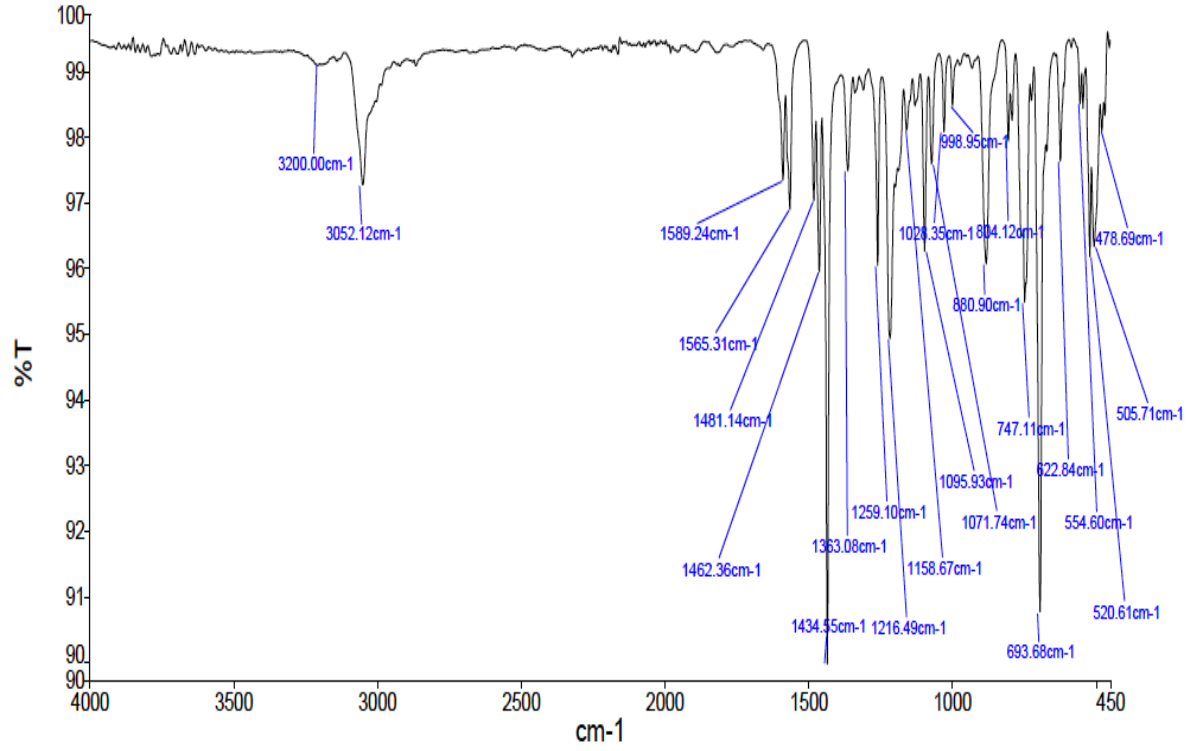


Figure S103. ATR-IR of [(^{Ph}L3)Ni(BPI)] (^{Ph}3). BPI = benzophenone imine.

[($^{p\text{-}tol}$L2)Ni(HC≡CPh)] ($^{p\text{-}tol}$5-Ph)

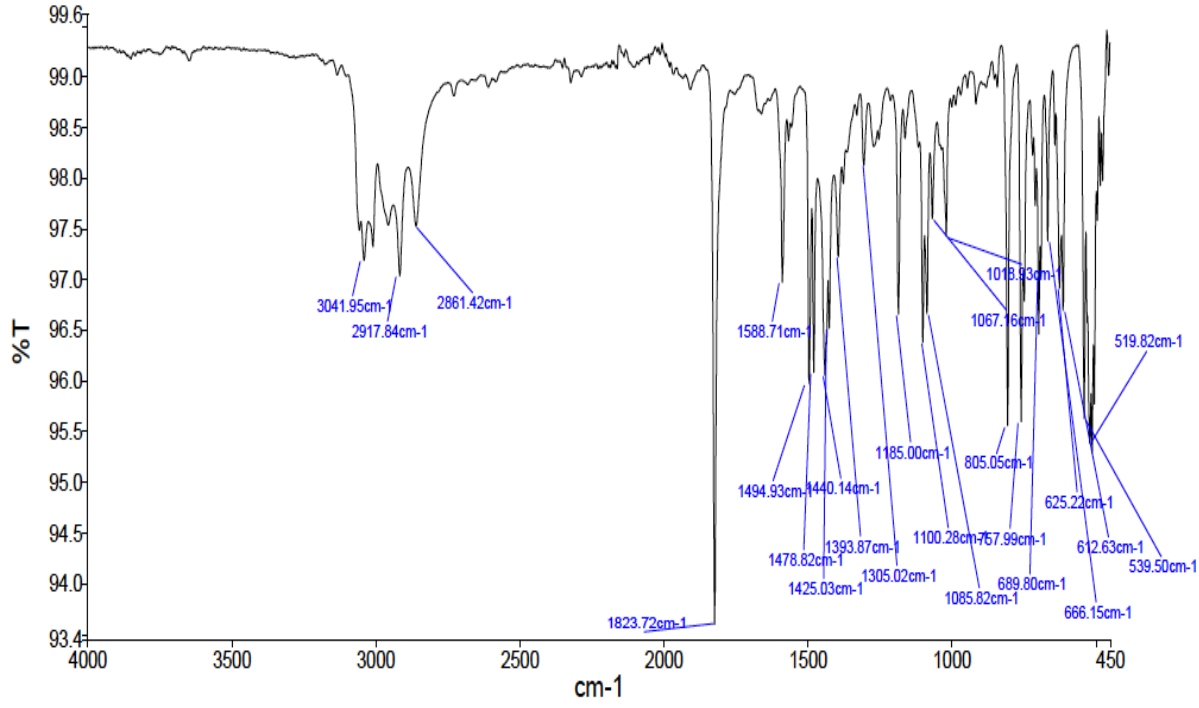


Figure S104. ATR-IR of [($^{p\text{-}tol}$L2)Ni(HC≡CPh)] ($^{p\text{-}tol}$5-Ph).

[($^{p\text{-tol}}$L2)Ni(DC≡CPh)]

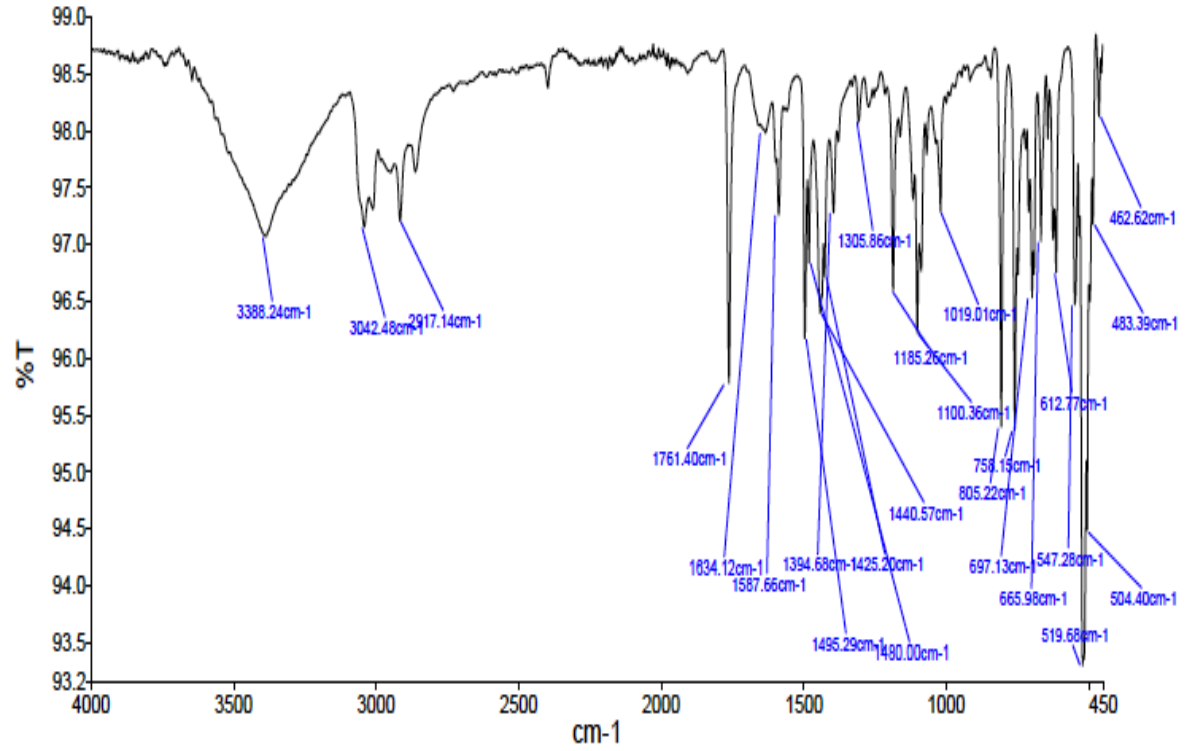


Figure S105. ATR-IR of [($^{p\text{-tol}}$**L2**)Ni(DC≡CPh)].

[(^{Ph}L3)Ni(HC≡CPh)] (^{Ph}6-Ph)

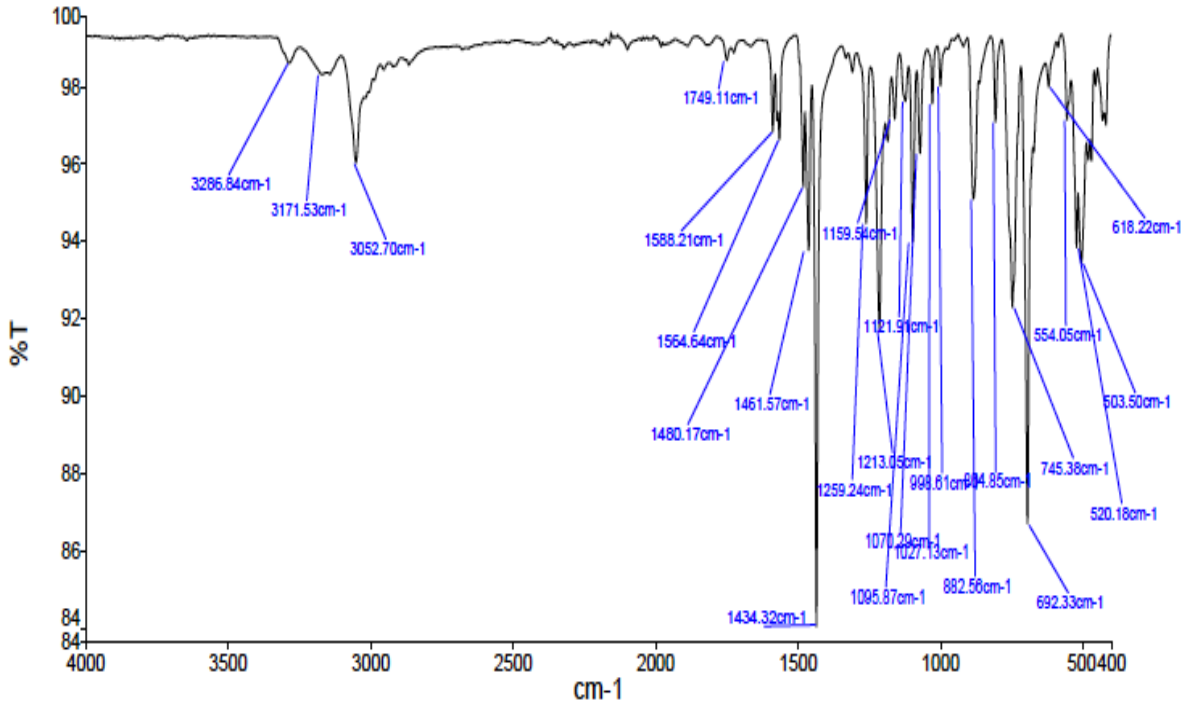


Figure S106. ATR-IR of [(^{Ph}**L3**)Ni(HC≡CPh)] (^{Ph}**6-Ph**).

[(^{Ph}L3)Ni(DC≡CPh)]

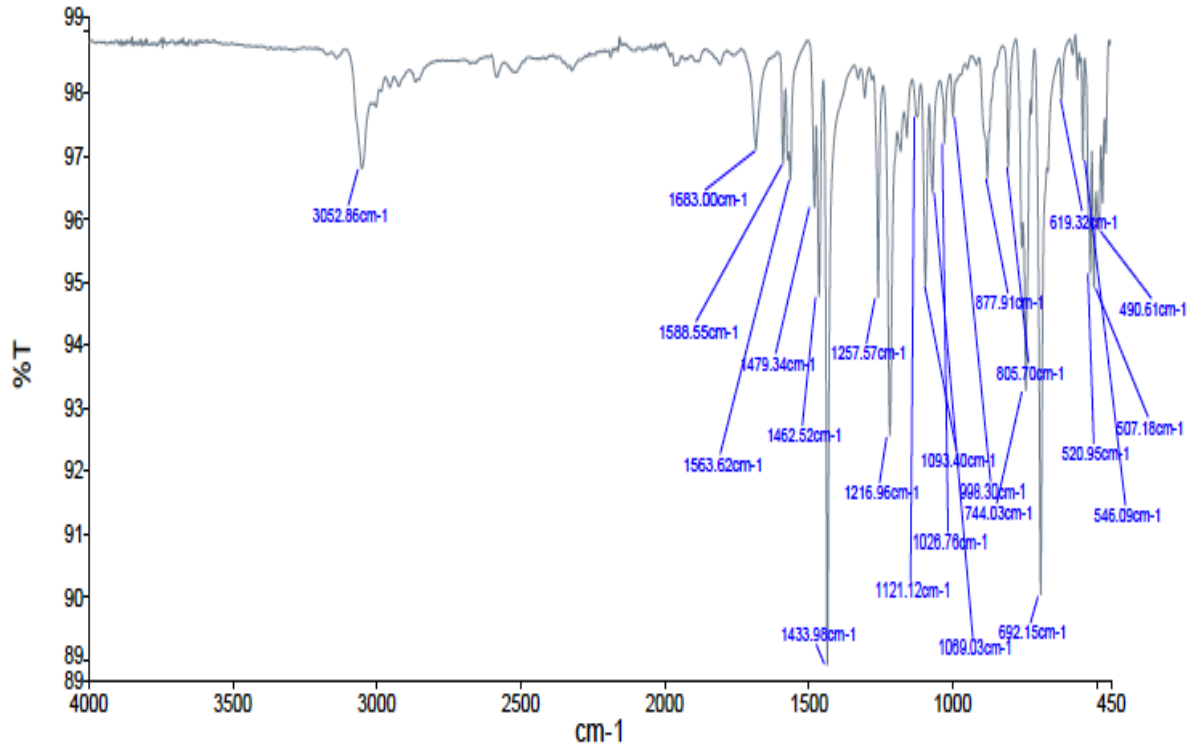


Figure S107. ATR-IR of [(^{Ph}**L3**)Ni(DC≡CPh)].

7. UV-Vis

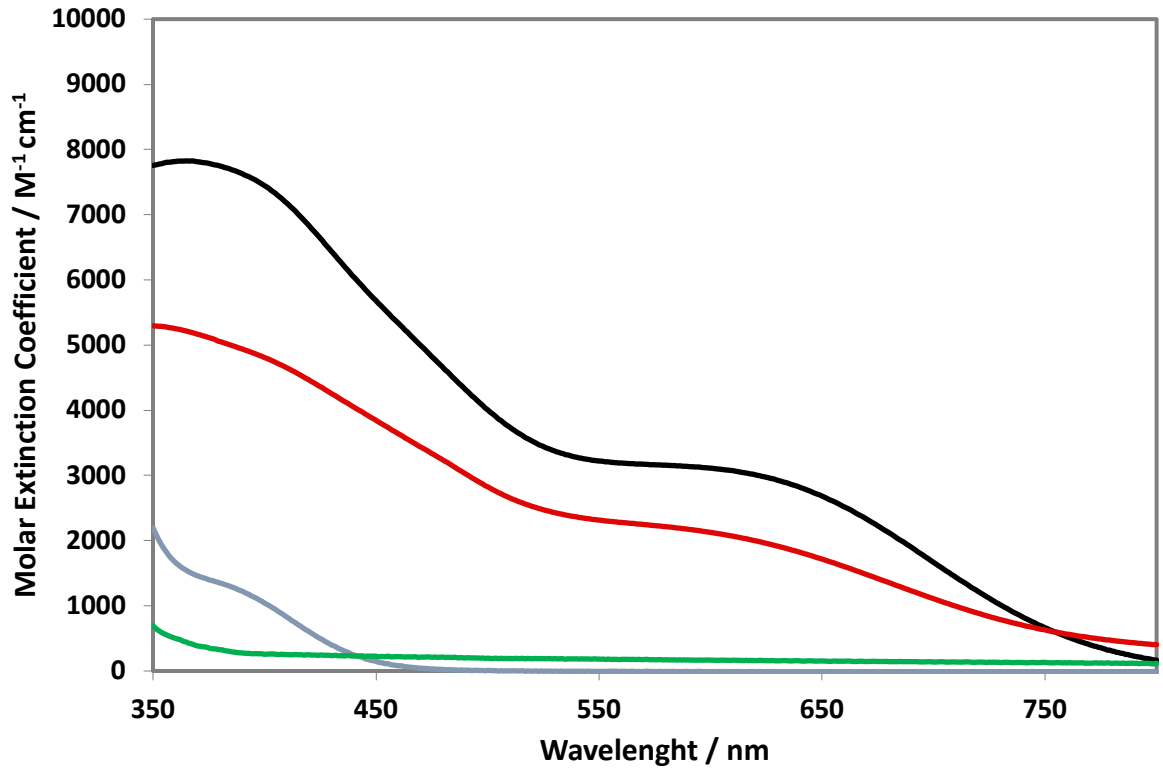


Figure S108. UV-vis spectrum of [(^{Ph}**L1**)Ni(BPI)] (black line = in toluene; red line = in THF)), the ligand ^{Ph}**L1** (light blue line, in toluene) and BPI (green line, in toluene).

