Supporting Information

for

Electronic Effects in Mixed N-Heterocyclic Carbene/Phosphite Indenylidene Ruthenium Metathesis Catalysts

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1. General Considerations

All reactions were performed under an inert atmosphere of argon or nitrogen using standard Schlenk and glovebox techniques. Solvents were dispensed from a solvent purification system. All other reagents were used without further purification. ^{1}H, ^{13}C-{^{1}H} and ^{31}P-{^{1}H} 1D and 2D Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker AVANCE 400 Ultrashield spectrometer using the residual solvent peak as reference ($CHCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; CH_2Cl_2, δ_H = 5.32 ppm, δ_C = 53.80 ppm) at 298K. Variable temperature NMR spectra were carried out in CD_2Cl_2 on a Bruker AVANCE 300 and a Bruker AVANCE 500. Gas chromatography (GC) analyses were performed on an Agilent 7890A apparatus equipped with a flame ionization detector and a (5%-Phenyl)-methylpolysiloxane column (30 m, 320 μm, film: 0.25 μm). Elemental analyses were performed by the London Metropolitan University Service. Calorimetric studies were performed using a CALVET C80 solution calorimeter. Flash chromatography was performed on silica gel 60 Å pore diameter and 40-63 μm particle size.

2. General procedure for the synthesis of phosphite ligands.

$P(O\text{-}C_6H_4\text{-}p\text{-}OMe)_3$ **1b**,[1] $P(O\text{-}C_6H_4\text{-}p\text{-}CF_3)_3$ **1c,**[2] $P(O\text{-}C_6H_4\text{-}p\text{-}Cl)_3$ **1d,**[1] and $P(O\text{-}C_6H_4\text{-}p\text{-}CN)_3$ **1f**[1] were synthesized according to literature procedures and $P(OC_6H_5)_3$ **1a** was commercially available (it was however distilled under inert atmosphere).

A Schlenk flask was charged with the corresponding *para*-substituted phenol, triethylamine (1.2 equiv.) and diethylether. The reaction mixture was stirred at room temperature for 1 hour under inert atmosphere. Phosphorus trichloride (0.33 equiv.) was then added dropwise. The reaction mixture was stirred at room temperature for 24 hours filtered through Celite, and the solvent was removed *in vacuo*. The resulting solid was dissolved in 30 mL of hexane and filtered through a pad of silica. The filtrate was then dried *in vacuo* to give the desired ligand.

Tri(*p*-methoxyphenyl)phosphite (1b).[1]

Starting with *p*-methoxyphenol (5 g, 40.3 mmol), triethylamine (1.2 equiv., 7.3 mL, 48.4 mmol) and phosphorus trichloride (0.33 equiv., 1.2 mL, 13.3 mmol) in 50 mL of diethylether, tri(*p*-methoxyphenyl)phosphite was obtained as a colorless oil (4.94 g, 92%).

^{1}H NMR (300 MHz, CD_2Cl_2, 298K) δ = 7.05 (m, 6H), 6.85 (m, 6H), 3.77 (s, 9H, O-Me); ^{31}P-{^{1}H} NMR (112 MHz, CD_2Cl_2, 298K) δ = 129.1.

These data were compared and found similar to literature data.[3]

Tri(*p*-trifluoromethylphenyl)phosphite (1c).[2]

Starting with *p*-trifluoromethylphenol (2 g, 12.3 mmol), triethylamine (1.2 equiv., 2.2 mL, 14.8 mmol) and phosphorus trichloride (0.33 equiv., 370 µL, 4.06 mmol) in 20 mL of diethylether, tri(*p*-trifluorophenyl)phosphite was obtained as a colorless solid (1.86 g, 80%).

^{1}H NMR (400 MHz, CD_2Cl_2, 298K) δ = 7.64 (d, ^3J (H,H) = 8.8 Hz, 6H), 7.27 (d, ^3J (H,H) = 8.8 Hz, 6H); ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 298K) δ = 125.9.

These data were compared and found similar to literature data.[2]

Tri(*p*-chlorophenyl)phosphite (1d).[1]

Starting with *p*-chlorophenol (5 g, 42.8 mmol), triethylamine (1.2 equiv., 7.7 mL, 51.4 mmol) and phosphorus trichloride (0.33 equiv., 1.3 mL, 14.1 mmol) in 50 mL of diethylether, tri(*p*-chlorophenyl)phosphite was obtained as a colorless solid (4.64 g, 78%).

^{1}H NMR (400MHz, CD_2Cl_2, 298K) δ = 7.32 (d, ^3J (H,H) = 8.8 Hz, 6H), 7.08 (d, ^3J (H,H) = 8.8 Hz, 6H); ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 298K) δ = 127.1.

These data were compared and found similar to literature data.[3]

Tri(*p*-pentafluorosulfurphenyl)phosphite (1e).

A Schlenk flask was charged with the corresponding *p*-pentafluorosulfurphenol (1.0 g, 4.5 mmol), triethylamine (1.2 equiv., 800 µL, 5.45 mmol) and diethylether (50 mL). The reaction mixture was stirred at room temperature under inert atmosphere for 1 hour. Phosphorus trichloride (0.33 equiv., 137 µL, 1.51 mmol) was added drop wise. The reaction mixture was stirred at room temperature for 24 hours. The solvent was removed *in vacuo*. Resulting solid was dissolved in 30 mL of hexane and filtered on a pad of silica. The supernatant was then dried *in vacuo*. Tri(*p*-pentafluorosulfurphenyl)phosphite was obtained as a colorless solid (0.76 g, 73%).

^{1}H NMR (400 MHz, CD_2Cl_2, 298K) δ = 7.78 (d, ^3J (H,H) = 9.5 Hz, 6H), 7.24 (d, ^3J (H,H) = 9.5 Hz, 6H); ^{13}C-{1H} NMR (101 MHz, CD_2Cl_2, 298K): δ = 153.6 (s, C_p), 150.2 (d, ^{2}J (C,P) = 19.0 Hz, C_i), 128.5 (p, J (C,F) = 4.1 Hz, C_m), 120.9 (d, ^3J (C,P) = 7.2 Hz, C_o); ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 298K): δ = 125.3.

Tri(*p*-cyanophenyl)phosphite (1f).[1]

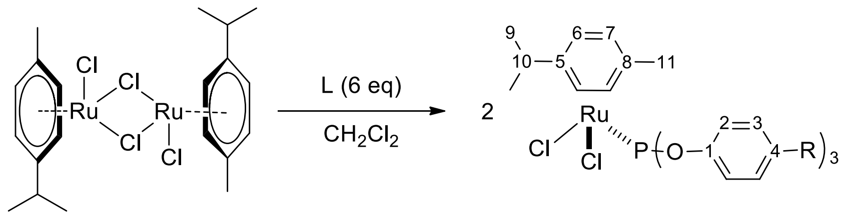
Starting with *p*-cyanophenol (3 g, 25.0 mmol), triethylamine (1.2 equiv., 4.5 mL, 30.0 mmol) and phosphorus trichloride (0.33 equiv., 750 µL, 8.3 mmol) in 30 mL of diethylether, the compound was then collected as a colorless solid (1.6 g, 50%).