8. X-ray crystallography data

X-ray crystal structure determinations

[(^{Ph}L1)Ni(BPI)] (^{Ph}1), CCDC 1882146. $C_{50}H_{39}NNiOP_2$ + disordered hexane, Fw = 790.47,* black needle, 0.27 × 0.10 × 0.04 mm^3, triclinic, $P\bar{1}$ (no. 2), a = 13.3161(5), b = 14.0105(6), c = 15.2863(6) Å, α = 72.192(3), β = 64.226(2), γ = 62.740(2) °, V = 2262.60(17) Å^3, Z = 2, D_x = 1.160 g/cm^3,* μ = 0.53 mm^{-1}.* The diffraction experiment was performed on a Bruker Kappa ApexII diffractometer with sealed tube and Triumph monochromator (λ = 0.71073 Å) at a temperature of 150(2) K up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.65 Å^{-1}. The Eval15 software[S4] was used for the intensity integration. A numerical absorption correction and scaling was performed with SADABS[S5] (correction range 0.85-1.00). A total of 38652 reflections were measured, 10404 reflections were unique (R_{int} = 0.036), of which 7922 were observed [I>2σ(I)]. The structure was solved with Patterson superposition methods using SHELXT.[S6] Least-squares refinement was performed with SHELXL-2014[S7] against F^2 of all reflections. The crystal structure contains large channels along the *c* axis (438.4 Å^3 / unit cell) filled with disordered hexane molecules. Their contribution to the structure factors was secured by back-Fourier transformation with the SQUEEZE algorithm.[S8] This resulted in 90 electrons / unit cell. Non-hydrogen atoms were refined freely with anisotropic displacement parameters. All hydrogen atoms were located in difference Fourier maps. The N-H hydrogen atom was refined freely with an isotropic displacement parameter, the C-H hydrogen atoms were refined with a riding model. 500 Parameters were refined with no restraints. R1/wR2 [I > 2σ(I)]: 0.0415 / 0.1034. R1/wR2 [all refl.]: 0.0616 / 0.1127. S = 1.015. Residual electron density between -0.73 and 0.63 e/Å^3. Geometry calculations and checking for higher symmetry was performed with the PLATON program.[S9]

[(^{Ph}L3)Ni(BPI)] (^{Ph}3), CCDC 1882147. $C_{49}H_{39}NNiOP_2$, Fw = 778.46, red needle, 0.40 × 0.08 × 0.04 mm^3, triclinic, $P\bar{1}$ (no. 2), a = 9.5744(3), b = 11.9148(5), c = 18.1503(7) Å, α = 102.462(2), β = 103.789(2), γ = 97.605(2) °, V = 1926.26(13) Å^3, Z = 2, D_x = 1.342 g/cm^3, μ = 0.63 mm^{-1}. The diffraction experiment was performed on a Bruker Kappa ApexII diffractometer with sealed tube and Triumph monochromator (λ = 0.71073 Å) at a temperature of 150(2) K up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.65 Å^{-1}. The Eval15 software[S4] was used for the intensity integration. A numerical absorption correction and scaling was performed with SADABS[S5] (correction range 0.83-1.00). A total of 44040 reflections were measured, 8867 reflections were unique (R_{int} = 0.045), of which 6688 were observed [I>2σ(I)]. The structure was solved with Patterson superposition methods using SHELXT.[S6] Least-squares refinement was performed with SHELXL-2016[S7] against F^2 of all reflections. Non-hydrogen atoms were refined freely with anisotropic displacement parameters. All hydrogen atoms were located in difference Fourier maps. The N-H hydrogen atom was refined freely with an isotropic displacement parameter, the C-H hydrogen atoms were refined with a riding model. 491

* Derived values do not contain the contribution of the disordered hexane

Parameters were refined with no restraints. R1/wR2 [I > 2σ(I)]: 0.0400 / 0.0913. R1/wR2 [all refl.]: 0.0621 / 0.1001. S = 1.035. Residual electron density between -0.43 and 0.85 e/Å^3. Geometry calculations and checking for higher symmetry was performed with the PLATON program.[S9]

[($^{p\text{-}tol}$L2)Ni(HC≡CPh)] ($^{p\text{-}tol}$5-Ph), CCDC 1882148. $C_{54}H_{47}NiOP_3$, Fw = 847.53, red needle, 0.47 × 0.12 × 0.04 mm^3, monoclinic, $P2_1/c$ (no. 14), a = 20.6558(15), b = 9.9242(9), c = 22.5170(13) Å, β = 109.612(5) °, V = 4348.0(6) Å^3, Z = 4, D_x = 1.295 g/cm^3, μ = 0.59 mm^{-1}. The diffraction experiment was performed on a Bruker Kappa ApexII diffractometer with sealed tube and Triumph monochromator (λ = 0.71073 Å) at a temperature of 150(2) K up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.59 Å^{-1}. The Eval15 software[S4] was used for the intensity integration. A numerical absorption correction and scaling was performed with SADABS[S5] (correction range 0.77-1.00). A total of 33894 reflections were measured, 7420 reflections were unique (R_{int} = 0.104), of which 4537 were observed [I>2σ(I)]. The structure was solved with Patterson superposition methods using SHELXT.[S6] Least-squares refinement was performed with SHELXL-2016[S7] against F^2 of all reflections. Non-hydrogen atoms were refined freely with anisotropic displacement parameters. Hydrogen atom H47 was located in a difference Fourier map and refined freely with an isotropic displacement parameter. All other hydrogen atoms were introduced in calculated positions and refined with a riding model. 529 Parameters were refined with no restraints. R1/wR2 [I > 2σ(I)]: 0.0618 / 0.1270. R1/wR2 [all refl.]: 0.1244 / 0.1511. S = 1.096. Residual electron density between -0.53 and 0.51 e/Å^3. Geometry calculations and checking for higher symmetry was performed with the PLATON program.[S9]

[(^{Ph}L3)Ni(HC≡CPh)] (^{Ph}6-Ph), CCDC 1882149. $C_{44}H_{34}NiOP_2 \cdot 1.5C_7H_8$, Fw = 837.56, yellow-orange block, 0.33 × 0.19 × 0.08 mm^3, triclinic, $P\overline{1}$ (no. 2), a = 10.3659(4), b = 14.4217(6), c = 16.3310(7) Å, α = 102.7809(13), β = 99.4257(13), γ = 110.5668(13) °, V = 2149.77(15) Å^3, Z = 2, D_x = 1.294 g/cm^3, μ = 0.57 mm^{-1}. The diffraction experiment was performed on a Bruker Kappa ApexII diffractometer with sealed tube and Triumph monochromator (λ = 0.71073 Å) at a temperature of 150(2) K up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.65 Å^{-1}. The Saint software[S10] was used for the intensity integration. A multiscan absorption correction and scaling was performed with SADABS[S5] (correction range 0.70-0.75). A total of 49178 reflections were measured, 9910 reflections were unique (R_{int} = 0.043), of which 7704 were observed [I>2σ(I)]. The structure was solved with Patterson superposition methods using SHELXT.[S6] Least-squares refinement was performed with SHELXL-2016[S7] against F^2 of all reflections. Non-hydrogen atoms were refined freely with anisotropic displacement parameters. One of the two independent toluene molecules was disordered on an inversion center. Hydrogen atom H37 was located in a difference Fourier map and refined freely with an isotropic displacement parameter. All other hydrogen atoms were introduced in calculated positions and refined with a riding model. 528 Parameters were refined with 147 restraints (molecular flatness, 1,2- and 1,3-distances and displacement parameters in the toluene molecules). R1/wR2 [I > 2σ(I)]: 0.0379 / 0.0855. R1/wR2 [all refl.]: 0.0611 / 0.0947.

S = 1.012. Residual electron density between -0.48 and 1.06 e/Å^3. Geometry calculations and checking for higher symmetry was performed with the PLATON program.[S9]

Packing molecular structure of [(^{Ph}L1)Ni(BPI)] (^{Ph}1)

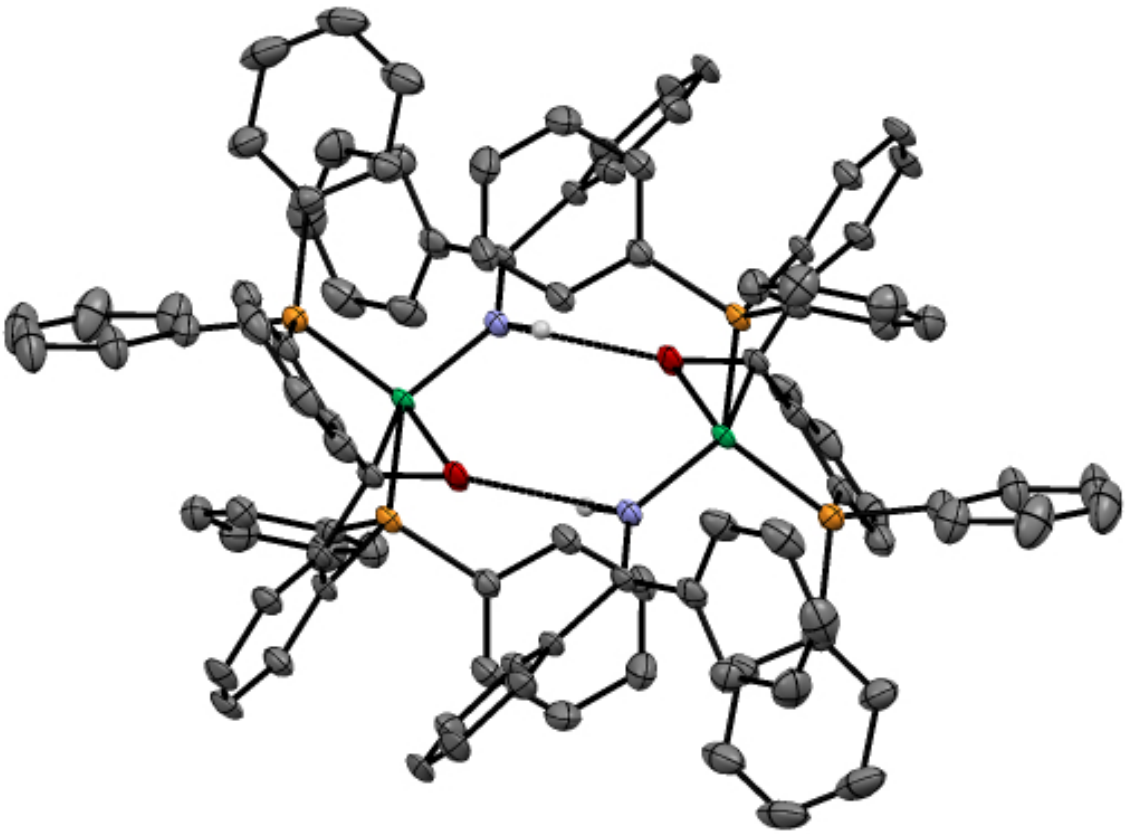


Figure S109. Molecular structure of [(^{Ph}**L1**)Ni(BPI)] (^{Ph}**1**) in the crystal (50% probability level). Carbons are shown in black, oxygen in red, phosphorous in orange, nickel in green, nitrogen in violet, and hydrogens from the imine moiety in white. Hexane solvent molecules and hydrogen atoms have been omitted for clarity.

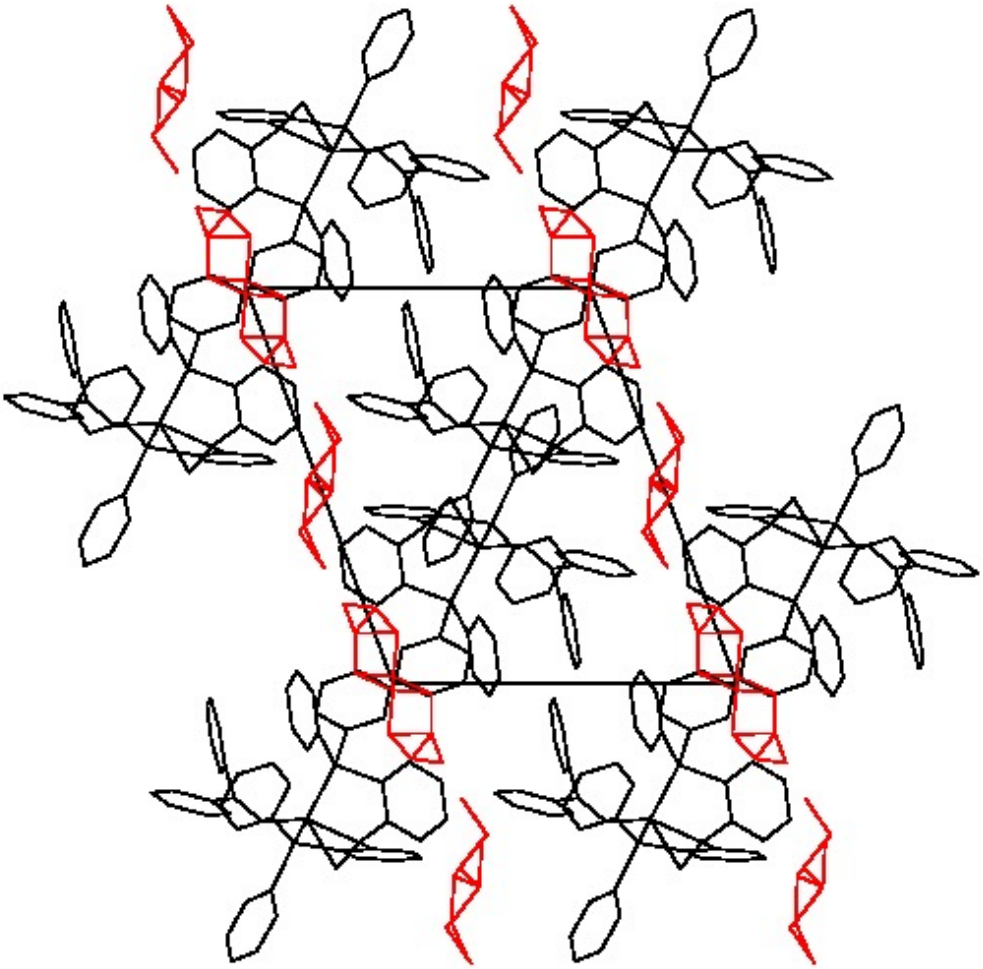
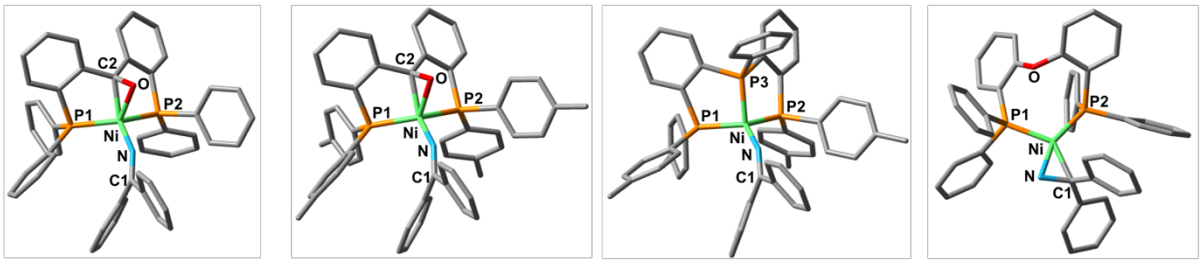


Figure S110. Packing of [(**^{Ph}L1**)Ni(BPI)] (**^{Ph}1**) in the crystal. The crystal structure contains channels along the c-axis, which are filled with disordered hexane molecules (in red). Hydrogen atoms have been omitted for clarity.

9. DFT computational details

Geometry optimizations of Ni(0)-benzophenone imine complexes and comparison

The structural differences between Ni(0)-benzophenone imine complexes (^{Ph}**1**, $^{p\text{-tol}}$**1**, $^{p\text{-tol}}$**2**, and ^{Ph}**3**) were explored by comparison of DFT properties obtained by geometry optimization at a B3LYP/6-31g(d,p) level of theory (Figure S109).



[(^{Ph}**L1**)Ni(BPI)] (^{Ph}**1**) [($^{p\text{-tol}}$**L1**)Ni(BPI)] ($^{p\text{-tol}}$**1**) [($^{p\text{-tol}}$**L2**)Ni(BPI)] ($^{p\text{-tol}}$**2**) [(^{Ph}**L3**)Ni(BPI)] (^{Ph}**3**)

Figure S111. Geometry optimization (B3LYP/6-31g(d,p)) of benzophenone imine complexes, ^{Ph}**1** – ^{Ph}**3**. Hydrogen atoms have been omitted for clarity.

Table S7 shows selected distances and angles from optimized structures. Complexes ^{Ph}**1**, $^{p\text{-tol}}$**1**, and ^{Ph}**3** adopt tetrahedral geometries while ^{Ph}**3** is trigonal planar. First, comparison of the phenyl-substituted ketone complex, ^{Ph}**1**, with the *para*-tolyl analogue, $^{p\text{-tol}}$**1**, suggests that the *para*-tolyl substituents do not affect significantly the geometry of the complex (no major differences in selected DFT properties). Similarly, the data reveal that there are only minor differences in geometry between $^{p\text{-tol}}$**1** and the tridentate phosphine complex $^{p\text{-tol}}$**2**. Indeed, the main distinction between $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2** resides in their central ketone and phosphine (Ph-P2) group. Finally, the bidentate mode of the ligand in ^{Ph}**3** (κ^2-(P1,P2)) affects the mode of binding of the BPI co-ligand (entry 8 to 12), compared to ^{Ph}**1**. Nevertheless, the bite angle of the ligand (entry 7) and the N–O distance (entry 5) are in the same range as those found for [(^{Ph}**L1**)Ni(Cl_2)],[S3] the bidentate Ni(II) analogue of ^{Ph}**1**.

Table S7. Selected DFT bond lengths and angles calculated by DFT calculation (B3LYP/6-31g(d,p)).

Entry	Property	^{Ph}**1**	$^{p\text{-tol}}$**1**	$^{p\text{-tol}}$**2**	^{Ph}**3**
1	C2 –O	1.32 Å	1.32 Å	-	-
2	∠ C2-Ni-O	39˚	39˚	-	-
3	Total ∠ C2	349˚	349˚	-	-
4	Ni–C2	1.93 Å	1.93 Å	-	-
5	Ni–O	1.95 Å	1.95 Å	-	3.38 Å
6	Ni–P3	-	-	2.13 Å	-
7	∠ P1-Ni-P2	128˚	128˚	122˚	108˚
8	C1–N	1.30 Å	1.30 Å	1.30 Å	1.38 Å
9	Total ∠ C1	360˚	360˚	360˚	350˚
10	∠ C1-Ni-N	13˚	13˚	13˚	42˚
11	Ni–C1	3.08 Å	3.08 Å	3.09 Å	1.98 Å
12	Ni–N	1.92 Å	1.92 Å	1.92 Å	1.86 Å

Natural bond orbital (NBO) analysis on Ni(0)-benzophenone imine complexes

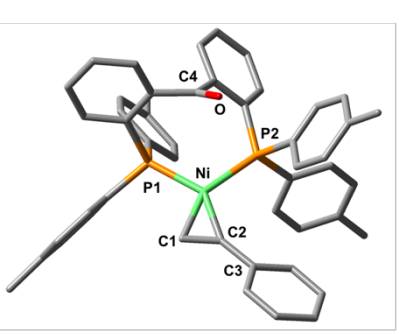
NBO analysis were performed on the benzophenone imine co-ligand and complexes $^{p\text{-tol}}$**1** – ^{Ph}**3** in order to further assign and understand the different coordination modes of the imine (Table S8). The binding of BPI through its Nitrogen atom in $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2** induces a slight decrease of the C–N Wiberg bond index (WBI), consistent with the observed shift of the calculated IR band from 1661 for BPI to 1592 ($^{p\text{-tol}}$**1**), 1559 ($^{p\text{-tol}}$**2**) 1292 cm^{-1} (^{Ph}**3**). However, the orbital interaction between the Ni center and the carbon atom is low, with Ni–C1 and Ni–N WBIs below 0.1, indicating that the σ-donation from the Nitrogen to the metal is dominating and the binding is best described by a η^1-fashion mode of BPI to nickel in $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2**. In contrast, the C–N WBI decreases upon binding from 1.86 in the free ligand imine to 1.33 in ^{Ph}**3**. The Ni–O WBIs in ^{Ph}**3** (0.37) is similar to the corresponding Ni–C1 WBIs (0.35), suggesting that back-donation into the π*(C1–N) orbital contributes equally to the bonding, in respect to the donation from the π(C1–N) orbital. The partially acceptor character of the C1–N moiety is additionally corroborated by a decrease of the total charge of the C1–N fragment by 0.39 upon coordination to ^{Ph}**3**. In accordance with the structures proposed, the total natural charge q(C1) + q(N) of $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2** is somehow similar to the free BPI. The preference for the η^1 (C1,N) mode in ^{Ph}**3** compared to the η^1(N) in $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2** (with limited back donation from Ni) can be attributed to (i) the flexibility of the bidentate ^{Ph}**L3** ligand (versus tridentate for $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2**) which gives less geometrical constrains; (ii) the geometry of ^{Ph}**L3** (trigonal planar vs pseudo tetrahedral) where the C1–N bond axis of BPI is parallel to the metal coordination plane, which is thought to make the π-backdonation from the high-lying in-plane *d* orbital with significant σ*(P–Ni) character more favorable in ^{Ph}**3** than for $^{p\text{-tol}}$**1** and $^{p\text{-tol}}$**2**.

Table S8. Selected Wiberg bond indexes (WBI) and natural charges (q) at a B3LYP/def2TZVP level of theory from the optimized geometries.