^{1}H NMR (300 MHz, CD_2Cl_2, 298K) δ = 7.68 (d, ^3J (H,H) = 9.0 Hz, 6H), 7.23 (d, ^3J (H,H) = 9.0 Hz, 6H); ^{31}P-{^{1}H} NMR (121 MHz, CD_2Cl_2, 298K): δ = 125.4.

3. Synthesis of [RuCl$_2$(η^6-cymene){P(OPh-*p*-R)$_3$}] (2a) and calorimetric experiments.

Complex [RuCl$_2$(η^6-cymene){P(O-C_6H_5)$_3$}] (**2a**) was already described.[4] Its characterization data were in agreement with the literature.

3.1. Numbering of atoms in complexes of the type [RuCl$_2$(η^6-cymene){P(OR$_3$)}].

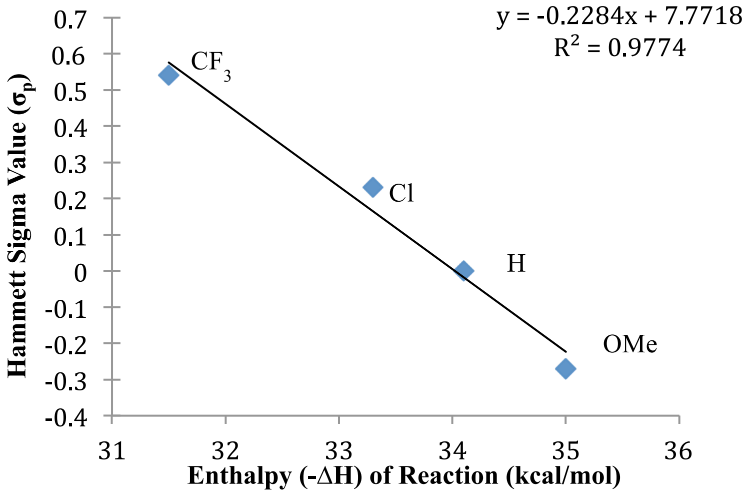


3.2 Calorimetric experiments Table 1.

3.2.1. Procedure for calorimetric experiments.

Two solutions containing separately the complex and the ligand were prepared: stock solution **A** containing 30 mg (0.048 mmol) of [Ru(µ-Cl)Cl(η^6-cymene)]$_2$ in CH_2Cl_2 (0.75 mL) and stock solution **B** containing the ligand **L** (0.293 mmol, 6 eq) in CH_2Cl_2 (2 mL). The first container of the cell was charged with stock solution **B** (0.75 mL) and the second container with stock solution **A** (0.3 mL). The cell was placed in the calorimeter and the temperature stabilised to 30 °C. The solutions were then mixed by inversion of the calorimeter and the thermogram recorded. The measured enthalpies of reaction are the average of at least three experiments.

3.2.2. Plot: Enthalpy of reaction (KCal.mol^{-1}) *vs* Hammett σ_p.



Therefore σ_{pSF5} is estimated to be around 0.87 following this plot.

3.2.3. Equation leading to BDE.

Reaction done in the vessel is described by this equation:

$$[Ru(\mu\text{-}Cl)Cl(n^6\text{-cymene})]_{2\,(sol)} + 2L_{(sol)} \xrightarrow[30°C]{DCM} 2\ [RuCl_2(n^6\text{-cymene})LCl_2]_{(sol)}$$

Considering it in term of energy and bond dissociation, we obtain the following equation:

$$2\,D(Ru-Cl) = 2\,D(Ru-L) + \Delta H_{rxn}$$

This equation could be modified to isolate and calculate the BDE of the inserted ligand directly from the enthalpy of reaction:

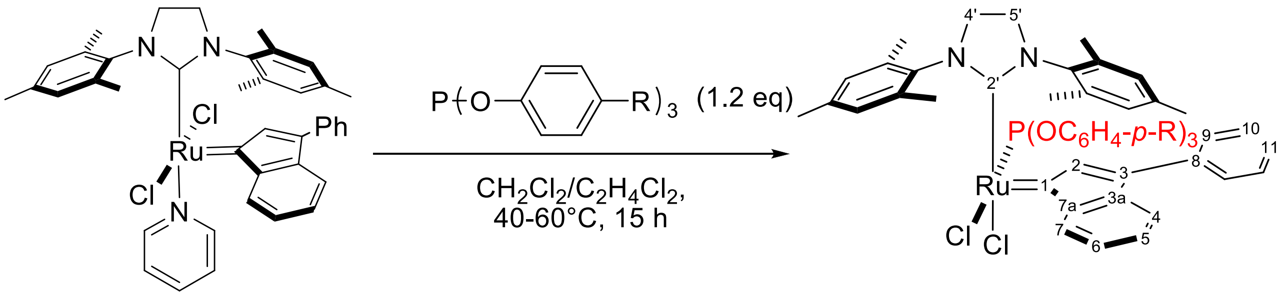
$$2\,D(Ru-L) = D(Ru-Cl) - \Delta H_{rxn}$$

$$D(Ru-L) = \frac{D(Ru-Cl) - \Delta H_{rxn}}{2}$$

Unfortunately the BDE Ru-Cl for [Ru(μ-Cl)Cl(η^6-cymene)]$_2$ is not described in the literature, therefore we were not able to calculate properly the absolute BDE. In order to compare different ligands we decided to deduce only the "relative" BDE. Starting from the previous equation, relative BDE were calculated using this general equation. That gives the value for Ru-L BDE (kcal.mol^{-1}):

$$D(Ru-L) = \frac{|-\Delta H_{rxn}|}{2}$$

4. Numbering of atoms in 3a-f.



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5. Procedures for catalysis

Substrates **4**,[5] **6**,[6] **8**,[7] **10**,[8] **12**,[8] **16**,[6] **18**,[9] **20**,[8] **22**,[10] **24**,[5] **26**,[5] **28**,[11] **30**,[12] **33**,[13] **34**,[13] **35**,[14] were synthesised according to literature procedures. Substrates **14**, methyl acrylate (**46**), 4-Chlorostyrene (**32**) are commercially available.

NMR spectra of the metathesis products **5**,[5] **7**,[6] **11**,[8] **13**,[15] **15**,[5] **17**,[6] **19**,[9] **21**,[5] **23**,[5] **25**,[5] **27**,[16] **29**,[16], **37**,[17] **38**,[18] **39**,[18] **40**,[19] were compared to previously reported analyses.

5.1. Procedure for Figure 3 – Comparative kinetic studies

A reaction tube (Radleys carousel 12 reactions station) was charged with a solution of di(methallyl)tosylamine **4** (0.5 mmol) in toluene (0.5 mL) and the ruthenium pre-catalyst (0.5 mol%) was added. The reaction mixture was stirred at 80°C and aliquots were taken every 5 minutes from 0 to 30 minutes, every 10 minutes from 30 minutes to 1 hour, every 30 minutes until 2 hours and every hour afterwards. Each aliquot was then added to a solution of 40 μL of ethylvinyl ether and toluene. All samples were then subjected to GC analysis to determine the conversion of **4** to **5**.

5.2. Procedure for Table 4- Catalytic comparison in RCM of complexes 3a-f.

In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **3a-f** (1 mol% from a stock solution of 0.0075 mmol in 2 mL of toluene), and extra volume of toluene to complete 0.5 mL. The mixture was stirred outside the glovebox at 110˚C during 24h. Afterwards aliquots were taken; samples were then subjected to GC analysis to determine the conversion. It was also was confirmed by ^{1}H NMR ($CDCl_3$).

5.3. Procedure for Table 5-Temperature profile of 3c.

In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **3c** (0.3 mol% from a stock solution of 5.9 mg in 2 mL of toluene), and extra volume of toluene to complete 0.5 mL. The mixture was stirred outside the glovebox at different temperatures during 17 h. Afterwards aliquots were taken; samples were then subjected to GC analysis to determine the conversion. It was also was confirmed by ^{1}H NMR ($CDCl_3$).

5.4. Procedure for Table 6- Comparisons of state-of-the-art catalysts

For commercially available **Gru-II**: In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **Gru-II** (from a stock solution of 31.8 mg in 1.5 mL of dichloromethane), and a volume of dichloromethane to complete 0.5 mL. The mixture was stirred outside the glovebox at reflux between 17 and 24h. Afterwards aliquots were taken; samples were then subjected to GC analysis to determine the conversion. It was also was confirmed by ^{1}H NMR ($CDCl_3$).

For commercially available **Hov-II**: In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **Hov-II** (from a stock solution of 23.4 mg in 1.5 mL of benzene), and a volume of benzene to complete 0.5 mL. The mixture was stirred outside the glovebox at 60˚C between 17 and 24h. Afterwards aliquots were taken; samples were then subjected to GC analysis to determine the conversion. It was also was confirmed by ^{1}H NMR ($CDCl_3$).

For commercially available ***cis*-Caz-1**: In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst ***cis*-Caz-1** (from a stock solution of 33 mg in 1.5 mL of toluene), and a volume of toluene to complete 0.5 mL. The mixture was stirred outside the glovebox at 110˚C between 17 and 24h. Afterwards aliquots were taken; samples were then subjected to GC analysis to determine the conversion. It was also was confirmed by ^{1}H NMR ($CDCl_3$).

For **3c**: In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **3c** (from a stock solution of 44.4 mg in 1.5 mL of toluene), and a volume of toluene to complete 0.5 mL. The mixture was stirred outside the glovebox at 110˚C between 17 and 24h. Afterwards aliquots were taken; samples were then subjected to GC analysis to determine the conversion. Then the solvent was evaporated. Flash chromatography (pentane/diethylether - 9:1 to 8:2 v:v) on silica gel afforded the title compounds.

5.5. Procedure for Table 7- Catalytic RCM and enyne metathesis at low catalyst loading

In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **3c** (from a stock solution of 5.9 mg in 2 mL of toluene), and extra volume of toluene to complete 0.5 mL. The mixture was stirred outside the glovebox at 80 ˚C between 1-24h. Afterwards the reaction was stopped and solvent was evaporated. Flash chromatography (pentane/diethylether - 9:1 to 8:2 v:v) on silica gel afforded the title compounds.

5.6. Procedure for Scheme 2 - Catalytic CM at low catalyst loading

In the glovebox, a vial was charged with a stirring bar, substrate (0.25 mmol), pre-catalyst **3c** (from a stock solution of 5.9 mg in 2 mL of toluene), and a volume of toluene was added to complete 2.5 mL. The mixture was stirred outside the glovebox at 80 ˚C between 17 and 24h. Afterwards the reaction was stopped and solvent was evaporated. Flash chromatography (pentane/diethylether - 9:1 to 8:2 v:v) on silica gel afforded the title compounds.

6. Crystallographic data

6.1. Crystallographic data for complexes 2b-f

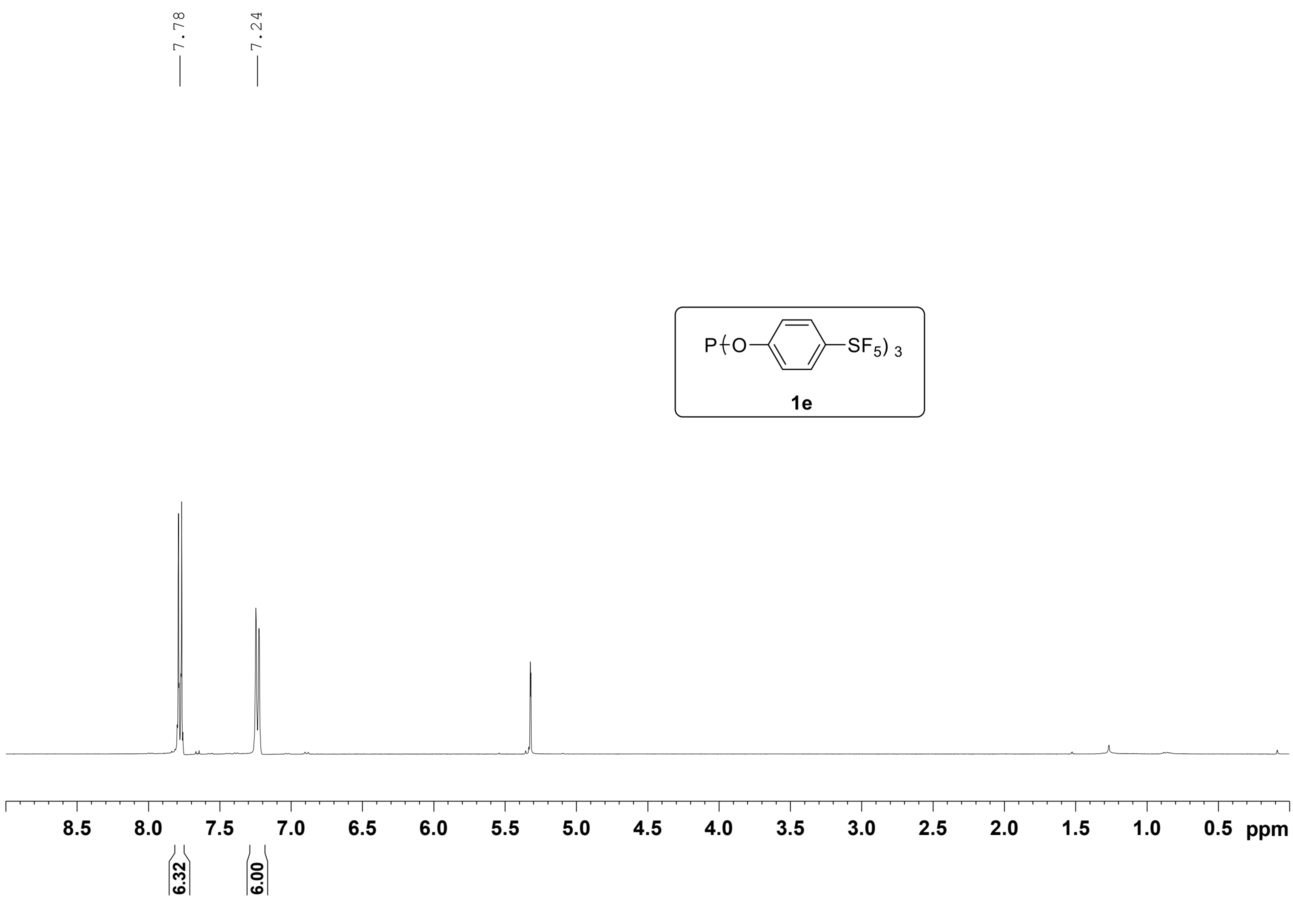
Complex	**2b**	**2c**	**2d**	**2e**	**2f**
CCDC number	CCDC 1023424	CCDC 1023425	CCDC 1023426	CCDC 1023427	CCDC 1023428
Formula	$C_{31}H_{35}Cl_2O_6PRu$	$C_{31}H_{26}Cl_2F_9O_3PRu$	$C_{28}H_{26}Cl_5O_3PRu$	$C_{28.25}H_{26.5}Cl_{2.5}F_{15}O_3PRuS_3$	$C_{31}H_{28}Cl_4N_3O_3PRu$
M /g.mol^{-1}	706.56	820.48	719.82	1015.85	776.45
Crystal system	Hexagonal	Triclinic	Triclinic	Monoclinic	Triclinic
Space group	$R\bar{3}$	$P\bar{1}$	$P\bar{1}$	$P2_1$	$P\bar{1}$
a/ Å	26.177(2)	13.5992(19)	12.8846(14)	12.849(2)	9.329(4)
b/ Å		13.6640(17)	13.4812(16)	20.749(4)	12.681(5)
c/ Å	24.576(4)	19.245(2)	18.7873(18)	14.436(3)	15.181(5)
α/ °		108.828(14)	76.882(14)		92.167(7)
β/ °		99.84(2)	73.593(14)	97.129(5)	102.588 (9)
γ/ °		102.742(16)	69.366(11)		109.537(9)
V/ Å^3	14585(4)	3185.8(9)	2900.0(6)	3818.7(13)	1639.8(11)
Z	18	4	2	4	2
ρ_{calcd}/g.cm^{-3}	1.448	1.711	1.649	1.767	1.572
μ (Mo Kα)/ mm^{-1}	0.738	0.796	1.086	0.895	0.890
T/ K	93(2)	93(2)	93(2)	93(2)	93(2)
Number of reflections	30076	20358	18767	23686	10614
Number of unique reflections	5938	12079	11091	10382	6407
R_{int}	0.0523	0.0598	0.0471	0.0622	0.0272
$R1$, w$R2$ ($I > 2\sigma(I)$)	0.0369, 0.0881	0.0628, 0.1048	0.0527, 0.0845	0.0516, 0.1068	0.0459, 0.0982
R, w$R2$ (all data)	0.0527, 0.1063	0.1370, 0.1328	0.1036, 0.1095	0.0684, 0.1197	0.0768, 0.1105
GOF	1.058	1.008	1.011	1.082	1.037