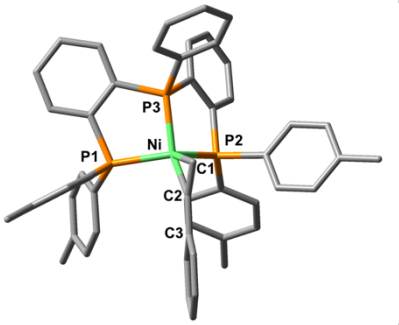
	BPI	$^{p\text{-tol}}$**1**	$^{p\text{-tol}}$**2**	^{Ph}**3**
WBI (C–N)	1.86	1.69	1.67	1.33
WBI (Ni–C1)	-	0.08	0.10	0.35
WBI (Ni–N)	-	0.23	0.25	0.37
q(C1)	0.26	0.26	0.23	-0.03
q(N)	-0.60	-0.67	-0.69	-0.80
q(C1) + q(N)	-0.44	-0.41	-0.46	-0.83

Geometry optimizations of Ni(0)-phenylacetylene complexes and comparison (complementary data to table 2)

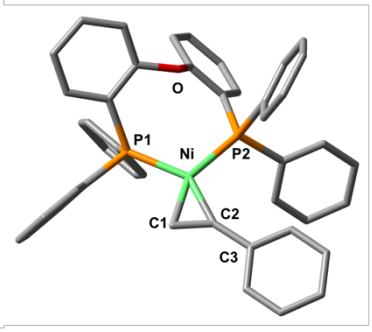
Table S9. Selected DFT bond distances and angles from the geometry optimizations (B3LYP/6-31g(d,p)) of diphenylacetylene complexes, $^{p\text{-tol}}$**4-Ph** – ^{Ph}**6-Ph**. Hydrogen atoms have been omitted for clarity.



[($^{p\text{-tol}}$**L1**)Ni(HC≡CPh)] ($^{p\text{-tol}}$**4-Ph**)



[($^{p\text{-tol}}$**L2**)Ni(HC≡CPh)] ($^{p\text{-tol}}$**5-Ph**)



[(^{Ph}**L3**)Ni(HC≡CPh)] (^{Ph}**6-Ph**)

Entry	Property	$^{p\text{-tol}}$**4-Ph**	$^{p\text{-tol}}$**5-Ph**	^{Ph}**6-Ph**
1	C4 –O	1.22 Å	-	-
2	∠ C4-Ni-O	92˚	-	-
3	Total ∠ around C2	355˚	-	-
4	Ni–C4	3.37 Å	-	-
5	Ni–O	3.64 Å	-	3.43 Å
6	Ni–P3	-	2.11 Å	-
7	∠ P1-Ni-P2	110˚	129˚	109˚
8	C1–C2	1.29 Å	1.26 Å	1.30 Å
9	∠ C1–C2–C3	141˚	150˚	150˚
11	Ni–C1	1.84 Å	1.94Å	1.84 Å
12	Ni–C2	1.89 Å	1.927Å	1.89 Å

Rotation of acetylene around Ni coordination plane of ^{Ph}6-H

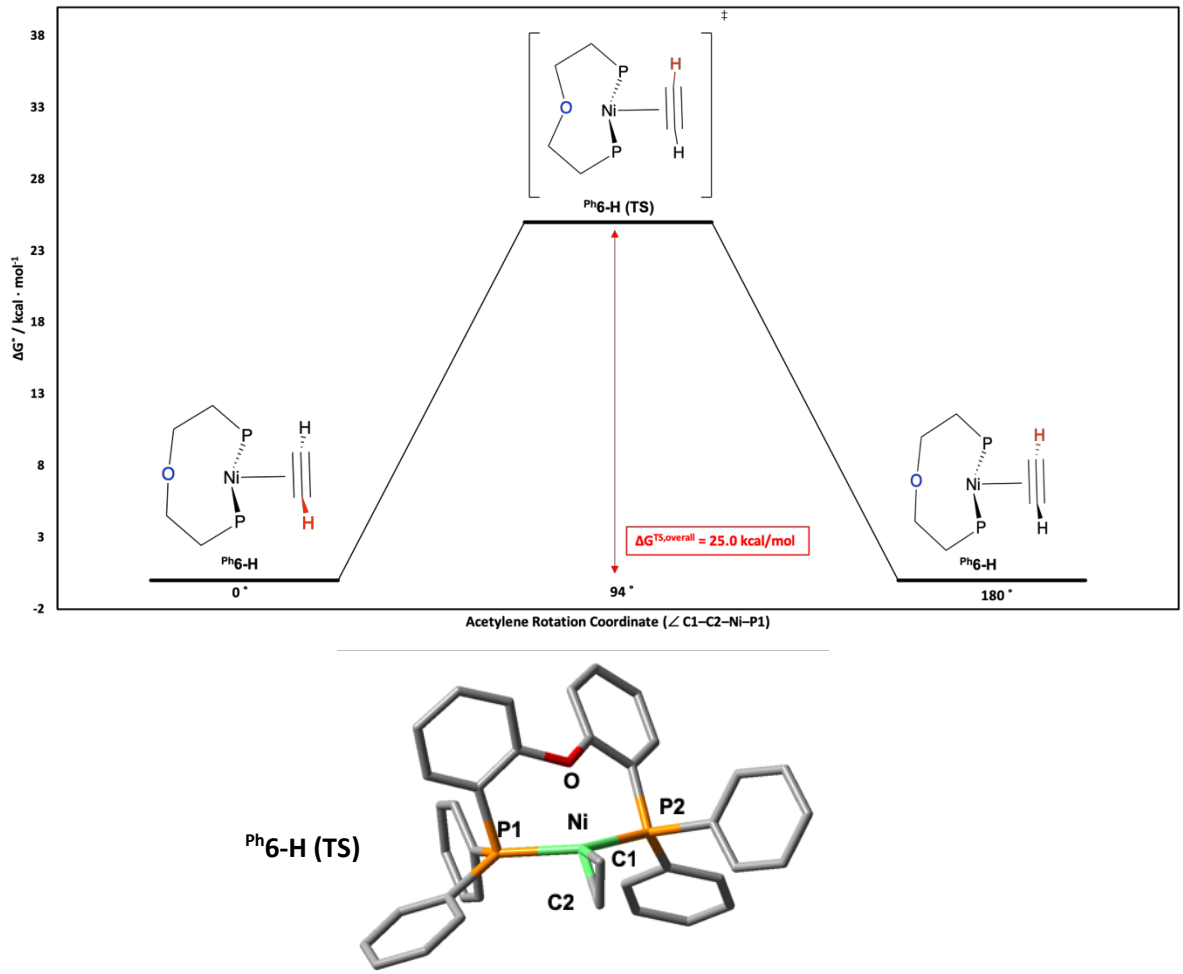
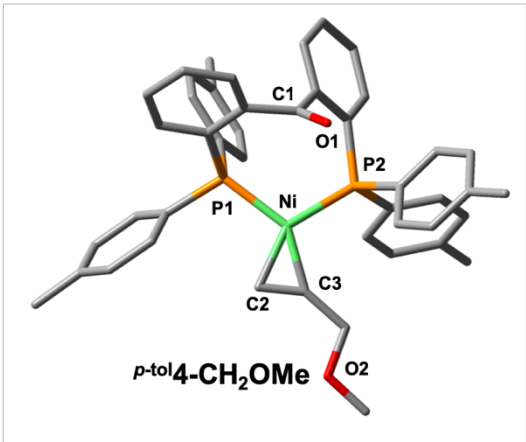
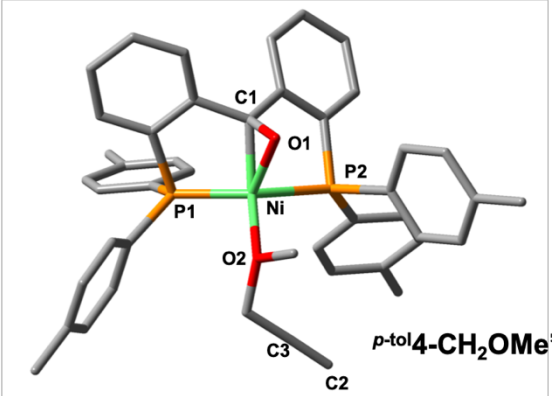


Figure S112. Top. Energy diagram for the rotation of acetylene around Ni-coordination plane of ^{Ph}**6-H** (∠ C1–C2–Ni–P1). $\Delta G^{\ddagger}$ = 25.0 kcal/mol. **Bottom.** Optimized geometry of the transition state (**^{Ph}6-H (TS)**) at a B3LYP/6-31g(d,p) level of theory under vacuum. The imaginary frequency (–120 cm^{-1}) found in the transition state is the rotation of acetylene around the C1–C2–Ni–P1 torsion angle. Selected bond lengths [Å] and angle [˚] for **^{Ph}6-H (TS)**. Ni–O = 2.21; Ni–P1 = 2.20; Ni–P2 = 2.21; C1–C2 = 1.26; ∠ P1–Ni–P2 = 124 ˚. Weak interaction of the central oxygen with Ni was found by NBO (WBI = 0.06). Hydrogen atoms have been omitted for clarity.

Coordination mode of methyl propargyl ether

Table S10. Structural and energetic differences between the two possible methyl propargyl ether complexes, **$^{p\text{-tol}}$4-PhCN – $^{p\text{-tol}}$4-PhCN''**, modelled at a B3LYP/6-31g(d,p) level of theory. Hydrogen atoms have been omitted for clarity.

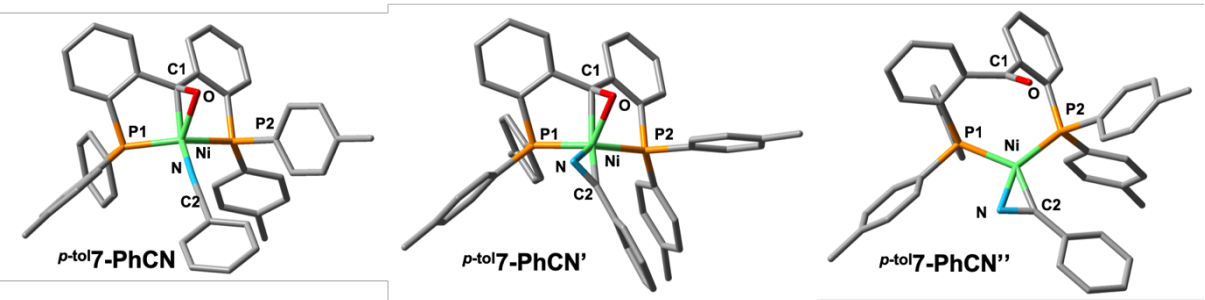




Entry	Property	$^{p\text{-tol}}$4-CH$_2$OMe	$^{p\text{-tol}}$4-CH$_2$OMe'
1	G (kcal/mol)	0	11.0
2	∠ P1–Ni–P2	113˚	131˚
4	Ni–C1	3.50 Å	1.89 Å
5	Ni–O1	3.86 Å	1.94 Å
6	C1–O1	1.21 Å	1.32 Å
7	C2–C3	1.28 Å	1.20 Å

Coordination mode of PhCN

Table S11. Structural and energetic differences between the three possible benzonitrile nickel complexes, **$^{p\text{-tol}}$7-PhCN – $^{p\text{-tol}}$7-PhCN''**, modelled at a B3LYP/6-31g(d,p) level of theory. Hydrogen atoms have been omitted for clarity.



Entry	Property	$^{p\text{-tol}}$7-PhCN	$^{p\text{-tol}}$7-PhCN'	$^{p\text{-tol}}$7-PhCN''
1	G (kcal/mol)	0	9.4	12.6
2	∠ P1–Ni–P2	129°	119°	112°
4	Ni–C1	1.93 Å	2.00 Å	3.40 Å
5	Ni–O	1.95 Å	1.97 Å	3.31 Å
6	C1–O	1.32 Å	1.30 Å	1.21 Å
7	Ni–C1	1.16 Å	1.20 Å	1.23 Å

DFT-simulated IR spectra

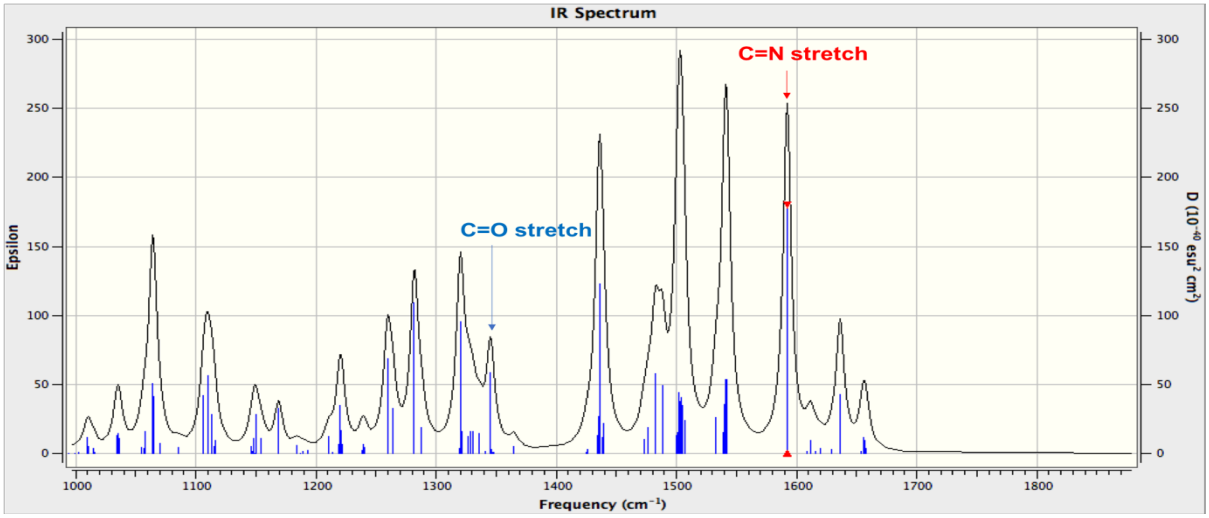


Figure S113. Simulated IR of [($^{p\text{-tol}}$**L1**)Ni(BPI)] ($^{p\text{-tol}}$**1**). BPI = benzophenone imine.

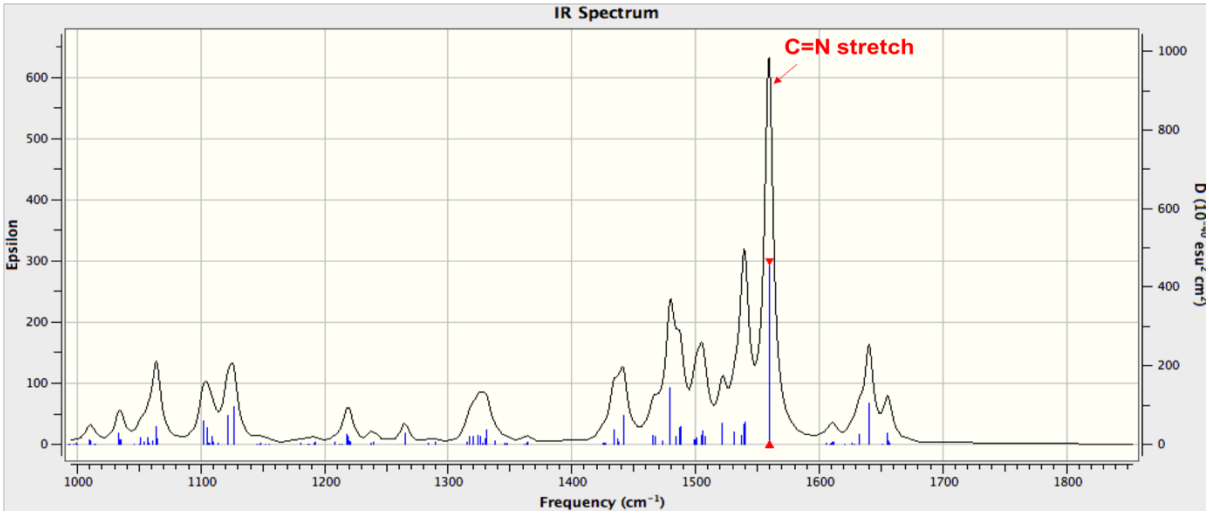


Figure S114. Simulated IR of [($^{p\text{-tol}}$**L2**)Ni(BPI)] ($^{p\text{-tol}}$**2**). BPI = benzophenone imine.

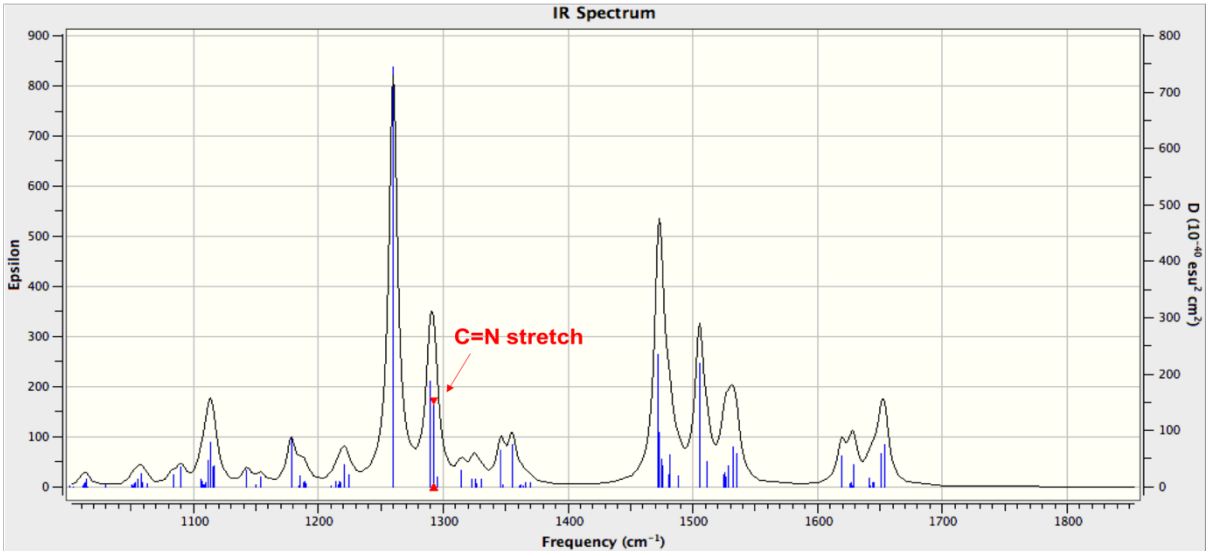


Figure S115. Simulated IR of [(^{Ph}**L3**)Ni(BPI)] (^{Ph}**3**). BPI = benzophenone imine.