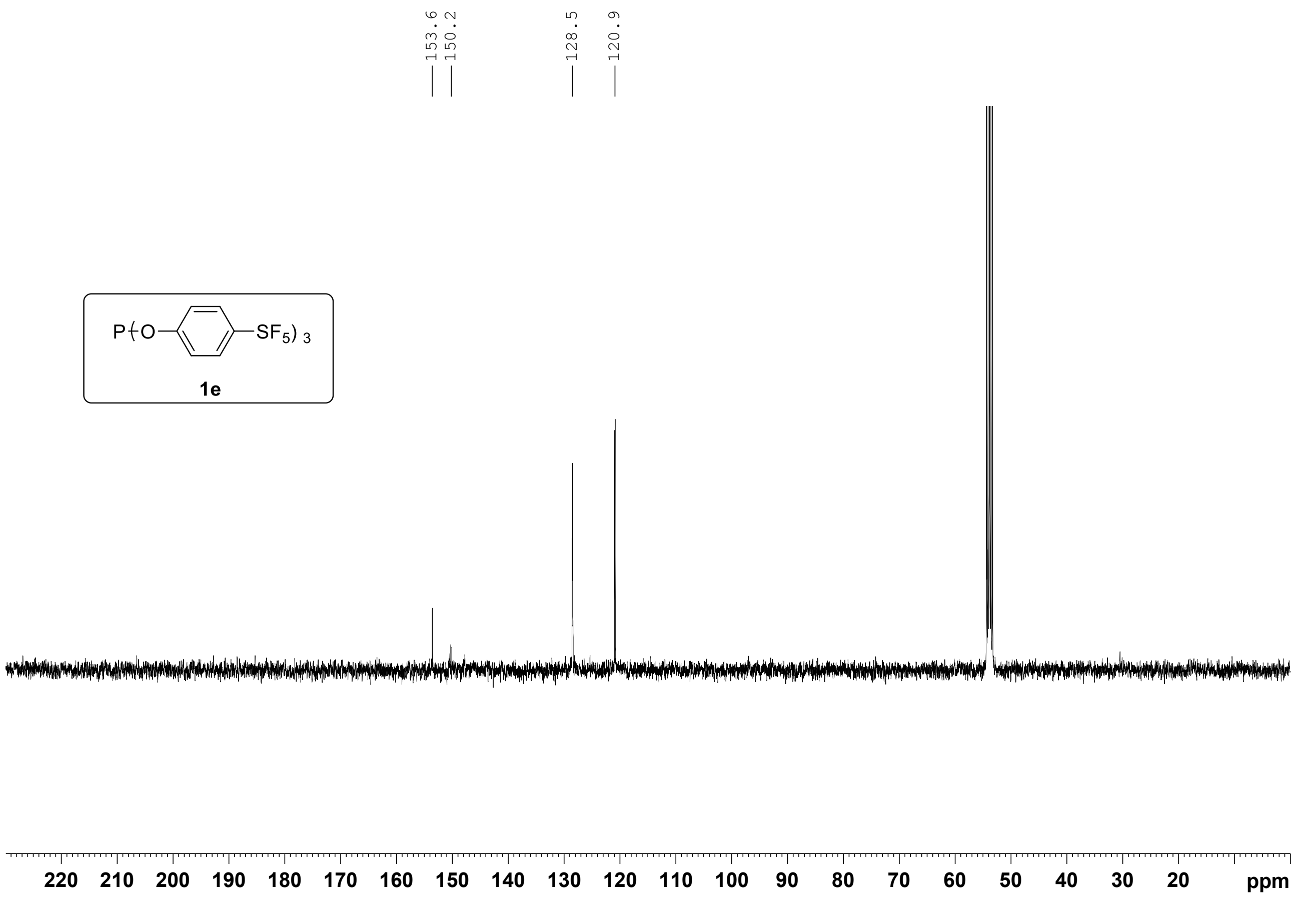
6.2. Crystallographic data for complexes 3b-f