Optimized structures

Compound: ^{Ph}1
Charge: 0
Multiplicity: 1
Lowest Frequency: 13.70 cm^{-1}
Energy: -4249.755572 Hartree

Ni	-0.13462000	-0.06755600	-0.67366900
P	0.21415800	2.00114200	-0.17604000
P	-1.78900200	-1.45611800	0.09802800
O	-0.63101900	-0.52212700	-2.50602500
N	1.52043400	-1.05146000	-0.62599000
C	-0.23409800	2.74048500	-1.80554000
C	2.60430100	-1.28133600	0.05474400
C	0.18168700	3.98930200	-2.28584200
C	2.71835700	-0.82658500	1.46277100
C	-0.11858000	4.36651700	-3.59410900
C	1.59695800	-0.84215300	2.30932900
C	-0.81398500	3.48689000	-4.42874900
C	1.70524000	-0.43910800	3.63919300
C	-1.22787700	2.24290000	-3.95203700
C	2.92951400	0.00894700	4.14076100
C	-0.96061800	1.86451300	-2.62898100
C	4.04806600	0.04018100	3.30582800
C	-1.34530400	0.50588800	-2.06889400
C	3.94733900	-0.38401700	1.98254100
C	-2.81967000	0.23493400	-1.82547800
C	3.73936400	-2.02151600	-0.56566500
C	-3.84829400	0.91164700	-2.49456900
C	4.49673300	-2.94894900	0.17103300
C	-5.18798900	0.58149600	-2.27899000
C	5.51305700	-3.68085600	-0.43962900
C	-5.52897000	-0.42818000	-1.38108700
C	5.80199400	-3.49189300	-1.79252100
C	-4.51906200	-1.09281300	-0.68331000
C	5.06564100	-2.56519800	-2.53287600
C	-3.17737600	-0.76044800	-0.88904700
C	4.04423100	-1.83773600	-1.92635400
C	1.94124200	2.63540100	0.05864500
C	2.90695200	2.19564600	-0.86353900
C	4.23440700	2.60464000	-0.75842900
C	4.62567200	3.45600700	0.27804800
C	3.67694900	3.89889900	1.19835900

C	2.34371800	3.49533300	1.08892800
C	-0.76651100	2.93455800	1.08174000
C	-1.72144200	3.90087900	0.73532900
C	-2.48402000	4.53240800	1.72028900
C	-2.29594300	4.21911700	3.06611400
C	-1.34575200	3.25957300	3.42430900
C	-0.59632400	2.61425400	2.44077000
C	-1.59400100	-3.19156600	-0.48867600
C	-2.18872800	-3.65869500	-1.66894000
C	-1.93142900	-4.95169900	-2.12915900
C	-1.07881600	-5.79718400	-1.41990800
C	-0.47302300	-5.33938000	-0.24720400
C	-0.72112600	-4.04588300	0.20822800
C	-2.53718500	-1.64707100	1.78021800
C	-3.05645800	-2.84471400	2.29505600
C	-3.59611000	-2.88937700	3.58241600
C	-3.63350700	-1.73897400	4.37105800
C	-3.12468300	-0.54007500	3.86644600
C	-2.57512100	-0.49713000	2.58616100
H	1.56147800	-1.50555700	-1.53985600
H	0.75927900	4.65160000	-1.64730800
H	0.20506300	5.33327900	-3.96922400
H	0.64398200	-1.17852900	1.91950100
H	-1.02366400	3.76785300	-5.45724500
H	0.83037700	-0.47960600	4.28189700
H	-1.74198800	1.55106200	-4.61254500
H	3.01211600	0.32863000	5.17557100
H	5.00183400	0.39491500	3.68508400
H	4.82007200	-0.35405000	1.33927600
H	-3.60513500	1.70700200	-3.18955800
H	4.27328600	-3.10626700	1.22092400
H	-5.96545200	1.12101700	-2.81314400
H	6.07818900	-4.40342600	0.14182200
H	-6.57041100	-0.68338400	-1.20787000
H	6.59769300	-4.05976100	-2.26542400
H	-4.77908800	-1.85092300	0.04980400
H	5.29122800	-2.40245800	-3.58258500
H	3.49094600	-1.10460200	-2.50644400
H	2.60957400	1.53277900	-1.67083600
H	4.96422000	2.25830000	-1.48494300
H	5.66113500	3.77301700	0.36379000
H	3.96957100	4.56676500	2.00390200
H	1.61893900	3.85751800	1.80955100
H	-1.87302600	4.15926700	-0.30728100

H	-3.22369900	5.27417200	1.43245500
H	-2.88629000	4.71546800	3.83085200
H	-1.19127000	3.00897300	4.47030400
H	0.12709900	1.85589300	2.72818100
H	-2.84890500	-3.00910200	-2.23251600
H	-2.40068400	-5.29655200	-3.04633300
H	-0.88193200	-6.80313200	-1.77930200
H	0.19837900	-5.98741600	0.30931000
H	-0.23500600	-3.69741000	1.11579900
H	-3.03670200	-3.74709000	1.69304200
H	-3.99215200	-3.82560400	3.96631300
H	-4.05450600	-1.77645400	5.37179500
H	-3.15043000	0.36333600	4.46943300
H	-2.17348400	0.43663900	2.20414800

Compound: $^{p\text{-tol}}$1
Charge: 0
Multiplicity: 1
Lowest Frequency: 12.17 cm^{-1}
Energy: -4407.038784 Hartree

Ni	0.04510800	0.19555800	-0.82255700
P	-1.18837900	-1.56297600	-0.61094100
P	2.21436100	0.50498200	-0.14583000
O	0.52727900	0.79619900	-2.61715800
N	-0.94347600	1.76134900	-0.30044100
C	-1.26572800	-2.04109100	-2.39188100
C	-1.71957500	2.28521200	0.60202100
C	-2.24884400	-2.84459200	-2.98428800
C	-1.91389400	1.61486400	1.91182800
C	-2.27372200	-3.00781200	-4.36866300
C	-0.85445800	0.92479600	2.52515000
C	-1.33119000	-2.34833000	-5.16273800
C	-1.02630600	0.32125000	3.76988100
C	-0.35206900	-1.54748000	-4.57442200
C	-2.26442700	0.37615400	4.41407000
C	-0.29515300	-1.40218100	-3.18110400
C	-3.32833600	1.04737300	3.80832300
C	0.72113200	-0.50972800	-2.48835600
C	-3.15269700	1.67027700	2.57452000
C	2.17002800	-0.96656300	-2.48238100
C	-2.40752600	3.58142300	0.34065000
C	2.70571200	-1.84563900	-3.43342600
C	-2.55003900	4.54848200	1.35099900

C	4.06085200	-2.18268500	-3.42153800
C	-3.13635700	5.78231100	1.07653300
C	4.90968100	-1.65467900	-2.45055900
C	-3.60371700	6.06992600	-0.20739400
C	4.38738000	-0.80228900	-1.47647700
C	-3.47925600	5.11402600	-1.21727200
C	3.03038000	-0.46873100	-1.47883800
C	-2.88650900	3.88261900	-0.94692100
C	-2.98674100	-1.39884400	-0.19498400
C	-3.70039800	-0.37504900	-0.84353600
C	-5.05105400	-0.16771300	-0.58592700
C	-5.74462700	-0.96777300	0.33529700
C	-5.03330500	-1.98348700	0.97949300
C	-3.67804700	-2.20213700	0.71848200
C	-0.67074000	-3.08699800	0.29230700
C	-0.28198400	-4.26396700	-0.36062800
C	0.16546100	-5.36902500	0.36512700
C	0.23326300	-5.34364500	1.76221900
C	-0.16131000	-4.16640000	2.41464200
C	-0.59354700	-3.05388700	1.69607400
C	2.80630200	2.23217200	-0.37753200
C	3.40285600	2.67027100	-1.56691400
C	3.74119400	4.01291300	-1.74095200
C	3.49582600	4.96223800	-0.74312900
C	2.89356600	4.52219700	0.44443700
C	2.54552600	3.18612400	0.62179000
C	3.09347300	-0.05359300	1.38109700
C	4.19736700	0.59317700	1.95713200
C	4.79511800	0.08961400	3.11271600
C	4.31940700	-1.07372100	3.73081700
C	3.22139700	-1.72143000	3.14905300
C	2.61393800	-1.21822100	2.00094600
H	-0.84232400	2.38841600	-1.10016600
H	-3.00657200	-3.31838100	-2.36679900
H	-3.03675000	-3.62868700	-4.82963500
H	0.10448700	0.87114800	2.02413500
H	-1.36727500	-2.45023100	-6.24399400
H	-0.18756000	-0.18887500	4.23501000
H	0.36010600	-1.01415400	-5.19704400
H	-2.39875500	-0.09854000	5.38182800
H	-4.29704700	1.08758600	4.29761600
H	-3.98443300	2.18886000	2.10995200
H	2.06103400	-2.27701500	-4.19043600
H	-2.18286800	4.33453400	2.34912200

H	4.44987000	-2.86466300	-4.17290500
H	-3.22460000	6.52243600	1.86651800
H	5.96310000	-1.91916000	-2.43623100
H	-4.06500100	7.03012200	-0.41843400
H	5.03342600	-0.42205800	-0.69040600
H	-3.85077300	5.32385200	-2.21592200
H	-2.81274200	3.13828200	-1.73466900
H	-3.18825500	0.26019800	-1.56049600
H	-5.57738100	0.62951800	-1.10611500
H	-5.54501200	-2.62223300	1.69561200
H	-3.16659000	-3.00799000	1.23332000
H	-0.32733500	-4.32078700	-1.44310400
H	0.46281800	-6.26935000	-0.16729500
H	-0.12700100	-4.11968000	3.50093600
H	-0.87838000	-2.15145000	2.23030300
H	3.60227600	1.96135500	-2.36264200
H	4.20669100	4.32609400	-2.67255100
H	2.69080400	5.23694500	1.23877900
H	2.07367500	2.88069000	1.55225200
H	4.59283200	1.49702600	1.50486900
H	5.65113200	0.60839900	3.53849500
H	2.83299100	-2.63168800	3.60020900
H	1.76085500	-1.73883600	1.57631700
C	-7.21349400	-0.74233300	0.60375800
H	-7.82277100	-1.00307000	-0.27015000
H	-7.56422800	-1.34843300	1.44365600
H	-7.42214100	0.30787300	0.83609200
C	0.74048700	-6.53210600	2.54335000
H	0.62592200	-7.46123100	1.97768700
H	1.80632100	-6.42467800	2.78087800
H	0.20785800	-6.64494100	3.49294200
C	4.95155200	-1.59661700	4.99855100
H	4.48638700	-1.15208700	5.88765600
H	4.84018100	-2.68181300	5.08303600
H	6.01920600	-1.36073200	5.04083000
C	3.83797100	6.41894500	-0.94655400
H	4.62499900	6.54431600	-1.69587700
H	2.96512900	6.98714700	-1.29227900
H	4.17813500	6.88549700	-0.01648200

Compound: *p*-tol2
Charge: 0
Multiplicity: 1
Lowest Frequency: 4.13 cm^{-1}
Energy: -4866.714056 Hartree

Ni	0.19424400	0.02034900	-0.21351700
P	-1.44407800	1.35634200	-0.66046500
P	-0.09203300	-2.08474000	0.19554800
N	1.70152100	0.75573300	0.73538200
C	-1.59949900	1.39326300	-2.52936400
C	2.09553600	1.37542200	1.81741600
C	-2.52707700	2.19995100	-3.20381500
C	1.14160900	1.71387300	2.89789600
C	-2.57102900	2.22584300	-4.59670200
C	-0.03378000	0.96231700	3.07983100
C	-1.67351800	1.45183900	-5.33549700
C	-0.91956400	1.26240500	4.11271100
C	-0.74040700	0.65392100	-4.67622800
C	-0.66504900	2.33281600	4.97271900
C	-0.69770500	0.60966200	-3.27443900
C	0.48689800	3.10086700	4.79120000
C	1.38342000	2.79211400	3.77084900
C	0.00482300	-2.15612400	-2.60527100
C	3.53591200	1.73311600	1.97191200
C	-0.10860000	-2.74202900	-3.87318200
C	4.21747800	1.53596300	3.18620500
C	-0.55244500	-4.05699500	-4.01160200
C	5.58066900	1.80520000	3.29018900
C	-0.88509200	-4.80229400	-2.87874800
C	6.29073000	2.28727700	2.18845900
C	-0.76222100	-4.23465700	-1.61057000
C	5.62596500	2.49563400	0.97905800
C	-0.31352000	-2.91502800	-1.46187900
C	4.26389300	2.22104300	0.87170400
C	-1.27991800	3.18268200	-0.32926700
C	0.01608300	3.71967200	-0.29352600
C	0.22514100	5.08242400	-0.09492400
C	-0.85053700	5.96241000	0.08238500
C	-2.14282000	5.42563600	0.05648200
C	-2.35722900	4.06230800	-0.14928900
C	-3.18416400	1.03685800	-0.11682400
C	-4.15768900	0.43764300	-0.92710600
C	-5.42228400	0.12517900	-0.41901500

C	-5.76270100	0.40308500	0.90794700
C	-4.78354900	0.99617900	1.72079000
C	-3.52055200	1.29911700	1.22467300
C	1.43655000	-2.90270900	0.85311900
C	2.20267200	-3.83371600	0.13984800
C	3.38677800	-4.34761800	0.67377500
C	3.84454700	-3.96010800	1.93659900
C	3.07266500	-3.03420100	2.65430800
C	1.89965700	-2.50816200	2.12158400
C	-1.43111000	-2.90586300	1.18342800
C	-1.21476400	-3.88485100	2.16282100
C	-2.28526100	-4.43677300	2.87027400
C	-3.60316300	-4.04159400	2.61986300
C	-3.81735600	-3.07017700	1.63086600
C	-2.75442500	-2.50731200	0.93184600
H	2.51945500	0.55569600	0.16029100
H	-3.21378200	2.82049400	-2.63644200
H	-3.29472500	2.85723700	-5.10465200
H	-0.24590100	0.15437300	2.38877500
H	-1.69450700	1.47751300	-6.42147300
H	-1.81123000	0.65566900	4.24278500
H	-0.02448300	0.08124000	-5.25747400
H	-1.35858800	2.56865500	5.77482300
H	0.68849800	3.94425000	5.44541700
H	2.27263300	3.39896400	3.63981200
H	0.14841500	-2.17140900	-4.75995600
H	3.67534800	1.15370700	4.04487000
H	-0.64361000	-4.49680700	-5.00089700
H	6.09118600	1.63321900	4.23348500
H	-1.23789100	-5.82464500	-2.98256500
H	7.35213800	2.50094300	2.27295100
H	-1.01910000	-4.81751400	-0.73116500
H	6.16597100	2.87968400	0.11852800
H	3.75315100	2.40292600	-0.06983700
H	0.86647300	3.05426800	-0.40539300
H	1.24172400	5.46842800	-0.06686100
H	-2.99715000	6.08329200	0.20083700
H	-3.37446200	3.68427800	-0.15335700
H	-3.93691100	0.21059400	-1.96471600
H	-6.15786000	-0.33574500	-1.07427800
H	-5.01577900	1.22052500	2.75964800
H	-2.78350700	1.74860200	1.88381100
H	1.87576100	-4.17079500	-0.83785200
H	3.96067500	-5.06860300	0.09606500

H	3.39976200	-2.71598500	3.64162200
H	1.33256600	-1.78280400	2.69802900
H	-0.20798300	-4.22565600	2.37951100
H	-2.08872900	-5.19436100	3.62574900
H	-4.82990200	-2.74293400	1.40744800
H	-2.95367900	-1.74891700	0.18170000
C	-0.62098100	7.44236700	0.27666400
H	-0.47784700	7.95178100	-0.68477900
H	-1.47139200	7.91814400	0.77371800
H	0.27330900	7.63348300	0.87824900
C	-7.13288300	0.08259300	1.45623000
H	-7.76627600	-0.38806600	0.69920900
H	-7.07227100	-0.59879100	2.31283400
H	-7.64571800	0.98701100	1.80423900
C	-4.75779600	-4.62017100	3.40248200
H	-5.07698700	-3.94060600	4.20293100
H	-5.62904200	-4.79306100	2.76224000
H	-4.48803300	-5.57111600	3.87105200
C	5.13652900	-4.49781700	2.50371500
H	5.45522800	-5.40501000	1.98248100
H	5.94691100	-3.76397900	2.41131100
H	5.03885600	-4.73559600	3.56815300
P	0.51516300	-0.39449200	-2.28582100
C	2.07971700	-0.22593600	-3.25160000
C	3.01146700	-1.27801700	-3.29848300
C	2.46173700	1.02104200	-3.77977900
C	4.26939700	-1.09628900	-3.87230700
H	2.75045100	-2.24634400	-2.88230100
C	3.71955200	1.20048800	-4.35468500
H	1.76554100	1.85417000	-3.74823000
C	4.62956100	0.14246300	-4.40629900
H	4.96966500	-1.92669000	-3.90361900
H	3.98797000	2.16986200	-4.76631800
H	5.60860300	0.28247400	-4.85522300

Compound: ^{Ph}3
Charge: 0
Multiplicity: 1
Lowest Frequency: 11.87 cm^{-1}
Energy: -4211.626391 Hartree

Ni	0.15095700	-0.65358400	0.32739600
P	0.89909000	1.29275500	-0.29748900
P	-2.05073300	-0.63144700	0.22563100

O	-1.76092800	2.00619400	1.17107500
N	0.25073600	-2.42065200	0.91499200
C	0.46550900	2.82407900	0.69200300
C	1.39670400	3.85862400	0.89474100
C	1.11722700	4.95536100	1.70976900
C	-0.11089500	5.04634400	2.36257500
C	-1.06463300	4.05041000	2.16582600
C	-0.78279500	2.97570200	1.32261300
C	-2.60325400	2.06456000	0.07233700
C	-3.13382000	3.25668900	-0.41591300
C	-4.02956600	3.20722700	-1.48505300
C	-4.39079700	1.98228900	-2.04584800
C	-3.84892500	0.79808900	-1.54274700
C	-2.93447500	0.82026700	-0.48267700
C	2.73820200	1.52312700	-0.38304800
C	3.47821000	1.29635400	0.78922200
C	4.86269800	1.45674400	0.79849200
C	5.53359400	1.83956300	-0.36488300
C	4.80910100	2.06613000	-1.53499400
C	3.42013800	1.91539100	-1.54434500
C	0.39239400	1.70521700	-2.02892200
C	0.53478900	0.69383400	-2.99586300
C	0.19274500	0.93134300	-4.32686000
C	-0.30601700	2.17808700	-4.71139900
C	-0.44981100	3.18684800	-3.75960400
C	-0.09642700	2.95494900	-2.42826200
C	-2.89076000	-0.87356500	1.85369100
C	-4.10583300	-0.25230000	2.17799200
C	-4.70572000	-0.47356300	3.41815000
C	-4.10598400	-1.32635500	4.34585700
C	-2.90240900	-1.95669200	4.02692400
C	-2.29297300	-1.73271200	2.79126000
C	-2.68604100	-2.01942700	-0.81541300
C	-2.23324400	-2.10747400	-2.14413600
C	-2.64580200	-3.15314600	-2.96814900
C	-3.50595300	-4.13729700	-2.47477300
C	-3.95430800	-4.06343300	-1.15673800
C	-3.55126800	-3.01000000	-0.33217900
C	1.54546300	-2.03227300	0.60808700
C	2.18307600	-2.62080300	-0.62547500
C	1.89148400	-3.94235000	-1.00789600
C	2.45124900	-4.50915900	-2.15341600
C	3.33360800	-3.77302500	-2.94425600
C	3.65234300	-2.46627300	-2.56957500

C	3.08687000	-1.90146900	-1.42628700
C	2.43511900	-1.78896400	1.79560100
C	3.82145100	-2.01134200	1.76267300
C	4.62174400	-1.77883400	2.88439900
C	4.06108600	-1.31366100	4.07204800
C	2.68036200	-1.09442500	4.12585900
C	1.88353800	-1.32941700	3.00979800
H	-0.13484200	-3.02488200	0.18727100
H	2.36719100	3.79752400	0.41827600
H	1.86716900	5.72923500	1.84177100
H	-0.32880400	5.88472000	3.01723900
H	-2.03170200	4.08358400	2.65658500
H	-2.85360800	4.20237000	0.03429900
H	-4.44983400	4.13082700	-1.87223800
H	-5.09347400	1.94579800	-2.87252800
H	-4.12817400	-0.15119500	-1.98610000
H	2.97249700	0.98413000	1.69663500
H	5.41434100	1.26595400	1.71364300
H	6.61344300	1.95697000	-0.35963100
H	5.32159500	2.36583000	-2.44491600
H	2.87226700	2.10339200	-2.46075800
H	0.92981500	-0.27746300	-2.70906400
H	0.31707600	0.14212700	-5.06286100
H	-0.57890400	2.36112300	-5.74666400
H	-0.83410100	4.16018000	-4.05106900
H	-0.20394900	3.75241500	-1.70102900
H	-4.58599500	0.40938200	1.46470700
H	-5.64412500	0.01935000	3.65679400
H	-4.57454500	-1.49812000	5.31089600
H	-2.42965200	-2.62298300	4.74305900
H	-1.35330200	-2.21896400	2.53977700
H	-1.55834600	-1.35104700	-2.53578300
H	-2.28919400	-3.20416100	-3.99287600
H	-3.82032400	-4.95731800	-3.11388100
H	-4.62147300	-4.82582000	-0.76463400
H	-3.90938600	-2.96299100	0.69043300
H	1.22975500	-4.54237200	-0.38963800
H	2.20447200	-5.53331900	-2.42042800
H	3.77215000	-4.21304600	-3.83537500
H	4.34228300	-1.87925000	-3.17006400
H	3.34527900	-0.88636300	-1.14974100
H	4.28417900	-2.37991100	0.85446400
H	5.69019800	-1.97004500	2.82415500
H	4.68315000	-1.13124100	4.94373900

H	2.22125300	-0.73962000	5.04505300
H	0.81378000	-1.16468700	3.07047400

Compound: $^{p\text{-tol}}$4-H
Charge: 0
Multiplicity: 1
Lowest Frequency: 14.15 cm^{-1}
Energy: -3927.597656 Hartree

Ni	0.03980300	-0.62904600	-1.35576800
P	-1.79327400	-0.35408800	-0.22586600
P	1.79007800	-0.04209600	-0.22513600
O	1.05928700	-2.98374500	0.85996500
C	-2.25726600	-1.86991500	0.75628700
C	-3.57828800	-2.32862100	0.86375300
C	-3.88401300	-3.51683700	1.53033200
C	-2.86399900	-4.28787500	2.08384400
C	-1.54399500	-3.85200200	1.98352300
C	-1.23677500	-2.64094200	1.35091300
C	0.21793200	-2.23941300	1.33956400
C	0.63290700	-1.02283700	2.13580800
C	0.21858800	-0.95959400	3.47103900
C	0.67893100	0.05395200	4.31128200
C	1.53839600	1.02479100	3.80520200
C	1.93107300	0.98354700	2.46493400
C	1.49744700	-0.03616100	1.61135000
C	-3.27523100	-0.10195800	-1.30720900
C	-3.73003900	-1.14975900	-2.12730500
C	-4.78272100	-0.95799500	-3.01710800
C	-5.41272300	0.28912500	-3.13973000
C	-4.95531500	1.33056800	-2.32715400
C	-3.90732000	1.14201500	-1.42371300
C	-2.02380300	1.00676700	1.01408600
C	-2.93969100	0.93135100	2.07505100
C	-3.11952600	2.00576800	2.94246800
C	-2.40191700	3.19909600	2.77973100
C	-1.48704900	3.27163000	1.72430800
C	-1.29854700	2.19418800	0.85751800
C	3.34504700	-1.01646500	-0.43253300
C	3.88602400	-1.83887700	0.56142200
C	5.06077800	-2.55534600	0.32983000
C	5.73099900	-2.48049400	-0.89546900
C	5.18951700	-1.65073800	-1.88697800
C	4.01956200	-0.93125000	-1.66162800

C	2.42023700	1.65713400	-0.60852000
C	3.67002600	2.12995100	-0.17132300
C	4.10695500	3.40868200	-0.50525800
C	3.32466100	4.25848200	-1.30249300
C	2.09239400	3.77876000	-1.75697900
C	1.64872500	2.49819000	-1.42050500
H	-4.37897000	-1.76185500	0.40169900
H	-4.91760400	-3.84330300	1.60042600
H	-3.09058000	-5.22541900	2.58276300
H	-0.73472000	-4.44764800	2.39468100
H	-0.46224400	-1.71428700	3.85327600
H	0.35700200	0.08820900	5.34774100
H	1.89244300	1.82886700	4.44391100
H	2.56517600	1.77383500	2.08012900
H	-3.26162900	-2.12656700	-2.06188500
H	-5.12015600	-1.79070800	-3.62995100
H	-5.42793300	2.30764100	-2.39447400
H	-3.58799600	1.97412700	-0.80582200
H	-3.51258400	0.02367100	2.23480400
H	-3.82992200	1.91669900	3.76126500
H	-0.90597600	4.17909600	1.57948100
H	-0.56767500	2.27785300	0.06098800
H	3.38444500	-1.93748000	1.51604700
H	5.46118200	-3.18630000	1.11983100
H	5.69320000	-1.56395000	-2.84691000
H	3.63432900	-0.28563300	-2.44497700
H	4.31422800	1.48605300	0.42004900
H	5.07622300	3.75135700	-0.15028300
H	1.47310400	4.40811400	-2.39124300
H	0.70226100	2.13573200	-1.81263000
C	-6.52947100	0.49946600	-4.13368700
H	-7.20573700	-0.36094400	-4.16554400
H	-7.12120400	1.38642500	-3.88995900
H	-6.13549300	0.63681600	-5.14839900
C	-2.62523600	4.37083200	3.70537800
H	-2.77092300	4.04275600	4.73948700
H	-1.77965000	5.06416500	3.68527500
H	-3.52003500	4.93735600	3.41839300
C	3.82012800	5.63373000	-1.68027400
H	4.63339000	5.57374000	-2.41368500
H	3.02339700	6.23927400	-2.12055300
H	4.21247200	6.17043300	-0.80996700
C	6.98237200	-3.28522200	-1.15328800
H	7.50808200	-3.51820500	-0.22253400

H	6.74553900	-4.23918000	-1.64108000
H	7.67553900	-2.75034000	-1.81015300
C	-0.53924300	-1.25899400	-3.01444900
C	0.74373200	-1.20965700	-2.98420500
H	1.66526600	-1.40380500	-3.51175700
H	-1.41268800	-1.48303300	-3.60850600

Compound: $^{p\text{-tol}}$4-H (I1)
Charge: 0
Multiplicity: 1
Lowest Frequency: 13.12 cm^{-1}
Energy: -3927.595708 Hartree

Ni	0.04297900	-1.18022700	-0.69822900
P	-1.88759000	-0.36535500	-0.06898500
P	1.91624400	-0.06105200	-0.17078500
O	0.70437100	-2.82959300	0.34526000
C	-2.37702700	-1.62785600	1.17734600
C	-3.67332900	-1.95345900	1.59722600
C	-3.87347000	-3.02775800	2.46457300
C	-2.78283500	-3.78913900	2.89321100
C	-1.49103200	-3.46574100	2.47697600
C	-1.27631200	-2.36953200	1.63170800
C	0.11250800	-1.98987400	1.14178600
C	1.01355000	-1.24707900	2.12577700
C	0.95055700	-1.47173200	3.50812100
C	1.89712000	-0.91461300	4.36876000
C	2.93180200	-0.12736000	3.86367700
C	2.99082500	0.12992400	2.49384900
C	2.01898500	-0.39006100	1.63247700
C	-3.30578800	-0.35762100	-1.25613600
C	-3.84628900	-1.57888500	-1.69484100
C	-4.86333100	-1.61123900	-2.64560300
C	-5.37343100	-0.43138400	-3.20426100
C	-4.83332300	0.78229800	-2.76574400
C	-3.81789900	0.82290200	-1.80962300
C	-2.05437800	1.26194400	0.78561900
C	-2.74719800	1.42484300	1.99424100
C	-2.86566300	2.68239600	2.58270000
C	-2.30575300	3.81960500	1.98623700
C	-1.61250700	3.65345700	0.78146000
C	-1.47675800	2.39561600	0.19485700
C	3.53502300	-0.70076800	-0.79497600
C	4.58831500	0.10868300	-1.23636000

C	5.78125800	-0.46101900	-1.68832400
C	5.96134500	-1.84694200	-1.70924000
C	4.90538800	-2.65211700	-1.25511200
C	3.71062100	-2.09712400	-0.80814100
C	2.04965500	1.75938100	-0.41032600
C	2.04739800	2.23137300	-1.73716000
C	2.08772300	3.59362100	-2.01505700
C	2.12156800	4.54354000	-0.98193200
C	2.10147300	4.07328900	0.33421800
C	2.06496000	2.70605200	0.62044400
H	-4.52411800	-1.39212400	1.22266200
H	-4.87827700	-3.28501900	2.78705900
H	-2.94178700	-4.64464700	3.54376200
H	-0.64773600	-4.07495100	2.78801800
H	0.16441100	-2.09674400	3.91646700
H	1.83209700	-1.10864400	5.43581100
H	3.68067500	0.29079600	4.52999800
H	3.78980000	0.74873000	2.09547000
H	-3.48356200	-2.51242000	-1.27543800
H	-5.27026100	-2.57050800	-2.95683000
H	-5.21611700	1.71522600	-3.17261600
H	-3.43525100	1.78558600	-1.48791100
H	-3.19457700	0.56636300	2.48376500
H	-3.40678100	2.78224700	3.52073800
H	-1.15695000	4.51483200	0.30050400
H	-0.91097500	2.29687100	-0.72673300
H	4.48850200	1.18883700	-1.23096900
H	6.58531000	0.18826900	-2.02697100
H	5.02082600	-3.73360600	-1.25281500
H	2.90659900	-2.73781200	-0.45649700
H	2.01321300	1.52360500	-2.56108200
H	2.08967100	3.92708300	-3.05014600
H	2.11347300	4.78554700	1.15568500
H	2.03531900	2.38430700	1.65493500
C	-6.45312600	-0.47425300	-4.25864200
H	-7.16597900	-1.28296400	-4.06965100
H	-7.01014900	0.46618200	-4.30042000
H	-6.02659900	-0.64599200	-5.25487300
C	-2.41730400	5.17550500	2.64131300
H	-3.35889300	5.27960000	3.18898100
H	-1.60489400	5.33552700	3.36136400
H	-2.36197400	5.98202700	1.90424800
C	2.19039400	6.01998200	-1.29114200
H	1.46406800	6.30303200	-2.06049400

H	1.99410700	6.62527200	-0.40184400
H	3.18149300	6.30033100	-1.66837500
C	7.24150700	-2.46515300	-2.21804100
H	8.03182800	-1.71730900	-2.32838100
H	7.60568000	-3.24499300	-1.54072400
H	7.09298700	-2.93590700	-3.19767500
C	0.58744500	-1.59905100	-2.58091000
C	-0.57015300	-2.02967500	-2.37939800
H	-1.48880400	-2.50089300	-2.67440300
H	1.49033500	-1.45638200	-3.14339200

Compound: *p*-tol4-H (TS1)
Charge: 0
Multiplicity: 1
Lowest Frequency: -113.70 cm^{-1}
Energy: -3927.591533 Hartree

Ni	0.09048200	-1.01677300	-0.82290300
P	-1.85956700	-0.39163200	-0.09567000
P	1.91468700	0.00248100	-0.16332100
O	1.00488900	-2.71789700	0.84058900
C	-2.31017100	-1.67273200	1.15249900
C	-3.59859700	-2.06012000	1.54063000
C	-3.77607900	-3.11195900	2.43976500
C	-2.66580400	-3.79167600	2.94598200
C	-1.37951800	-3.40476800	2.57183200
C	-1.19551100	-2.32991000	1.69285700
C	0.22195400	-1.89450900	1.36033500
C	0.82552200	-0.78940200	2.22278600
C	0.52322900	-0.70794800	3.58631200
C	1.18234000	0.21138500	4.40553700
C	2.14467500	1.06319200	3.86778400
C	2.44109600	1.00055500	2.50354000
C	1.78690400	0.08504300	1.67626400
C	-3.20202900	-0.46672300	-1.35961200
C	-3.82332400	-1.67423800	-1.71043700
C	-4.74652300	-1.72591700	-2.75506300
C	-5.07393300	-0.58313300	-3.49409400
C	-4.43686300	0.61753600	-3.15415200
C	-3.51797600	0.67722900	-2.10903600
C	-2.26490400	1.20463800	0.76040500
C	-3.58744500	1.56237100	1.07896700
C	-3.86458400	2.73705500	1.76955100
C	-2.83477900	3.60223600	2.17159200

C	-1.52186700	3.24750600	1.85143700
C	-1.23977700	2.06753900	1.15937000
C	3.51654600	-0.84432300	-0.48991800
C	4.05373500	-1.77230300	0.41242200
C	5.22588100	-2.46079600	0.10621300
C	5.89463100	-2.26037100	-1.10787300
C	5.34858200	-1.33961900	-2.01071500
C	4.17811700	-0.64421400	-1.71137700
C	2.26593700	1.72922900	-0.71024000
C	3.49784400	2.37340700	-0.49964900
C	3.70170500	3.68200000	-0.92874300
C	2.69109000	4.39416400	-1.59191100
C	1.47377100	3.74429400	-1.82131600
C	1.26381200	2.43360300	-1.39074700
H	-4.46663300	-1.56279100	1.11948000
H	-4.77865500	-3.41224700	2.73045700
H	-2.80311000	-4.62630800	3.62753100
H	-0.51097000	-3.93377900	2.95212900
H	-0.22798700	-1.36539800	4.01114900
H	0.93647200	0.26327400	5.46235600
H	2.65246300	1.78574000	4.50010200
H	3.16150600	1.69332700	2.08112300
H	-3.58587100	-2.58323300	-1.16767800
H	-5.21677700	-2.67479900	-3.00179500
H	-4.66202300	1.52032400	-3.71706500
H	-3.04701300	1.62616700	-1.87121500
H	-4.41110000	0.92663400	0.76961000
H	-4.89700300	2.99097300	1.99893700
H	-0.70281900	3.89944800	2.14391000
H	-0.21018400	1.82384900	0.93100600
H	3.54406400	-1.97197400	1.34741700
H	5.62688700	-3.17083500	0.82568200
H	5.84623500	-1.16142400	-2.96106700
H	3.78671100	0.06928200	-2.43055800
H	4.31294000	1.83978800	-0.02037400
H	4.66453700	4.15686200	-0.75526000
H	0.68027400	4.26532700	-2.35113400
H	0.31476400	1.94534600	-1.59133400
C	-6.09340200	-0.63603000	-4.60640400
H	-5.83112700	0.04464000	-5.42222700
H	-6.18081700	-1.64429700	-5.02130800
H	-7.08832100	-0.34312600	-4.24784800
C	-3.14478200	4.86667000	2.93609200
H	-3.46127200	4.64112200	3.96173700

H	-2.27184000	5.52218200	2.99672800
H	-3.95876900	5.42895000	2.46613900
C	2.91218700	5.82095100	-2.03301600
H	2.78050000	6.51745500	-1.19555600
H	3.92599300	5.96882000	-2.41816200
H	2.20554500	6.11235800	-2.81497800
C	7.14617000	-3.03553400	-1.44403800
H	7.77478800	-2.49397400	-2.15719300
H	7.74397700	-3.23826200	-0.55006200
H	6.90139500	-4.00498200	-1.89603000
C	-0.48782300	-2.08461600	-2.30527300
C	0.76030800	-1.87802600	-2.39816000
H	1.70616200	-2.02637300	-2.89108200
H	-1.39438900	-2.48839500	-2.72452100

Compound: *p*-tol4-H (TS2)
Charge: 0
Multiplicity: 1
Lowest Frequency: -95.13 cm^{-1}
Energy: -3927.588061 Hartree

Ni	-0.14252300	-1.17805400	-0.32334900
P	-2.07773200	-0.22651300	-0.04677400
P	2.03425500	-0.04253100	-0.20492000
O	0.61951400	-2.23818400	1.09084100
C	-2.52369600	-1.06722300	1.53521900
C	-3.80549000	-1.30401900	2.04429500
C	-3.95893400	-2.01579400	3.23423300
C	-2.83396000	-2.49213500	3.91281400
C	-1.55416900	-2.24177000	3.41582300
C	-1.38879000	-1.51478700	2.23065200
C	-0.02236700	-1.22369800	1.63264800
C	0.83804900	-0.17312700	2.30198100
C	0.61042300	0.25369100	3.61632400
C	1.45788000	1.17798200	4.23132200
C	2.54464100	1.70178200	3.53599800
C	2.76872200	1.30801700	2.21458400
C	1.92514300	0.38626000	1.58832000
C	-3.39239100	-0.70581900	-1.24014200
C	-3.93522900	-2.00044800	-1.22245900
C	-4.82067800	-2.41666500	-2.21422200
C	-5.18767300	-1.56710800	-3.26621600
C	-4.62629300	-0.28485500	-3.29504900
C	-3.74198400	0.13986700	-2.30425100

C	-2.42697500	1.55855100	0.29375600
C	-3.72407800	2.09683600	0.33901200
C	-3.92924100	3.43348900	0.66878800
C	-2.85261500	4.28067900	0.97113900
C	-1.56348900	3.73947900	0.93631800
C	-1.35184000	2.40097400	0.60239000
C	3.42435600	-1.24082600	-0.32903200
C	4.02376200	-1.84433900	0.78318100
C	5.02819100	-2.79907700	0.61900900
C	5.46471700	-3.18609600	-0.65256000
C	4.85926300	-2.58321800	-1.76435900
C	3.85205700	-1.63521100	-1.60817700
C	2.74887100	1.48391600	-0.96976000
C	4.12435500	1.75823000	-1.05171100
C	4.58523900	2.92613100	-1.65569900
C	3.69570000	3.86319500	-2.20043400
C	2.32624700	3.58311500	-2.12993200
C	1.86029600	2.41184500	-1.53270500
H	-4.68131200	-0.95752200	1.50361600
H	-4.95340300	-2.20942400	3.62609900
H	-2.95535700	-3.06255500	4.82942200
H	-0.68068900	-2.61922900	3.93937600
H	-0.23626700	-0.13937200	4.16743800
H	1.26085700	1.48906000	5.25349000
H	3.20478700	2.42406000	4.00753900
H	3.59107600	1.74616400	1.65772500
H	-3.66244800	-2.68921400	-0.42951300
H	-5.22961800	-3.42342100	-2.17289300
H	-4.88268800	0.39293400	-4.10583900
H	-3.32743000	1.14202100	-2.35973300
H	-4.58040100	1.47098800	0.10768400
H	-4.94283700	3.82700100	0.69644400
H	-0.71023300	4.36950100	1.17438600
H	-0.34087400	2.00764100	0.59416800
H	3.70651200	-1.56989300	1.78308300
H	5.48093900	-3.25007100	1.49894600
H	5.17809600	-2.86359300	-2.76564500
H	3.39911300	-1.19110100	-2.49060900
H	4.84062600	1.04710500	-0.65190700
H	5.65557300	3.11281900	-1.70801500
H	1.61414400	4.28423700	-2.55853500
H	0.79247200	2.21313000	-1.50862800
C	-6.16976000	-2.01477900	-4.32189500
H	-7.20494300	-1.85501300	-3.99463000

H	-6.03459200	-1.46050300	-5.25523200
H	-6.06204700	-3.08131800	-4.54195700
C	-3.08347800	5.73531000	1.30302100
H	-2.22356700	6.16877200	1.82107400
H	-3.25239000	6.32715500	0.39470000
H	-3.96457900	5.86522300	1.93954600
C	4.20348500	5.13767300	-2.83128400
H	5.09261100	4.95550500	-3.44346300
H	3.44356900	5.60041600	-3.46718400
H	4.48437300	5.87318500	-2.06711700
C	6.53228700	-4.23992300	-0.82648900
H	7.17971800	-4.01838800	-1.68095300
H	7.16242000	-4.32194600	0.06395300
H	6.08929900	-5.22790900	-1.00470500
C	-0.23563300	-1.61441400	-2.29798600
C	-0.11648300	-2.67391800	-1.66200500
H	0.02654100	-3.70503100	-1.40989100
H	-0.36098800	-0.97142200	-3.14651100

Compound: $^{p\text{-tol}}$4-CH_2OMe
Charge: 0
Multiplicity: 1
Lowest Frequency: 10.30 cm^{-1}
Energy: -4081.435743 Hartree

Ni	0.03250100	-1.16459500	0.21259300
P	-1.89418100	-0.14067700	0.28019400
P	1.67100700	0.25159700	0.03395900
O	0.82943300	1.39444300	2.99309000
C	-2.42743100	0.78399300	1.82003000
C	-3.75091200	0.71212500	2.28425000
C	-4.14506700	1.32243800	3.47590400
C	-3.21012500	2.00101000	4.25423800
C	-1.89050900	2.08107300	3.81660200
C	-1.50013900	1.50958700	2.59790200
C	-0.05655400	1.71326900	2.21816900
C	0.25506500	2.49788800	0.96390500
C	-0.30808900	3.77365700	0.85808600
C	0.03447600	4.61907200	-0.19798700
C	0.92524100	4.17296400	-1.16914200
C	1.46874900	2.88777900	-1.08501300
C	1.15659800	2.03540900	-0.02069300
C	-3.30326500	-1.33250500	0.09813800
C	-3.49768400	-2.30355600	1.09706100