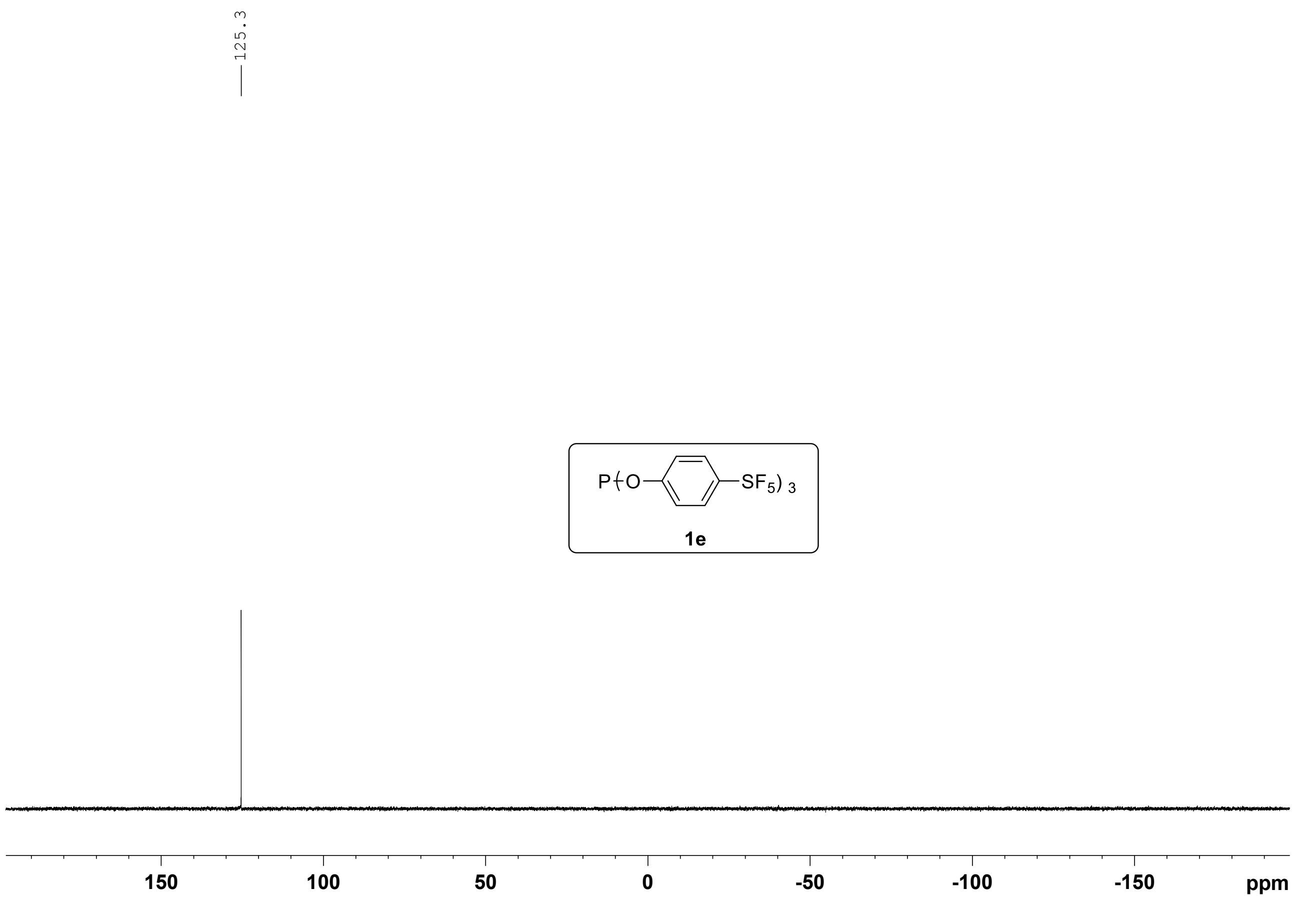
Complex	**3b**	**3c**	**3d**	**3e**	**3f**
CCDC number	CCDC 1023429	CCDC 1023430	CCDC 1023431	CCDC 1023432	CCDC 1023433
Formula	$C_{57}H_{57}Cl_2N_2O_6PRu$	$C_{57}H_{48}Cl_2F_9N_2O_3PRu$	$C_{54}H_{48}Cl_5N_2O_3PRu$	$C_{54}H_{48}Cl_2F_{15}N_2O_3PRuS_3$	$C_{57}H_{48}Cl_2N_5O_3PRu$
M /g.mol^{-1}	1069.04	1182.95	1082.29	1357.09	1053.99
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/c$	$P2_1/n$
a/ Å	10.600(3)	10.840(3)	10.688(3)	16.522(9)	10.6380(6)
b/ Å	29.872(9)	32.588(10)	30.998(9)	39.79(2)	29.5028(16)
c/ Å	16.619(5)	16.079(5)	15.794(5)	9.596(6)	15.8896(11)
β/ °	92.943(5)	93.378(5)	93.633(8)	101.371(10)	95.072(7)
V/ Å^3	5255(3)	5670(3)	5222(3)	6185(6)	4967.4(5)
Z	4	4	4	4	4
ρ_{calcd}/g.cm^{-3}	1.351	1.386	1.376	1.457	1.409
μ (Mo Kα)/ mm^{-1}	0.482	0.472	0.630	0.554	0.506
T/ K	93(2)	93(2)	93(2)	93(2)	93(2)
Number of reflections	53374	51138~~7~~	30460	63477	49634
Number of unique reflections	9633	10316	8885	13235	10713
R_{int}	0.0893	0.0698	0.0804	0.1444	0.0611
R1, wR2 (I > 2σ(I))	0.0717, 0.1835	0.0687~~9~~, 0.149~~50~~5	0.1306, 0.3006	0.0869, 0.2137	0.0896, 0.1319
R, wR2 (all data)	0.0855, 0.1918	0.0734~~5~~, 0.152~~3~~2	0.1634, 0.3180	0.1364, 0.2441	0.1672, 0.1545
GOF	1.137	1.093~~5~~	1.121	1.033	1.083

7. NMR Spectra of phosphite ligands 1e

^{1}H NMR (400 MHz, CD_2Cl_2, 298K), ^{13}C-{1H} NMR (101 MHz, CD_2Cl_2, 298K) and ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 298K):