C	-4.50722200	-3.25288100	0.98503300
C	-5.35456700	-3.28353900	-0.13424000
C	-5.15484900	-2.32181000	-1.12710700
C	-4.14866000	-1.35743900	-1.01525800
C	-2.25859800	1.06725400	-1.07610700
C	-3.18378900	2.11315100	-0.95242000
C	-3.46238900	2.95088700	-2.03111100
C	-2.83287800	2.77415800	-3.26979000
C	-1.91341300	1.72530000	-3.39290900
C	-1.62669600	0.88921500	-2.31507300
C	2.97904500	0.23664700	1.33512400
C	3.82687700	1.32722800	1.57757400
C	4.82265500	1.25330800	2.54860800
C	5.00102700	0.09540100	3.31735800
C	4.14314500	-0.98500000	3.08243800
C	3.14452700	-0.91576000	2.11207900
C	2.63496000	0.04801300	-1.53878700
C	3.92641500	0.55950100	-1.74014100
C	4.58982800	0.37234700	-2.95170100
C	3.99480000	-0.33412600	-4.00562400
C	2.71537400	-0.86232300	-3.79712800
C	2.04923800	-0.67841500	-2.58587600
H	-4.48498200	0.15535800	1.71401800
H	-5.17989900	1.25130800	3.79821100
H	-3.50119300	2.45797000	5.19534100
H	-1.14124700	2.59196100	4.41330900
H	-1.01194000	4.10906800	1.61431000
H	-0.40219100	5.61111900	-0.26284100
H	1.19142500	4.81475800	-2.00412000
H	2.13529900	2.54389500	-1.86773900
H	-2.84956100	-2.31396400	1.96845900
H	-4.63780800	-3.98754300	1.77626000
H	-5.79605400	-2.31915600	-2.00526000
H	-4.03112200	-0.62494200	-1.80583200
H	-3.69459000	2.27720400	-0.00910800
H	-4.18404000	3.75522800	-1.90875100
H	-1.41122900	1.56110600	-4.34323100
H	-0.90401600	0.08869100	-2.43756000
H	3.69621700	2.25244000	1.02382100
H	5.46658300	2.11292600	2.71969100
H	4.24916400	-1.89147000	3.67356400
H	2.46758000	-1.75167200	1.97192300
H	4.42993800	1.09514200	-0.94261000
H	5.59226800	0.77489400	-3.07715100

H	2.23690100	-1.43684400	-4.58654600
H	1.07509400	-1.13343300	-2.43262000
C	-6.43151100	-4.33424700	-0.25948200
H	-7.04455500	-4.38971900	0.64680300
H	-7.09528500	-4.12741700	-1.10338100
H	-5.99838300	-5.32972800	-0.41447700
C	-3.11429700	3.70230100	-4.42686700
H	-2.40176500	4.53657500	-4.44649900
H	-3.03037400	3.18331400	-5.38647100
H	-4.11736800	4.13380100	-4.36009500
C	4.70691900	-0.50965500	-5.32525700
H	5.79108100	-0.57029600	-5.19099400
H	4.37647700	-1.41599300	-5.84077700
H	4.51004100	0.33650500	-5.99564200
C	6.05672300	0.03270000	4.39498000
H	6.40711800	-0.99160000	4.55325300
H	6.92255500	0.65369200	4.14552900
H	5.66351100	0.39350000	5.35370600
C	-0.45516600	-2.95161600	0.17405600
C	0.82009000	-2.85385200	0.01565700
H	-1.29319400	-3.63113900	0.20778200
C	2.05742500	-3.61238200	-0.25925200
C	2.95303200	-5.75535900	-0.60895000
H	2.66284200	-6.80835600	-0.65170500
O	1.79031500	-5.00890200	-0.33387800
H	2.50218500	-3.26239400	-1.20758500
H	2.81567700	-3.41667700	0.51885300
H	3.72035800	-5.63223600	0.17366500
H	3.40768000	-5.47461300	-1.57374500

Compound: $^{p\text{-tol}}$4-CH_2OMe'
Charge: 0
Multiplicity: 1
Lowest Frequency: 5.35 cm^{-1}
Energy: -4081.418216 Hartree

Ni	-0.08412400	-0.86677200	0.28543100
P	-2.07605300	-0.11314600	0.15103800
P	1.95420000	0.15540000	0.05956800
O	0.55271900	-1.64179000	1.95223700
C	-2.57743200	-0.42781300	1.90219200
C	-3.88012700	-0.53895500	2.40280500
C	-4.08548900	-0.84952900	3.74672600
C	-2.98942600	-1.05303400	4.58970800

C	-1.69050800	-0.92842900	4.09609900
C	-1.47131200	-0.59802400	2.75232200
C	-0.08281800	-0.49286500	2.14547300
C	0.78052500	0.69067900	2.53357200
C	0.57063500	1.43998000	3.69882400
C	1.41275200	2.50040400	4.03714300
C	2.47757900	2.83994100	3.20568700
C	2.68376800	2.12290800	2.02569800
C	1.84285100	1.06309500	1.67378400
C	-3.29422400	-1.06162200	-0.85749800
C	-3.70456400	-2.33929100	-0.44222800
C	-4.49475600	-3.13966500	-1.26511600
C	-4.89837800	-2.70510000	-2.53489100
C	-4.47274900	-1.43892600	-2.95570700
C	-3.68369600	-0.63113300	-2.13660000
C	-2.56756100	1.65399300	-0.10906900
C	-3.89576900	2.07371900	-0.28651000
C	-4.20753100	3.42620000	-0.40395100
C	-3.21032100	4.40940600	-0.33505900
C	-1.88824100	3.98910300	-0.15200300
C	-1.57014300	2.63546100	-0.04074100
C	3.43743400	-0.92416800	0.25204000
C	3.80319400	-1.44339300	1.50295700
C	4.84893000	-2.35900500	1.61544500
C	5.56571200	-2.79112800	0.49309900
C	5.18772000	-2.28319200	-0.75714800
C	4.14166400	-1.37059100	-0.87891800
C	2.53702900	1.44868900	-1.13006800
C	3.86425700	1.90138400	-1.22737800
C	4.21846500	2.88924600	-2.14325700
C	3.26548100	3.46316800	-2.99736100
C	1.94798000	3.00024900	-2.91232800
C	1.59076800	2.00579800	-2.00090600
H	-4.73209600	-0.40676900	1.74201900
H	-5.09597300	-0.94450000	4.13430400
H	-3.14866000	-1.31502600	5.63211800
H	-0.84078200	-1.10484300	4.74909200
H	-0.26203800	1.19611100	4.34870700
H	1.23007200	3.06251000	4.94895100
H	3.13468100	3.66638100	3.46119100
H	3.48959700	2.41651000	1.36102000
H	-3.40227300	-2.71014900	0.53210300
H	-4.80223900	-4.12201900	-0.91408200
H	-4.76238700	-1.07689600	-3.93950500

H	-3.37338400	0.34527000	-2.49673200
H	-4.69406000	1.34048200	-0.34766000
H	-5.24318500	3.72482900	-0.54960200
H	-1.09274800	4.72832200	-0.09873400
H	-0.53578800	2.34010400	0.10350700
H	3.25272800	-1.14658300	2.38785500
H	5.11116100	-2.74575900	2.59756200
H	5.71898400	-2.60789500	-1.64918800
H	3.86988300	-1.00363500	-1.86404000
H	4.63211800	1.46606700	-0.59507600
H	5.25340500	3.21954600	-2.19871300
H	1.19163200	3.41432200	-3.57481000
H	0.56485600	1.65049700	-1.96678200
C	-5.78187100	-3.56275600	-3.40868300
H	-5.60535700	-4.62834500	-3.23371000
H	-6.84364400	-3.37313400	-3.20650700
H	-5.61348800	-3.36040500	-4.47064400
C	-3.55769700	5.87588300	-0.42803400
H	-2.71698100	6.46322500	-0.80856200
H	-4.41619000	6.04455600	-1.08537600
H	-3.81900800	6.28230700	0.55713600
C	3.65244400	4.55380600	-3.96735300
H	4.61754300	4.34626800	-4.44084400
H	2.90549100	4.67102800	-4.75757400
H	3.74579200	5.52124700	-3.45826400
C	6.72151300	-3.75403700	0.62614300
H	6.82512700	-4.38211400	-0.26418300
H	7.67174400	-3.22073900	0.75801100
H	6.59723800	-4.41148800	1.49189600
C	-0.35019600	-2.58673800	-2.34660800
C	1.69745200	-2.01712100	-3.96819600
C	0.87619700	-3.61542600	-0.55502800
H	1.85441000	-3.47771900	-1.02583800
H	0.96739900	-3.54032100	0.52676300
H	0.45875800	-4.58971800	-0.83912400
O	-0.02816500	-2.57146600	-0.95287500
C	0.77962000	-2.26698600	-3.22386500
H	2.50443400	-1.78396300	-4.62399500
H	-1.15073200	-1.85487400	-2.47356700
H	-0.75416400	-3.57593900	-2.60643700

Compound: $^{p\text{-tol}}$4-Ph
Charge: 0
Multiplicity: 1
Lowest Frequency: 13.64 cm^{-1}
Energy: -4158.667385 Hartree

Ni	0.04661600	-1.05537100	0.02991400
P	-2.02410700	-0.36803200	0.24558600
P	1.42069100	0.65166700	0.08824300
O	0.56213300	0.68154700	3.18737900
C	-2.64819700	0.00768300	1.96952100
C	-3.93590500	-0.36105300	2.38938800
C	-4.35999000	-0.16373700	3.70482900
C	-3.48917800	0.38368500	4.64438600
C	-2.20570300	0.75570600	4.24995700
C	-1.79306800	0.60236100	2.92058500
C	-0.41146400	1.10218300	2.58617800
C	-0.30233500	2.26072600	1.62175200
C	-1.06842300	3.39781100	1.90010100
C	-0.93777200	4.55213600	1.12785500
C	-0.05778600	4.55676500	0.05003600
C	0.68717900	3.41335500	-0.25236600
C	0.59106000	2.25621700	0.52734100
C	-3.23160500	-1.66655500	-0.29639900
C	-3.37317800	-2.84074100	0.46507700
C	-4.21744600	-3.86596600	0.05096100
C	-4.94195900	-3.77117700	-1.14693800
C	-4.79397900	-2.60684200	-1.90507800
C	-3.95608300	-1.56879900	-1.48959300
C	-2.61034000	1.08720500	-0.74060300
C	-3.72588100	1.86038800	-0.38682600
C	-4.16418600	2.89758000	-1.20691400
C	-3.51124200	3.19845400	-2.41005300
C	-2.40138000	2.42271700	-2.76335100
C	-1.95411400	1.38891800	-1.94083300
C	2.84634600	0.62877600	1.26126700
C	3.42596600	1.80326800	1.76360600
C	4.52571200	1.74732300	2.61700200
C	5.08079700	0.52056300	3.00306100
C	4.49515600	-0.64833600	2.50377900
C	3.39389600	-0.59924100	1.65065200
C	2.22423900	1.02509700	-1.54137900
C	3.35732900	1.84160200	-1.68517900
C	3.91288200	2.07868000	-2.94115200

C	3.36573800	1.50746800	-4.09858100
C	2.25138500	0.67343700	-3.95172200
C	1.69346500	0.43231500	-2.69639200
H	-4.61359500	-0.82913300	1.68510900
H	-5.36585200	-0.45474500	3.99349500
H	-3.80202300	0.51614500	5.67579000
H	-1.50717000	1.17507700	4.96756300
H	-1.76486200	3.37964900	2.73314400
H	-1.52936400	5.43210000	1.36168000
H	0.04374600	5.44282300	-0.57005600
H	1.34224800	3.42454000	-1.11596200
H	-2.82158100	-2.94902200	1.39390600
H	-4.31441400	-4.75763100	0.66606400
H	-5.34614700	-2.50194400	-2.83589100
H	-3.87565700	-0.67931700	-2.10433000
H	-4.25897100	1.65454700	0.53577600
H	-5.03166100	3.48201600	-0.90887000
H	-1.87425400	2.63089700	-3.69123200
H	-1.08167100	0.81455100	-2.23391800
H	3.00580100	2.77108800	1.50725800
H	4.95494400	2.67216200	2.99564900
H	4.90199300	-1.61562500	2.78807300
H	2.95282600	-1.52172700	1.29363300
H	3.82313100	2.28196200	-0.80963000
H	4.79424700	2.71049500	-3.02277400
H	1.82274700	0.19177400	-4.82707300
H	0.85898600	-0.25683800	-2.60234100
C	-5.83267700	-4.90104400	-1.60437800
H	-6.43897800	-5.29249500	-0.78071700
H	-6.51055200	-4.57958900	-2.40003300
H	-5.24139200	-5.73876000	-1.99417400
C	-3.97372400	4.34229300	-3.28011400
H	-3.52961500	5.29112400	-2.95377100
H	-3.68756000	4.19198900	-4.32507800
H	-5.06050800	4.46360200	-3.23913200
C	3.95677800	1.78993000	-5.45870200
H	5.04314200	1.90983900	-5.40653800
H	3.73684000	0.98502900	-6.16577300
H	3.54883900	2.71669900	-5.88163000
C	6.24997900	0.46015200	3.95661700
H	6.88041600	-0.41253500	3.76127000
H	6.87521000	1.35516000	3.88279000
H	5.90791200	0.38708100	4.99667600
C	-0.21225400	-2.86616900	-0.18828700

C	1.04824700	-2.61672000	-0.34064800
H	-0.97298300	-3.62940800	-0.26581400
C	2.31997000	-3.28535600	-0.57466500
C	3.37150800	-2.67316500	-1.27979300
C	2.52124800	-4.59712300	-0.09754400
C	4.56880700	-3.34836100	-1.51182600
H	3.23895200	-1.66202600	-1.64808300
C	3.72238900	-5.26536400	-0.31844300
H	1.72059800	-5.07861600	0.45573800
C	4.75267700	-4.64565800	-1.03077800
H	5.36337900	-2.85577400	-2.06574900
H	3.85535100	-6.27408900	0.06367900
H	5.68912800	-5.16789900	-1.20527300

Compound: *p*-tol5-Ph
Charge: 0
Multiplicity: 1
Lowest Frequency: 8.99 cm^{-1}
Energy: -4618.360448 Hartree

Ni	-0.03161400	-0.53504300	0.55036400
P	-1.84206900	0.53832200	-0.25069600
P	-0.37820500	-2.11452900	-0.83528300
P	1.96127700	-0.15708200	-0.33648300
C	-2.31182000	-0.36840400	-1.81082700
C	-1.68716500	-1.60802900	-2.05327500
C	-2.04114800	-2.35076700	-3.18806100
C	-2.98386700	-1.86151500	-4.09085000
C	-3.58455100	-0.62130800	-3.86476800
C	-3.25343100	0.11719500	-2.72931400
C	-3.31545200	0.27091400	0.83299200
C	-4.43436500	-0.49345500	0.47722900
C	-5.47953700	-0.69545700	1.38127800
C	-5.44816000	-0.14071000	2.66452200
C	-4.32980700	0.62876000	3.01680800
C	-3.27886700	0.82426700	2.12583600
C	-6.56663200	-0.37940300	3.65051900
C	-2.05962300	2.30407700	-0.77072800
C	-3.20115500	3.07184500	-0.49828900
C	-3.28823600	4.39738400	-0.92643900
C	-2.24755700	4.99963600	-1.64246900
C	-1.11007300	4.22791000	-1.91750500
C	-1.01209300	2.90856000	-1.48374800
C	-2.33200700	6.44254700	-2.07982400

C	-0.86447100	-3.82031800	-0.34221400
C	0.11208900	-4.74807000	0.05608500
C	-0.25528600	-5.99787000	0.55402500
C	-1.60362500	-6.34011500	0.67135200
C	-2.58224400	-5.42045500	0.29177200
C	-2.21702400	-4.17036600	-0.20799300
C	2.19397700	-1.45838900	-1.65936700
C	1.14500000	-2.37453000	-1.86427400
C	1.30607600	-3.41565900	-2.79110900
C	2.48607600	-3.53928600	-3.52150300
C	3.52438400	-2.62592500	-3.32518500
C	3.37987500	-1.59888200	-2.39453100
C	3.47097400	-0.46313300	0.70179400
C	3.35623400	-1.35325400	1.78072100
C	4.46373000	-1.67010600	2.56561600
C	5.72021100	-1.10680100	2.31193400
C	5.83170500	-0.21554000	1.23751100
C	4.72939000	0.10272700	0.44554100
C	6.90808800	-1.42325100	3.18864100
C	2.41401300	1.41039000	-1.20546100
C	2.67154100	2.55112600	-0.42184300
C	2.92555400	3.78432800	-1.01235800
C	2.91976000	3.93876600	-2.40765000
C	2.64036000	2.81024000	-3.18468300
C	2.39384800	1.56572900	-2.59826300
C	3.22463900	5.27549700	-3.04097600
C	-0.22473000	-1.26607900	2.34205400
C	0.09544700	-0.04020300	2.45224400
C	0.40592500	1.10692900	3.27161300
C	0.71638400	0.95285000	4.64027400
C	1.00651800	2.05664900	5.43522800
C	0.98982500	3.34513700	4.89061500
C	0.68162100	3.51503900	3.54023100
C	0.39941400	2.41005500	2.73721300
H	-1.57874100	-3.31502900	-3.37234900
H	-3.24343400	-2.44244700	-4.97130200
H	-4.31293700	-0.23164900	-4.57037700
H	-3.72640400	1.07853300	-2.55416600
H	-4.50412000	-0.92917400	-0.51378400
H	-6.33751600	-1.29098300	1.07762500
H	-4.27692600	1.07519800	4.00702800
H	-2.42169800	1.41351800	2.43665900
H	-7.47672000	-0.72147400	3.14928400
H	-6.80920700	0.53032000	4.20950700

H	-6.28991100	-1.14448700	4.38660100
H	-4.02833700	2.63704000	0.05258800
H	-4.18435200	4.97141100	-0.70163200
H	-0.28377500	4.66478000	-2.47265600
H	-0.11185400	2.34280200	-1.69912800
H	-3.36922800	6.78681300	-2.12722500
H	-1.80126600	7.10120300	-1.38078600
H	-1.88034600	6.58985500	-3.06611000
H	1.16438200	-4.49426500	-0.02800100
H	0.51423000	-6.70501400	0.85086800
H	-1.88884800	-7.31392800	1.05857700
H	-3.63432900	-5.67493500	0.38434200
H	-2.98880300	-3.46238500	-0.49241200
H	0.51776700	-4.14968100	-2.92529900
H	2.59973700	-4.35117200	-4.23422100
H	4.44985200	-2.72303900	-3.88571100
H	4.20035300	-0.90788000	-2.22853900
H	2.38887200	-1.78330200	2.01848000
H	4.34672100	-2.36264400	3.39596700
H	6.79576100	0.23665600	1.01566200
H	4.85356900	0.80407300	-0.37329500
H	6.84636600	-2.43686400	3.59616700
H	7.84877000	-1.33537200	2.63663400
H	6.96580800	-0.73432300	4.04082300
H	2.66842000	2.47137600	0.66170600
H	3.12737500	4.64555900	-0.37959900
H	2.62035400	2.89902400	-4.26839700
H	2.18412800	0.71474900	-3.23777300
H	2.69136400	6.08915400	-2.53793100
H	2.94524900	5.29076600	-4.09823200
H	4.29484100	5.50919500	-2.98031000
H	-0.51277700	-2.19462300	2.80746300
H	0.72787400	-0.04667300	5.06426600
H	1.24642100	1.91454600	6.48570600
H	1.21589900	4.20533200	5.51424100
H	0.66141400	4.51181200	3.10781500
H	0.15773100	2.54050100	1.68707700

Compound: ^{Ph}6-H
Charge: 0
Multiplicity: 1
Lowest Frequency: 17.21 cm^{-1}
Energy: -3732.211826 Hartree

Ni	-0.03662200	-0.22379800	-1.57094200
P	-1.81978800	-0.03538200	-0.35420500
P	1.73221700	-0.07733900	-0.32660400
O	-0.23488000	1.78610700	1.15811100
C	-1.59446600	-0.10760800	1.47761800
C	-0.68551400	0.80860600	2.02992300
C	-0.31175900	0.76432200	3.37049700
C	-0.86321900	-0.21985700	4.19244000
C	-1.77794000	-1.13633700	3.67541900
C	-2.13874800	-1.07783400	2.32735500
C	-2.75724200	1.54271800	-0.59108400
C	-3.47961600	2.16503300	0.43768200
C	-4.18540500	3.34494000	0.19787400
C	-4.18209100	3.91812600	-1.07452700
C	-3.46500200	3.30780200	-2.10447100
C	-2.75508200	2.13118500	-1.86397300
C	-3.11105600	-1.33562900	-0.62517000
C	-4.46686400	-1.14970400	-0.31336400
C	-5.39064400	-2.17507200	-0.51747200
C	-4.97376300	-3.40288800	-1.03546400
C	-3.62984000	-3.59766500	-1.35551400
C	-2.70741800	-2.56925900	-1.15656100
C	2.10472800	1.50408900	0.59271600
C	1.07576700	2.22899200	1.22335000
C	1.31111900	3.45248900	1.84967500
C	2.60323300	3.97240700	1.89549700
C	3.65018500	3.26204400	1.31043400
C	3.39793200	2.04930500	0.66795200
C	1.92107900	-1.36691800	0.99066300
C	2.76698300	-1.21829200	2.10002500
C	2.90319500	-2.24660700	3.03248500
C	2.19905000	-3.44103200	2.86812800
C	1.35460000	-3.60024600	1.76930100
C	1.21474000	-2.56894600	0.83961800
C	3.29588600	-0.29257500	-1.29758300
C	4.14444000	-1.39688400	-1.14907700
C	5.26530600	-1.54824600	-1.97082800
C	5.55906100	-0.59601000	-2.94475000
C	4.71930900	0.51023100	-3.10137200
C	3.59506000	0.65541900	-2.29200100
C	0.60401000	-0.46506900	-3.29406900
C	-0.68298900	-0.52135200	-3.29505200
H	0.39781600	1.48600100	3.76011100
H	-0.57637000	-0.26383200	5.23896400