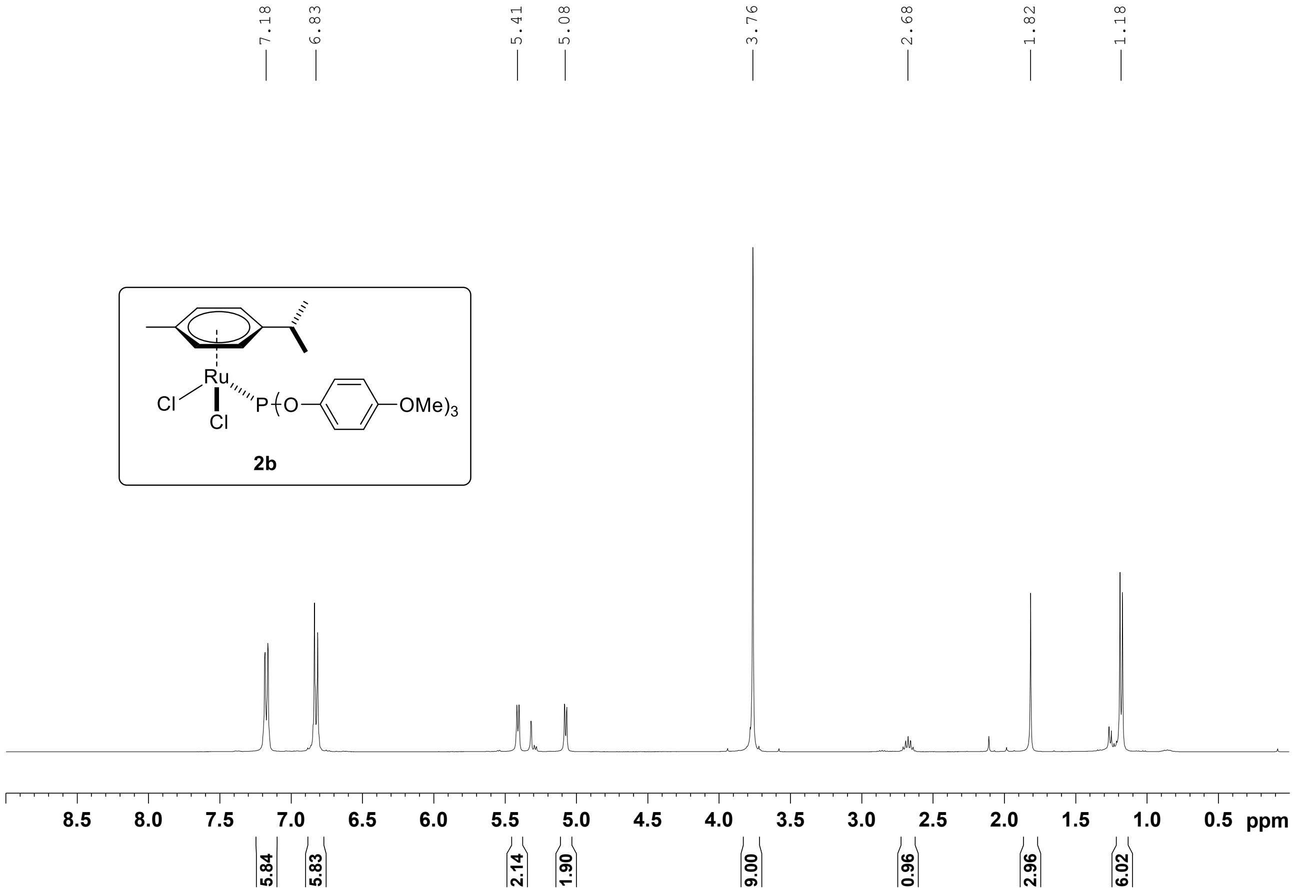


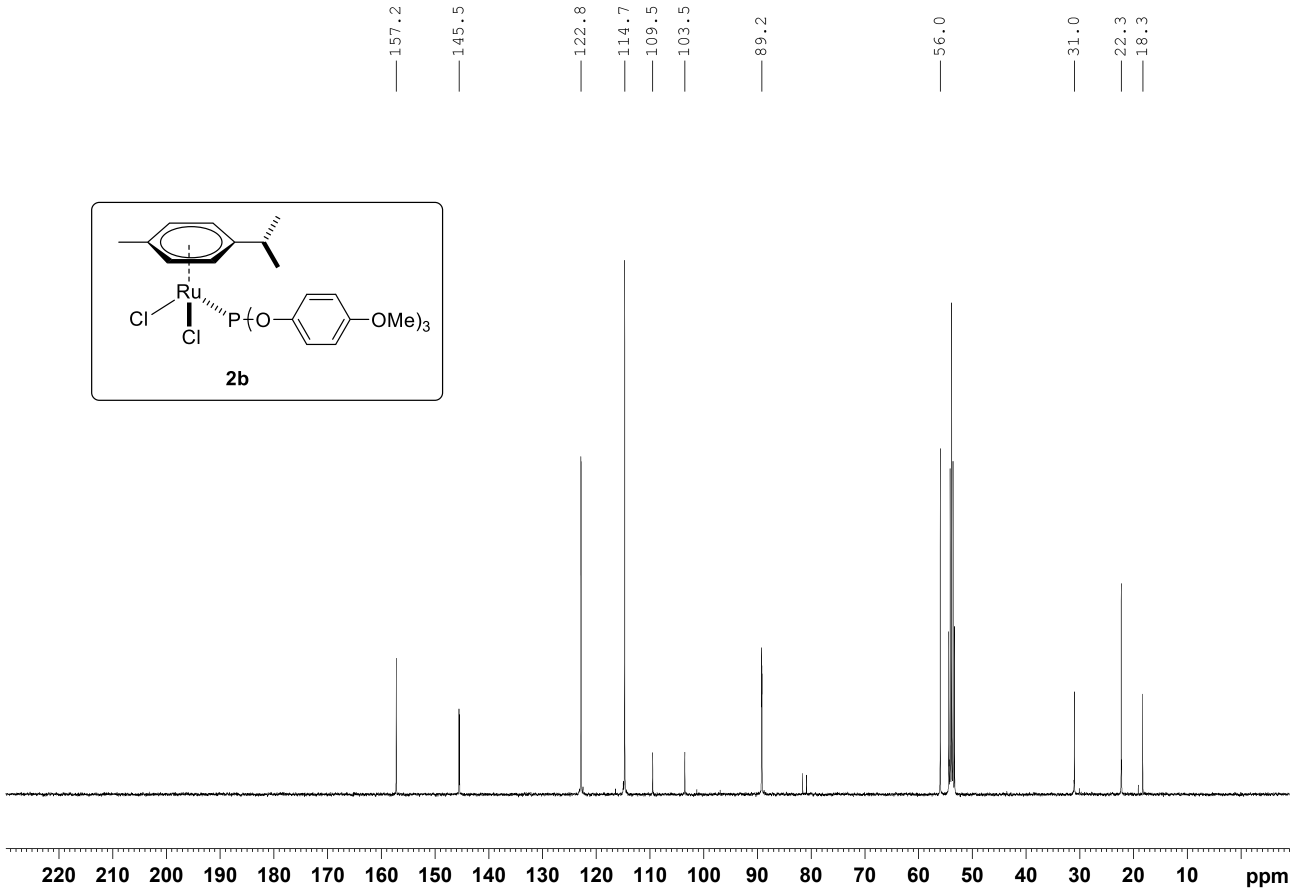

153.6
150.2
128.5
120.9
P(O-C6H4-SF5)3
1e
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


125.3
P(O-C6H4-SF5)3
1e
150 100 50 0 -50 -100 -150 ppm

8. NMR Spectra of Complexes 2b-f

^{1}H NMR (400 MHz, CD_2Cl_2, 298K), ^{13}C-{^{1}H} NMR (101 MHz, CD_2Cl_2, 298K) and ^{31}P-{^{1}H} NMR (121 MHz, CD_2Cl_2, 298K) of **2b**

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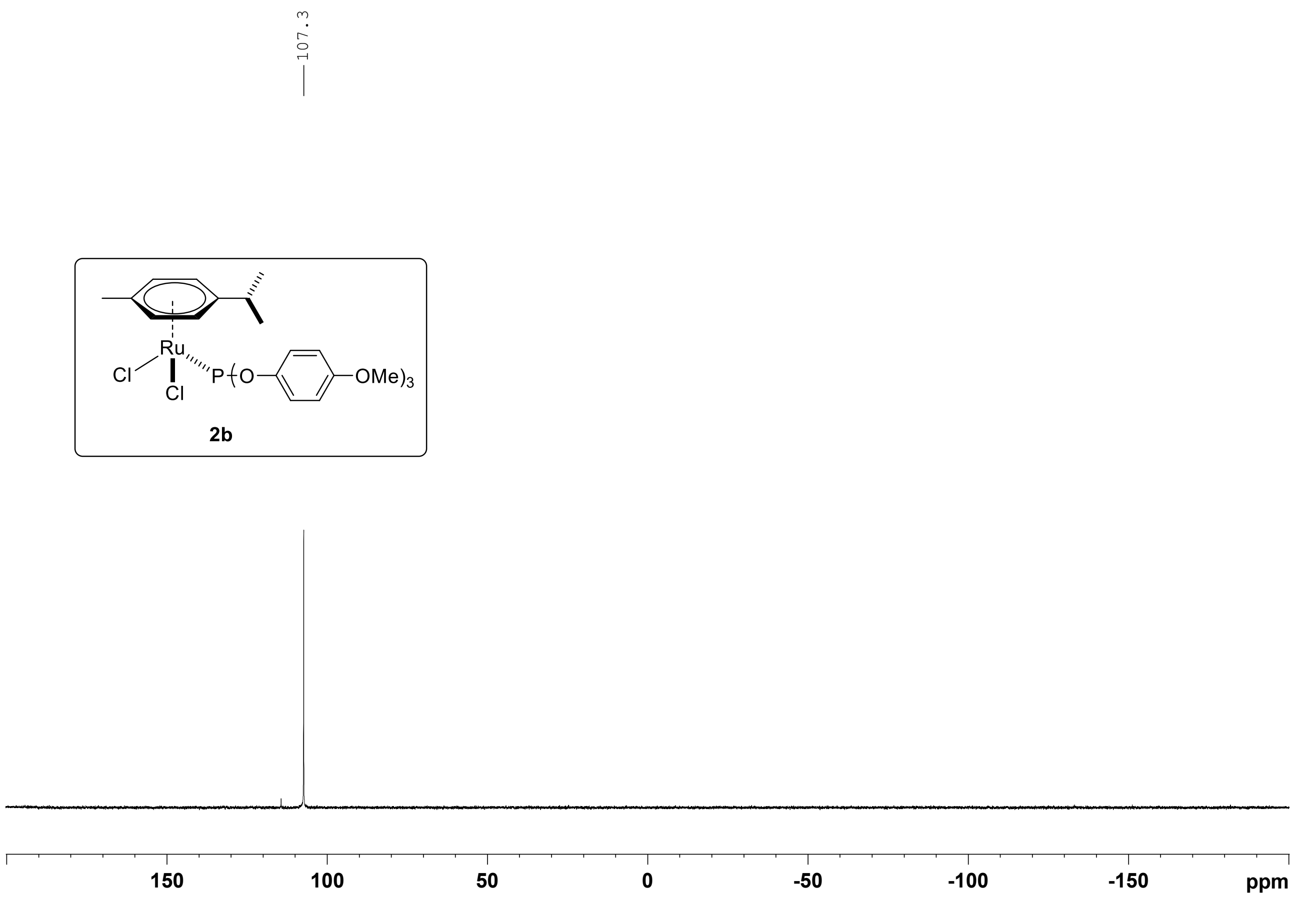
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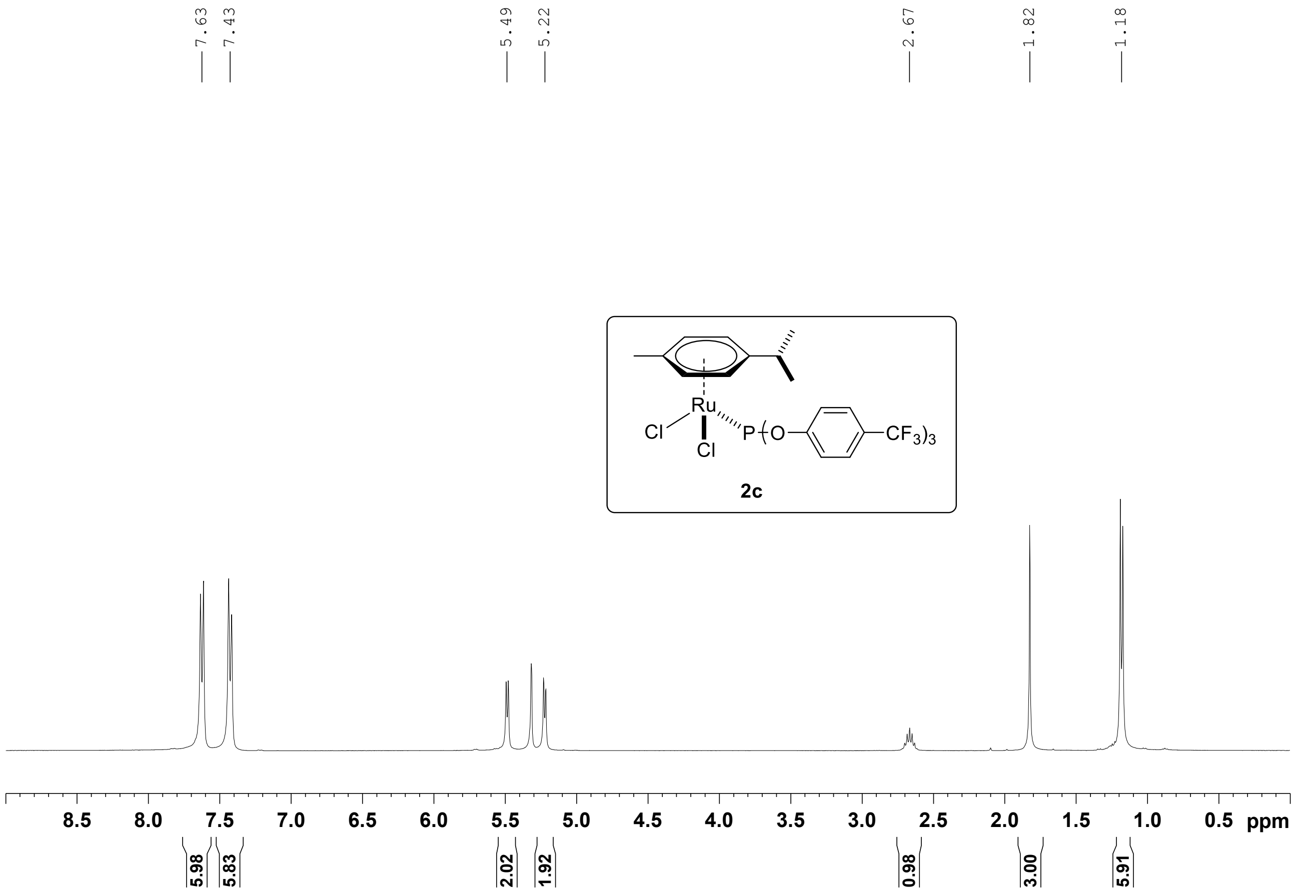
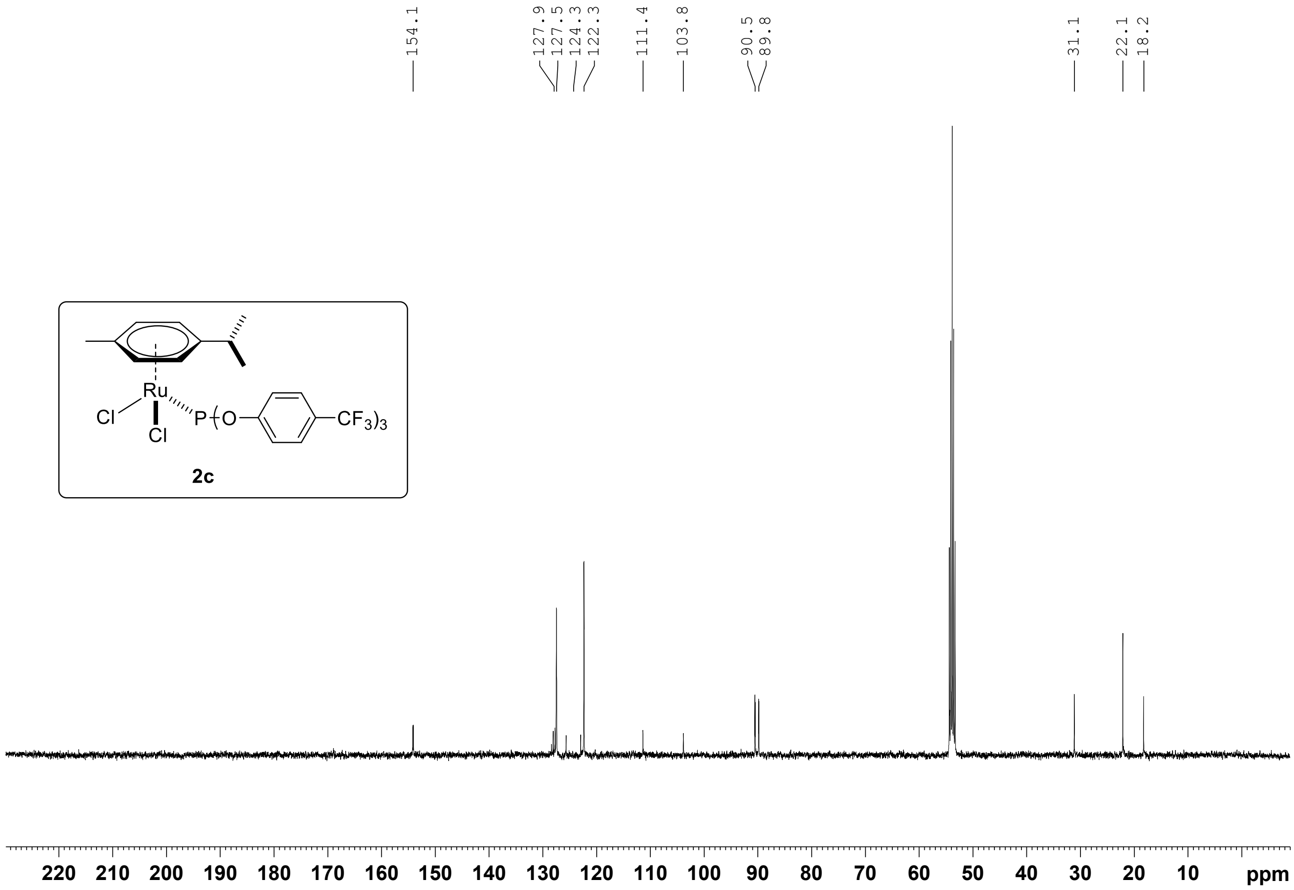
150 100 50 0 -50 -100 -150 ppm