H	-2.20763900	-1.90001900	4.31636500
H	-2.84056300	-1.80216500	1.92851300
H	-3.48264000	1.73419300	1.43424300
H	-4.73600000	3.81674100	1.00711300
H	-4.73002800	4.83759000	-1.26017300
H	-3.45040900	3.75125600	-3.09606600
H	-2.17966600	1.66975800	-2.66044800
H	-4.80591000	-0.19734300	0.08169600
H	-6.43729200	-2.01299200	-0.27544900
H	-5.69450600	-4.19964500	-1.19612200
H	-3.29901300	-4.54579800	-1.76981100
H	-1.66808000	-2.70885600	-1.43821800
H	0.46974600	3.98136300	2.28509000
H	2.78693500	4.92463500	2.38390400
H	4.66315500	3.65160400	1.34364800
H	4.22120200	1.52307900	0.19886300
H	3.32023800	-0.29489500	2.23926900
H	3.55995200	-2.11457300	3.88780900
H	2.30561800	-4.24121000	3.59503200
H	0.79947800	-4.52436600	1.63644100
H	0.54770800	-2.68972600	-0.00892000
H	3.93467600	-2.14606700	-0.39368500
H	5.90915300	-2.41396000	-1.84319600
H	6.43173600	-0.71413700	-3.58051900
H	4.93674500	1.25704100	-3.85980400
H	2.93964600	1.51009500	-2.43205400
H	1.50543500	-0.53685500	-3.88569000
H	-1.56526300	-0.67070000	-3.90119300

Compound: ^{Ph}6-H (TS)
Charge: 0
Multiplicity: 1
Lowest Frequency: -120.55 cm^{-1}
Energy: -3732.168155 Hartree

Ni	0.02359700	-0.94252800	-0.84727800
P	1.98727400	-0.04309100	-0.35213600
P	-1.91030300	0.00204200	-0.36613000
O	0.02887600	-1.40188000	1.31455000
C	1.91234700	0.03833200	1.49389000
C	0.85293700	-0.62146800	2.13860400
C	0.65018000	-0.50607500	3.51319400
C	1.53180200	0.26827600	4.26854800
C	2.60204700	0.92169200	3.65973100

C	2.78065300	0.80663800	2.28204900
C	3.42357900	-1.15263300	-0.68708300
C	4.16500200	-1.79920900	0.31226200
C	5.18531100	-2.69195000	-0.02327500
C	5.48483100	-2.94880000	-1.36099000
C	4.75023000	-2.31449000	-2.36592000
C	3.72343800	-1.43376200	-2.03247500
C	2.65222900	1.63179900	-0.77044600
C	3.97617400	1.88818000	-1.15625100
C	4.38184100	3.18415100	-1.48435500
C	3.47628000	4.24298700	-1.41988700
C	2.15695400	3.99892500	-1.03024600
C	1.74702100	2.70485500	-0.71754300
C	-2.33287900	-1.11397400	1.06199000
C	-1.26970300	-1.73876100	1.72782800
C	-1.46562500	-2.72900900	2.68479700
C	-2.77123300	-3.08334400	3.03240300
C	-3.85198700	-2.45493200	2.41443200
C	-3.63192500	-1.48584600	1.43335000
C	-2.13250000	1.69785500	0.33882000
C	-2.34170300	1.96402500	1.69942400
C	-2.40900800	3.27899600	2.16725800
C	-2.28450300	4.34933100	1.28278300
C	-2.08244200	4.09817200	-0.07769000
C	-1.99738100	2.78744000	-0.54190100
C	-3.42196500	-0.17546500	-1.42309700
C	-4.53240700	0.68110600	-1.35104700
C	-5.63861000	0.48319800	-2.17922500
C	-5.65381400	-0.57386800	-3.09015400
C	-4.55476400	-1.43054500	-3.17100700
C	-3.44548800	-1.23326300	-2.34840100
C	0.04326800	-1.65939100	-2.61335900
C	0.05222700	-2.64622900	-1.81832000
H	-0.18402800	-1.00044300	3.99318900
H	1.37166300	0.35812100	5.33887800
H	3.28523500	1.52501400	4.24927400
H	3.59470500	1.33653400	1.79755700
H	3.94764000	-1.60642300	1.35759600
H	5.74919800	-3.18330200	0.76498600
H	6.28011700	-3.64176500	-1.62014300
H	4.97063000	-2.51416500	-3.41082600
H	3.14318200	-0.96373400	-2.82124100
H	4.69328600	1.07563300	-1.20639000
H	5.41014400	3.36439600	-1.78582400

H	3.79414200	5.25010800	-1.67438600
H	1.44243300	4.81560800	-0.97654500
H	0.71625600	2.52160400	-0.42900700
H	-0.60994700	-3.22170100	3.13351500
H	-2.93728500	-3.85772700	3.77497000
H	-4.86761400	-2.73195800	2.68027800
H	-4.47730300	-1.02937600	0.92891100
H	-2.45515200	1.14334500	2.40031500
H	-2.56725100	3.46390000	3.22618200
H	-2.34224800	5.37068100	1.64747500
H	-1.98771300	4.92474100	-0.77659600
H	-1.82497800	2.60199600	-1.59939500
H	-4.53332100	1.50836600	-0.64909500
H	-6.48916400	1.15581400	-2.10990600
H	-6.51471000	-0.72642300	-3.73491700
H	-4.55623800	-2.25229200	-3.88168900
H	-2.58674200	-1.89160700	-2.43016600
H	0.02603000	-1.25531600	-3.61364400
H	0.08027600	-3.71572500	-1.68412300

Compound: ^{Ph}6-Ph
Charge: 0
Multiplicity: 1
Lowest Frequency: 9.73 cm^{-1}
Energy: -3963.281922 Hartree

Ni	0.26847200	1.00785700	-0.11841400
P	1.25518700	-0.93462300	-0.01006200
P	-1.89231600	0.70580100	0.00194600
O	-1.02923800	-1.88933100	-1.43497500
C	0.20772700	-2.36616400	0.50958600
C	-0.93209400	-2.62566900	-0.26570000
C	-1.86697800	-3.59346300	0.09301700
C	-1.66062000	-4.33161400	1.25939000
C	-0.53149600	-4.10347300	2.04479700
C	0.39443500	-3.12760200	1.66939900
C	1.98336900	-1.53181400	-1.60253000
C	2.18623600	-2.89091500	-1.88749800
C	2.74485100	-3.28625200	-3.10322700
C	3.10579100	-2.32904400	-4.05329500
C	2.89762300	-0.97596600	-3.78480100
C	2.33588800	-0.58017400	-2.57006300
C	2.64729000	-1.06111000	1.20644300
C	3.69459500	-1.98796300	1.09252500

C	4.69661200	-2.05154900	2.06171700
C	4.66517400	-1.19287000	3.16172900
C	3.63230100	-0.26271800	3.28277100
C	2.63556400	-0.19400900	2.30914800
C	-2.81065700	-0.25625000	-1.31039800
C	-2.26355400	-1.42995600	-1.86022200
C	-2.88560900	-2.12167100	-2.89903000
C	-4.10868900	-1.67506400	-3.39517800
C	-4.69791300	-0.53790300	-2.84484300
C	-4.05314700	0.15788200	-1.82157100
C	-2.51822700	-0.04440000	1.57648800
C	-3.77197100	-0.66263900	1.69431100
C	-4.20471900	-1.16163000	2.92284600
C	-3.39324200	-1.04631100	4.05313000
C	-2.14430500	-0.43374200	3.94808000
C	-1.70913100	0.05927200	2.71732300
C	-2.82779900	2.30525300	-0.05146900
C	-3.54981900	2.80802900	1.03786300
C	-4.17935300	4.05403500	0.96022300
C	-4.10293900	4.81109100	-0.20696700
C	-3.38406600	4.31961900	-1.30017000
C	-2.74700000	3.08345600	-1.21995300
C	0.37531500	2.84035400	-0.23180900
C	1.57918400	2.35969200	-0.21383500
C	2.97240600	2.78461100	-0.20873800
C	4.03737700	1.88688100	-0.39416700
C	5.35978700	2.32822100	-0.39820400
C	5.65242700	3.67949100	-0.20995200
C	4.60706900	4.58783900	-0.01872300
C	3.28743600	4.14708100	-0.02012300
H	-2.73843600	-3.76237600	-0.52991300
H	-2.38513400	-5.08710600	1.54872800
H	-0.37107500	-4.67902600	2.95123000
H	1.26381800	-2.94630000	2.29142700
H	1.89204400	-3.64563800	-1.16429500
H	2.89378100	-4.34253800	-3.30956400
H	3.53898200	-2.63769400	-5.00047900
H	3.16534800	-0.22507700	-4.52251800
H	2.15711400	0.47136400	-2.36858100
H	3.73776500	-2.65629200	0.23899600
H	5.50387700	-2.77066100	1.95458300
H	5.44707100	-1.24145500	3.91420700
H	3.60888700	0.42077500	4.12653700
H	1.85557400	0.55761600	2.38502500

H	-2.39262900	-2.99907300	-3.30436100
H	-4.59495300	-2.21336600	-4.20312800
H	-5.65504400	-0.18285800	-3.21466900
H	-4.51831200	1.05197400	-1.42356600
H	-4.41373000	-0.75775900	0.82417600
H	-5.17718800	-1.64032200	2.99700200
H	-3.73186900	-1.43503600	5.00926700
H	-1.50470500	-0.34342600	4.82129000
H	-0.73182300	0.52571000	2.63372500
H	-3.62531500	2.23159500	1.95302200
H	-4.73247100	4.42801200	1.81720500
H	-4.59500900	5.77754500	-0.26618400
H	-3.31408000	4.90262600	-2.21412200
H	-2.17858700	2.71767600	-2.07015200
H	-0.22633100	3.73607600	-0.29162700
H	3.81925200	0.83553000	-0.53762900
H	6.16376600	1.61245200	-0.54626100
H	6.68313500	4.02280700	-0.21059400
H	4.82301900	5.64258100	0.13003200
H	2.47612000	4.85343300	0.12839000

Compound: $^{p\text{=tol}}$7-PhCN
Charge: 0
Multiplicity: 1
Lowest Frequency: 10.20 cm^{-1}
Energy: -4174.765422 Hartree

Ni	0.03472200	-0.31569000	-0.65651900
P	2.07877200	0.23379400	-0.23921700
P	-1.90277200	0.79256800	-0.11940600
O	-0.54216300	-0.38195800	-2.52591200
C	2.61363800	0.62639900	-1.95778600
C	-0.44155400	-3.09849100	0.42770300
C	3.93165800	0.63000900	-2.43215100
C	4.18074200	0.80406800	-3.79290500
C	3.11156600	0.95007700	-4.68117300
C	1.79833400	0.94348400	-4.21029200
C	1.53523600	0.80168300	-2.84091400
C	0.12167600	0.73350200	-2.28267900
C	-0.71056400	2.00538900	-2.29817300
C	-0.69961000	-4.42055700	0.89307700
C	-0.47380400	3.06698800	-3.18122000
C	0.35406200	-5.20909900	1.39333600
C	-1.32407300	4.17416900	-3.22031800

C	0.09256000	-6.49904900	1.84461900
C	-2.42471300	4.24612600	-2.36884600
C	-1.20672300	-7.01149400	1.80050000
C	-2.65506700	3.21301400	-1.45879200
C	-2.25234300	-6.22950200	1.30255100
C	-1.80313500	2.10677600	-1.40873500
C	-2.00890400	-4.93671500	0.84918400
C	3.29175000	-1.07197500	0.26546300
C	3.16588200	-2.33526300	-0.33880700
C	4.03959800	-3.37114100	-0.01931500
C	5.06408100	-3.19298400	0.92287900
C	5.18713500	-1.93515200	1.52129600
C	4.31967400	-0.88900700	1.19881700
C	2.56413900	1.68560600	0.79001000
C	3.11858000	2.85555400	0.25524600
C	3.40599700	3.94798900	1.07515600
C	3.16041500	3.90983600	2.45200900
C	2.61166900	2.73491600	2.98687400
C	2.30795200	1.64721400	2.17169600
C	-3.39149800	-0.20353400	-0.53727700
C	-3.90474100	-0.25281300	-1.84151700
C	-4.95355300	-1.11335100	-2.16156200
C	-5.52424900	-1.95816600	-1.20144700
C	-5.00327300	-1.91456500	0.09876200
C	-3.94951500	-1.06127800	0.42509500
C	-2.41040500	1.73603400	1.38584900
C	-3.73768300	1.95592200	1.78407000
C	-4.02490700	2.70403400	2.92603100
C	-3.00399600	3.26216200	3.70519500
C	-1.67981500	3.04729000	3.30036200
C	-1.38634100	2.29231100	2.16747900
H	4.75654200	0.47080200	-1.74336800
H	5.20187800	0.80422200	-4.16355500
H	3.30229900	1.05586400	-5.74564500
H	0.97078200	1.02511700	-4.90858200
H	0.38194200	3.03320900	-3.84548800
H	1.35968900	-4.80233700	1.41679800
H	-1.11988100	4.98266000	-3.91711700
H	0.90467900	-7.10739700	2.23060900
H	-3.08605900	5.10742200	-2.39467000
H	-1.40401800	-8.01925800	2.15318300
H	-3.48314500	3.28684700	-0.76006400
H	-3.26136600	-6.62856100	1.26797200
H	-2.81289300	-4.31833600	0.46377200

H	2.38136800	-2.50257800	-1.07124400
H	3.92953900	-4.33331800	-0.51475700
H	5.97853000	-1.76407800	2.24739600
H	4.45368800	0.07472100	1.67833300
H	3.32849400	2.91700400	-0.80751700
H	3.83405500	4.84512500	0.63421400
H	2.41661800	2.67314500	4.05510300
H	1.86951200	0.75554800	2.61305100
H	-3.47492700	0.37783800	-2.61127500
H	-5.33625700	-1.12691600	-3.17949400
H	-5.43263800	-2.55158900	0.86917900
H	-3.57065600	-1.05238800	1.44361200
H	-4.55469800	1.53909800	1.20385400
H	-5.06219700	2.86106600	3.21319900
H	-0.86500500	3.47246400	3.88188300
H	-0.35035900	2.13691700	1.88149700
C	5.98867800	-4.32925800	1.28947200
H	6.23246000	-4.94435500	0.41746300
H	6.92564900	-3.96066100	1.71671900
H	5.52979900	-4.99233400	2.03384700
C	3.44802000	5.10345500	3.33085100
H	4.24098200	5.72853900	2.91001200
H	2.55900100	5.73698300	3.44172600
H	3.75431500	4.79719800	4.33591800
C	-3.31766100	4.04593900	4.95719300
H	-3.29068400	3.40260000	5.84587800
H	-2.59247700	4.84955300	5.11861400
H	-4.31498400	4.49320100	4.91067100
C	-6.64655100	-2.90152500	-1.56424500
H	-7.35648600	-2.43296100	-2.25335000
H	-6.26493200	-3.80260100	-2.06089800
H	-7.20033400	-3.22599100	-0.67823200
N	-0.23184500	-2.01887100	0.04345600

Compound: $^{p=tol}$7-PhCN'
Charge: 0
Multiplicity: 1
Lowest Frequency: 11.06 cm^{-1}
Energy: -4174.752997 Hartree

Ni	0.00586700	0.73883400	-0.84177300
P	-2.10527300	0.18258800	-0.27635000
P	1.71531900	-0.60694100	-0.18046800
O	0.59948300	0.35462700	-2.68184800

C	-2.72166500	-0.07609400	-1.99486100
C	0.47582600	2.58106600	-0.28425200
C	-4.03493300	0.09175400	-2.44653400
C	-4.32727300	-0.06111700	-3.80304500
C	-3.30759800	-0.36953500	-4.70639600
C	-1.99604200	-0.53775600	-4.25828400
C	-1.69574100	-0.39891300	-2.89871400
C	-0.28620900	-0.54467700	-2.36006400
C	0.24026500	-1.93834600	-2.10054900
C	1.34938500	3.35727900	0.58450700
C	-0.22009800	-3.05394900	-2.81128500
C	1.74213900	2.86745400	1.83735000
C	0.36890200	-4.30648700	-2.63440200
C	2.55543100	3.63743600	2.66722600
C	1.42436000	-4.46431100	-1.73729500
C	2.99677300	4.89376600	2.24804000
C	1.87354000	-3.36647100	-1.00100700
C	2.61317300	5.38461600	0.99717600
C	1.27900200	-2.11183200	-1.15955600
C	1.78829800	4.62712000	0.17008600
C	-3.26594900	1.43470400	0.42305200
C	-3.36457900	2.68622000	-0.21298700
C	-4.20447400	3.67242300	0.29523400
C	-4.96607100	3.45822000	1.45325600
C	-4.86146600	2.21384600	2.08219000
C	-4.02649500	1.21484400	1.57873000
C	-2.54664200	-1.36271000	0.62535500
C	-3.40802200	-2.34057900	0.10827400
C	-3.71491700	-3.48142900	0.84828400
C	-3.18443700	-3.68236500	2.12894100
C	-2.32751000	-2.70147200	2.64460300
C	-2.00362100	-1.56624600	1.90305200
C	3.40111100	-0.15139800	-0.79020700
C	4.54892000	-0.88705200	-0.45633700
C	5.79602300	-0.53103700	-0.96442100
C	5.94057100	0.56418600	-1.82656000
C	4.79290100	1.29406300	-2.15701500
C	3.54150600	0.94513300	-1.65093600
C	2.04551500	-1.23444600	1.52328400
C	2.93135800	-0.54579600	2.37073900
C	3.10914400	-0.93989700	3.69514900
C	2.41117000	-2.03100500	4.22984300
C	1.52769500	-2.71336400	3.38565100
C	1.34089500	-2.32263700	2.05947300

H	-4.81780400	0.36942400	-1.74708900
H	-5.34467800	0.07764500	-4.15728900
H	-3.53251700	-0.46641600	-5.76482500
H	-1.19908800	-0.75476500	-4.96340400
H	-1.03607300	-2.93858600	-3.51675500
H	1.40122200	1.88707200	2.15176400
H	0.00368000	-5.15786200	-3.20191200
H	2.84750900	3.25382100	3.64039600
H	1.88813600	-5.43678200	-1.59985300
H	3.63757900	5.48865600	2.89236000
H	2.67410800	-3.49928000	-0.27976100
H	2.95419200	6.36186900	0.66795000
H	1.47839500	5.00242500	-0.79962600
H	-2.77393400	2.88724300	-1.09920300
H	-4.26736300	4.62986400	-0.21670800
H	-5.44560100	2.01633500	2.97791000
H	-3.97952500	0.25957500	2.08994500
H	-3.84252300	-2.21263100	-0.87759000
H	-4.38395400	-4.22658200	0.42442200
H	-1.89955800	-2.82946900	3.63580800
H	-1.32004300	-0.83281800	2.32127300
H	4.47779200	-1.73403400	0.21882800
H	6.67169200	-1.11266500	-0.68575100
H	4.87652900	2.15140000	-2.82029600
H	2.66525700	1.51533100	-1.93567700
H	3.49967700	0.29638200	1.98914200
H	3.81063600	-0.39467300	4.32237000
H	0.97772300	-3.57044000	3.76729100
H	0.64525600	-2.87558900	1.43889300
C	-5.85513800	4.54623600	2.00601900
H	-6.46996300	4.99836300	1.22035900
H	-6.52520000	4.16179100	2.77999500
H	-5.26217400	5.35359200	2.45287200
C	-3.50249500	-4.93186700	2.91472100
H	-4.51161100	-5.29480500	2.69765300
H	-2.80658100	-5.74316900	2.66672600
H	-3.42831800	-4.75766200	3.99219700
C	2.59025100	-2.43974400	5.67219200
H	1.92843300	-1.86522700	6.33263800
H	2.35779300	-3.49837400	5.82043500
H	3.61546100	-2.26640800	6.01349300
C	7.28869900	0.92860600	-2.40048900
H	8.10042200	0.67489800	-1.71188000
H	7.47727200	0.38921000	-3.33729700

H	7.35291800	1.99763900	-2.62356700
N	-0.35926500	2.67114200	-1.15470100

Compound: $^{p=tol}$7-PhCN''
Charge: 0
Multiplicity: 1
Lowest Frequency: 12.06 cm^{-1}
Energy: -4174.749956 Hartree

Ni	0.05568100	0.99496200	-0.01583700
P	-2.05135200	0.30860700	-0.19773200
P	1.46326900	-0.64701400	-0.17639900
O	0.45368400	-0.35516200	-3.12045500
C	-2.73530200	-0.12497900	-1.88163000
C	0.93007900	2.57588200	0.43313600
C	-4.07128700	0.14554600	-2.21762400
C	-4.55619900	-0.07771300	-3.50651900
C	-3.70274700	-0.55172700	-4.50156000
C	-2.37138800	-0.82206500	-4.19140800
C	-1.89363500	-0.63807700	-2.88835900
C	-0.45495800	-0.99453300	-2.61781200
C	-0.18853800	-2.24252600	-1.81532600
C	2.12350300	3.34608600	0.78825400
C	-0.84193700	-3.41947700	-2.20050400
C	3.28502600	2.71669800	1.25548400
C	-0.54379600	-4.63408300	-1.58353800
C	4.40681300	3.46903200	1.60146700
C	0.39163000	-4.66574700	-0.55282800
C	4.38601700	4.85858500	1.47329300
C	1.02052100	-3.48805100	-0.14040700
C	3.23336000	5.49568300	1.00387000
C	0.75070200	-2.26318200	-0.76122900
C	2.10860000	4.74786300	0.66812900
C	-3.27142500	1.60067500	0.32120800
C	-3.21628500	2.85158400	-0.31804200
C	-4.12554400	3.85389500	0.00159100
C	-5.11521300	3.65717700	0.97564000
C	-5.16881100	2.41183100	1.60768900
C	-4.26598900	1.39579400	1.28522400
C	-2.52920200	-1.11829900	0.87110500
C	-3.18953100	-2.26281600	0.41150300
C	-3.50810700	-3.30270500	1.28684400
C	-3.19200700	-3.23144300	2.64741900
C	-2.54369200	-2.07636300	3.10898500

C	-2.21030400	-1.04178600	2.23829200
C	2.89085200	-0.43731200	-1.32887300
C	3.68122200	-1.52009000	-1.74323300
C	4.75948300	-1.32666900	-2.60348300
C	5.08447800	-0.04977900	-3.08162600
C	4.29423200	1.02692900	-2.66425400
C	3.21288700	0.83836000	-1.80477100
C	2.26675400	-1.13179400	1.41898900
C	3.65119600	-1.09170300	1.62862200
C	4.19431900	-1.39435400	2.87980500
C	3.38102500	-1.75187200	3.95881700
C	1.99559800	-1.80241000	3.74300700
C	1.44691400	-1.49150100	2.50296900
H	-4.73654100	0.55534000	-1.46602900
H	-5.59637500	0.13666000	-3.73377000
H	-4.06651100	-0.70262500	-5.51361400
H	-1.68937700	-1.17796100	-4.95803900
H	-1.57714000	-3.38347500	-2.99885400
H	3.29686400	1.63678300	1.34983400
H	-1.04503800	-5.54317000	-1.90199700
H	5.29884500	2.96903600	1.96791700
H	0.62806700	-5.60279900	-0.05687100
H	5.26258400	5.44371900	1.73696200
H	1.72298700	-3.52535300	0.68460200
H	3.21264400	6.57731200	0.90333700
H	1.20589700	5.23139700	0.30916200
H	-2.44757800	3.04533600	-1.05597700
H	-4.05985800	4.81198900	-0.50844700
H	-5.93022800	2.22553900	2.36139400
H	-4.35084100	0.44049500	1.79024700
H	-3.46425000	-2.34703600	-0.63437400
H	-4.01943800	-4.18221300	0.90300500
H	-2.29901600	-1.98533800	4.16470500
H	-1.71198200	-0.15645000	2.62536000
H	3.45206400	-2.52483800	-1.40106400
H	5.35655700	-2.18175500	-2.91206000
H	4.52242200	2.02890600	-3.01887400
H	2.60661300	1.68598200	-1.50736300
H	4.31572100	-0.82519500	0.81408900
H	5.27261000	-1.35363200	3.01393600
H	1.33670900	-2.08504300	4.56086900
H	0.37054100	-1.54332300	2.37211500
C	-6.07274500	4.76544100	1.34196400
H	-6.43385700	5.29331600	0.45312600

H	-6.94128100	4.38217200	1.88519000
H	-5.58684500	5.51146900	1.98293300
C	-3.51616000	-4.36724500	3.58778900
H	-4.33163700	-4.98600000	3.20258600
H	-2.64786400	-5.02265900	3.73058100
H	-3.80748600	-3.99839000	4.57621600
C	3.96506700	-2.05366000	5.31774300
H	3.80473700	-1.21873300	6.01085900
H	3.50011200	-2.93752300	5.76696000
H	5.04266400	-2.23040300	5.26029200
C	6.23018200	0.15040700	-4.04433200
H	7.03700400	-0.56659300	-3.86356900
H	5.90112800	0.01339900	-5.08208700
H	6.64689100	1.15885000	-3.96652300
N	-0.26453800	2.82717400	0.24334100

Compound: $^{p\text{=tol}}$16-MCP
Charge: 0
Multiplicity: 1
Lowest Frequency: 7.91 cm^{-1}
Energy: -4004.993040 Hartree

Ni	0.00530800	-0.22494600	0.05167200
P	-2.17850000	-0.05053800	0.02113400
P	2.18021500	-0.07268500	0.14746400
O	0.15010700	1.24861900	1.29468100
C	-2.53282500	-0.01173500	1.82105400
C	-3.82854200	0.01205700	2.34543000
H	-4.68067500	-0.09318000	1.67990000
C	-4.02876500	0.16183500	3.71778000
H	-5.03438400	0.16147500	4.12752100
C	-2.92381600	0.33543100	4.54991500
H	-3.06538100	0.49813900	5.61486200
C	-1.62967100	0.31111500	4.02607600
H	-0.79417300	0.49802800	4.68934000
C	-1.40101400	0.09204700	2.65867000
C	-0.03404300	0.11355800	2.00882400
C	1.19578200	-0.42593500	2.68776400
C	1.25313900	-0.98563100	3.97337500
H	0.34637600	-1.12828300	4.54540300
C	2.46894300	-1.37903100	4.54037300
H	2.47512300	-1.79833000	5.54278600
C	3.66122500	-1.23491500	3.83751600
H	4.60711100	-1.52849900	4.28229800

C	3.61766000	-0.75859500	2.52373100
H	4.53056800	-0.72689300	1.93664200
C	2.40425200	-0.39628200	1.94289100
C	-2.76086200	1.56660800	-0.62764700
C	-2.73031600	1.79719700	-2.01500400
H	-2.38671000	1.01377500	-2.68231300
C	-3.11681000	3.02703300	-2.53844000
H	-3.08914400	3.17950900	-3.61478400
C	-3.52724100	4.07581200	-1.70197300
C	-3.53086000	3.84844700	-0.32242000
H	-3.82932800	4.64851900	0.35033600
C	-3.15643400	2.61453200	0.21248300
H	-3.16709600	2.47686500	1.28726700
C	-3.33579600	-1.30833100	-0.64999500
C	-4.41873100	-0.99735800	-1.48172700
H	-4.59538800	0.02630600	-1.79105200
C	-5.28963000	-1.99781900	-1.91792600
H	-6.12209900	-1.73093800	-2.56420800
C	-5.11413800	-3.33093700	-1.53587200
C	-4.03749900	-3.63397100	-0.68906400
H	-3.88197000	-4.66090300	-0.36752600
C	-3.16103000	-2.64577700	-0.25558200
H	-2.33179500	-2.91002600	0.38937100
C	2.91060400	1.57372300	-0.23056500
C	4.29789400	1.77432100	-0.17507300
H	4.96219700	0.94781500	0.05668300
C	4.84503000	3.03091400	-0.42858000
H	5.92296900	3.16333300	-0.37740700
C	4.02905700	4.12307400	-0.74734100
C	2.64443900	3.91593600	-0.79702700
H	1.98736700	4.74933900	-1.03331700
C	2.08796700	2.66459000	-0.54255400
H	1.01349600	2.53373800	-0.56599500
C	3.26918400	-1.26531300	-0.71698300
C	3.46305100	-2.56202300	-0.21320100
H	3.02158200	-2.84514500	0.73558100
C	4.22051800	-3.49132400	-0.91859600
H	4.36227500	-4.48664400	-0.50429000
C	4.79557100	-3.17102700	-2.15704800
C	4.57964100	-1.88667200	-2.66649000
H	5.00393400	-1.61454900	-3.62962300
C	3.82683800	-0.94642700	-1.96241800
H	3.67755200	0.03988400	-2.38777200
C	5.63115200	-4.18155900	-2.90520400

C	4.62236800	5.47747800	-1.05218100
C	-3.96051800	5.40127000	-2.28038300
C	-6.03830400	-4.41704500	-2.03039200
H	5.61602300	5.58940800	-0.60889700
H	4.72760400	5.62871000	-2.13389900
H	3.98828900	6.28528400	-0.67397300
H	-4.00271100	6.17847400	-1.51247300
H	-3.27605200	5.73769300	-3.06610300
H	-4.95760000	5.32939700	-2.73222400
H	-6.96961500	-4.00215900	-2.42573800
H	-5.56887700	-4.99755600	-2.83412400
H	-6.29178900	-5.12143600	-1.23148500
H	6.60917500	-4.31951200	-2.42781800
H	5.14479500	-5.16242400	-2.92859600
H	5.80974000	-3.86793800	-3.93733000
C	0.11073700	0.09001700	-1.90372500
C	0.14642700	-1.09556600	-2.55079800
H	0.20011500	-1.18650600	-3.63795900
H	0.13016400	1.04270000	-2.43196400
C	0.06361000	-2.10966200	-0.38248300
C	0.12535900	-2.30095400	-1.71731500
H	0.17829100	-3.28654800	-2.18285300
H	0.07323200	-2.94167700	0.32127000

Compound: $^{p\text{=tol}}$17-MCP
Charge: 0
Multiplicity: 1
Lowest Frequency: 9.25 cm^{-1}
Energy: -4464.696221 Hartree

Ni	0.09881600	-0.55709700	-0.81518700
P	-1.96071300	-0.16885700	-0.06827200
P	0.45638700	-1.77520800	0.94143100
P	1.67931400	0.80990500	-0.12612600
C	0.34069700	-1.98609100	-2.13225800
C	-2.21974300	-1.24093800	1.43673000
C	-1.12257400	-2.00141400	1.88098200
C	-1.27307000	-2.87562600	2.96781300
C	-2.49808800	-2.98157600	3.62269800
C	-3.58746100	-2.22240400	3.18836500
C	0.25075500	-1.58336400	-3.42672000
C	-3.44987100	-1.36506800	2.09832900
C	-0.01868400	-0.16149700	-3.58107800
C	1.58921600	-0.87130600	2.09874700

C	2.12187100	0.34234000	1.62542800
C	2.96761400	1.08792800	2.45934200
C	3.27617200	0.63935800	3.74218700
C	2.75361800	-0.57045200	4.20563300
C	-0.12409200	0.50691900	-2.40964000
C	1.91717500	-1.32371300	3.38482100
C	1.16821600	-3.46702500	0.84878100
C	2.55151500	-3.67597700	0.95382300
C	3.09129700	-4.94916800	0.76925800
C	2.25975200	-6.02906500	0.47045800
C	0.88389600	-5.82810900	0.34820500
C	0.34152500	-4.55633100	0.53005100
C	-2.47375500	1.50971700	0.49946100
C	-2.57004400	1.88179500	1.84637400
C	-2.90135200	3.19123300	2.20350500
C	-3.14307400	4.17000500	1.23535300
C	-3.03272600	3.79738000	-0.11294800
C	-2.69990900	2.49748400	-0.47684500
C	-3.50010500	5.58624600	1.61811900
C	-3.38708100	-0.67718600	-1.13152300
C	-4.67859900	-0.14553800	-0.99506000
C	-5.72593800	-0.60779800	-1.79087900
C	-5.52098900	-1.61148700	-2.74584600
C	-4.22661400	-2.12783600	-2.88669100
C	-3.17198900	-1.67140200	-2.09779500
C	-6.66136300	-2.13120600	-3.58824900
C	1.44206900	2.63438600	-0.05686300
C	1.69794300	3.41181600	-1.19994900
C	1.44057900	4.77988800	-1.20387200
C	0.91674500	5.42428900	-0.07451500
C	0.64266300	4.64365400	1.05355500
C	0.89252500	3.27128900	1.06395400
C	0.67080000	6.91425000	-0.07842800
C	3.31300800	0.64739400	-0.98550800
C	3.49245900	-0.41165100	-1.88446200
C	4.72208800	-0.59855800	-2.51909100
C	5.80239700	0.25703800	-2.28143800
C	5.61199400	1.32484800	-1.39144500
C	4.38996000	1.51953700	-0.75443300
C	7.13874000	0.03605000	-2.94884500
H	-3.64760500	5.68466700	2.69722300
H	-4.41987300	5.91581000	1.12203100
H	-2.71011600	6.28786300	1.32431300
H	-0.43985100	-3.49362600	3.28742200

H	-6.32874900	-2.38216800	-4.60019200
H	-7.46861700	-1.39727700	-3.66823100
H	-7.09071500	-3.04307800	-3.15407400
H	1.61328900	7.47427200	-0.03779800
H	0.06902300	7.22313500	0.78116400
H	0.14967200	7.23171600	-0.98792800
H	-2.60662900	-3.66214900	4.46223700
H	7.60512800	0.98367100	-3.23687900
H	7.03981000	-0.58038800	-3.84669300
H	7.83790700	-0.47557300	-2.27533300
H	-4.54694100	-2.30982900	3.69006000
H	-4.30805600	-0.79968200	1.74962200
H	3.37916900	2.02880700	2.10951600
H	3.92700200	1.23106100	4.37965600
H	2.99599600	-0.92398600	5.20359800
H	1.51869900	-2.26521100	3.74882100
H	3.20992900	-2.84428200	1.18213000
H	4.16385800	-5.09525400	0.85912400
H	2.68128000	-7.01983800	0.32829300
H	0.23024000	-6.66126400	0.10670200
H	-0.72902900	-4.41063700	0.42516900
H	-2.39805100	1.14973800	2.62852700
H	-2.98051200	3.45025000	3.25684500
H	-3.20975300	4.53804200	-0.88927400
H	-2.62031300	2.23937900	-1.52866300
H	-4.86938800	0.64782200	-0.27918300
H	-6.71734200	-0.17691700	-1.67112100
H	-4.03478800	-2.89194500	-3.63641700
H	-2.17072900	-2.06545200	-2.24928100
H	2.10276600	2.94233000	-2.09059900
H	1.65152200	5.35762400	-2.10084300
H	0.22221200	5.11247200	1.93959800
H	0.65400000	2.69851700	1.95380700
H	2.66067100	-1.07680100	-2.10141100
H	4.83584300	-1.42196600	-3.22006400
H	6.43040400	2.01536300	-1.20036400
H	4.27175600	2.37053800	-0.09086500
H	-0.32561200	1.57927500	-2.36964400
H	-0.13090600	0.30975000	-4.56043000
H	0.36588800	-2.24304100	-4.29106900
H	0.54483800	-3.03896200	-1.91530300

Compound: ^{Ph}18-MCP
Charge: 0
Multiplicity: 1
Lowest Frequency: 8.60 cm^{-1}
Energy: -3809.595106 Hartree

Ni	-0.01873900	-0.81508900	1.32427100
P	-1.75411200	0.05495400	0.22161800
P	1.78135400	-0.10696800	0.19680200
O	-0.17182200	-1.11352800	-1.86237200
C	-1.53308300	0.77658100	-1.47146600
C	-0.69088100	0.07638800	-2.35128000
C	-0.44694700	0.52038800	-3.64902700
C	-1.05118300	1.69862900	-4.08883600
C	-1.89424000	2.41337600	-3.23939200
C	-2.13320700	1.95023100	-1.94380700
C	-2.90042900	-1.33888800	-0.19214500
C	-4.00198900	-1.14663900	-1.04152600
C	-4.84655300	-2.21025500	-1.35593300
C	-4.59456600	-3.48106700	-0.83319200
C	-3.49726600	-3.68136600	0.00362000
C	-2.65411500	-2.61643700	0.32737500
C	-2.79958700	1.30382800	1.08436600
C	-4.07203400	1.00948000	1.59324300
C	-4.78145000	1.96656300	2.32231200
C	-4.23325500	3.22833900	2.54917200
C	-2.96332100	3.52903000	2.05159400
C	-2.24762300	2.57202400	1.33440700
C	2.17853600	-1.10758600	-1.31166000
C	1.12661600	-1.50153800	-2.16176900
C	1.33460800	-2.36621000	-3.23420700
C	2.61862800	-2.84357800	-3.49656600
C	3.67940200	-2.46482300	-2.67522900
C	3.45686600	-1.61353500	-1.59193200
C	1.74225300	1.65142800	-0.38095400
C	1.99544400	2.06738500	-1.69238500
C	1.96961300	3.42483100	-2.02378700
C	1.70526700	4.38261300	-1.04649800
C	1.46583700	3.97862700	0.26973900
C	1.48244400	2.62474700	0.59952800
C	3.37797400	-0.03226100	1.14439300
C	4.46924800	0.70479600	0.64713700
C	5.65954500	0.79242000	1.36634700
C	5.77770000	0.15616400	2.60408900

C	4.70004200	-0.56717600	3.11125600
C	3.50762900	-0.66481200	2.38931300
H	0.20728200	-0.04724900	-4.30147000
H	-0.86456000	2.05011100	-5.09935300
H	-2.36901100	3.32782300	-3.58131400
H	-2.78848800	2.51428000	-1.28912800
H	-4.19756500	-0.16610700	-1.46519200
H	-5.69732600	-2.04805000	-2.01176600
H	-5.25052600	-4.31074800	-1.08176800
H	-3.29216600	-4.66757700	0.40970200
H	-1.80107300	-2.76574200	0.97958500
H	-4.50978600	0.03207200	1.42371900
H	-5.76521800	1.72158700	2.71223900
H	-4.78791600	3.97146600	3.11462300
H	-2.52596700	4.50751300	2.22880400
H	-1.25691200	2.81275200	0.95989300
H	0.48384000	-2.66796300	-3.83605300
H	2.78292000	-3.51798400	-4.33144400
H	4.67990600	-2.84056500	-2.86592800
H	4.28592400	-1.34881900	-0.94582200
H	2.21296700	1.33444600	-2.46146100
H	2.16092400	3.72985000	-3.04854000
H	1.69001500	5.43734400	-1.30492300
H	1.27146300	4.71869500	1.04085000
H	1.30631000	2.32069800	1.62853600
H	4.38580000	1.22820700	-0.30012700
H	6.49003400	1.36577700	0.96428800
H	6.70244100	0.23044000	3.16934800
H	4.77933000	-1.06063400	4.07560500
H	2.67937500	-1.24291200	2.78788100
C	0.88937800	-2.37671400	1.99083600
C	-1.14646100	-1.12770300	2.85825200
C	0.34907300	-2.93257600	3.09662700
H	1.70629900	-2.88453200	1.46705700
C	-0.78481500	-2.16896900	3.63571500
H	-1.93273300	-0.44146500	3.18480900
H	0.68714800	-3.86788400	3.54974600
H	-1.26068100	-2.42833200	4.58429400

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