^{1}H NMR (400 MHz, CD_2Cl_2, 298K), ^{13}C-{^{1}H} NMR (101 MHz, CD_2Cl_2, 298K) and ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 298K) of **2c**

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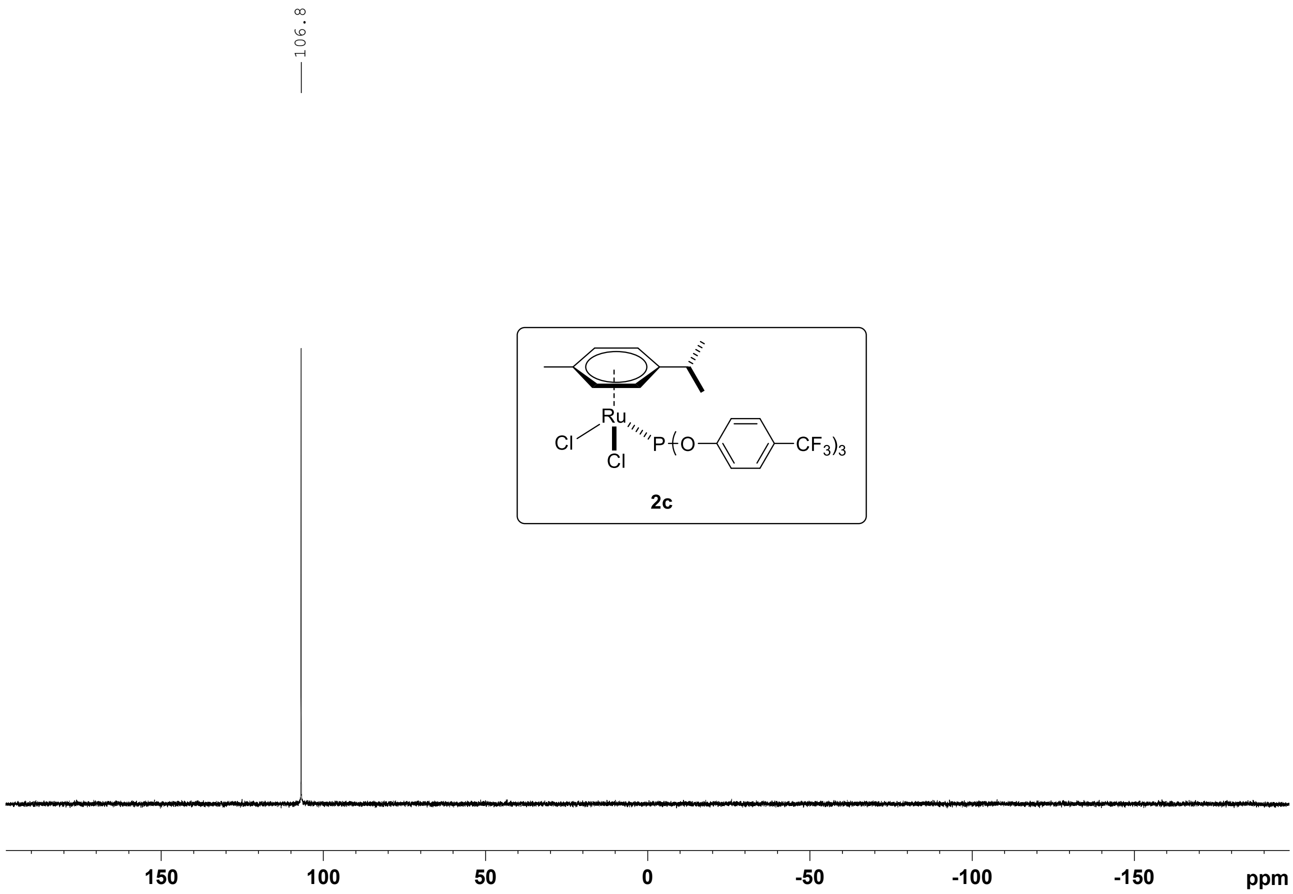
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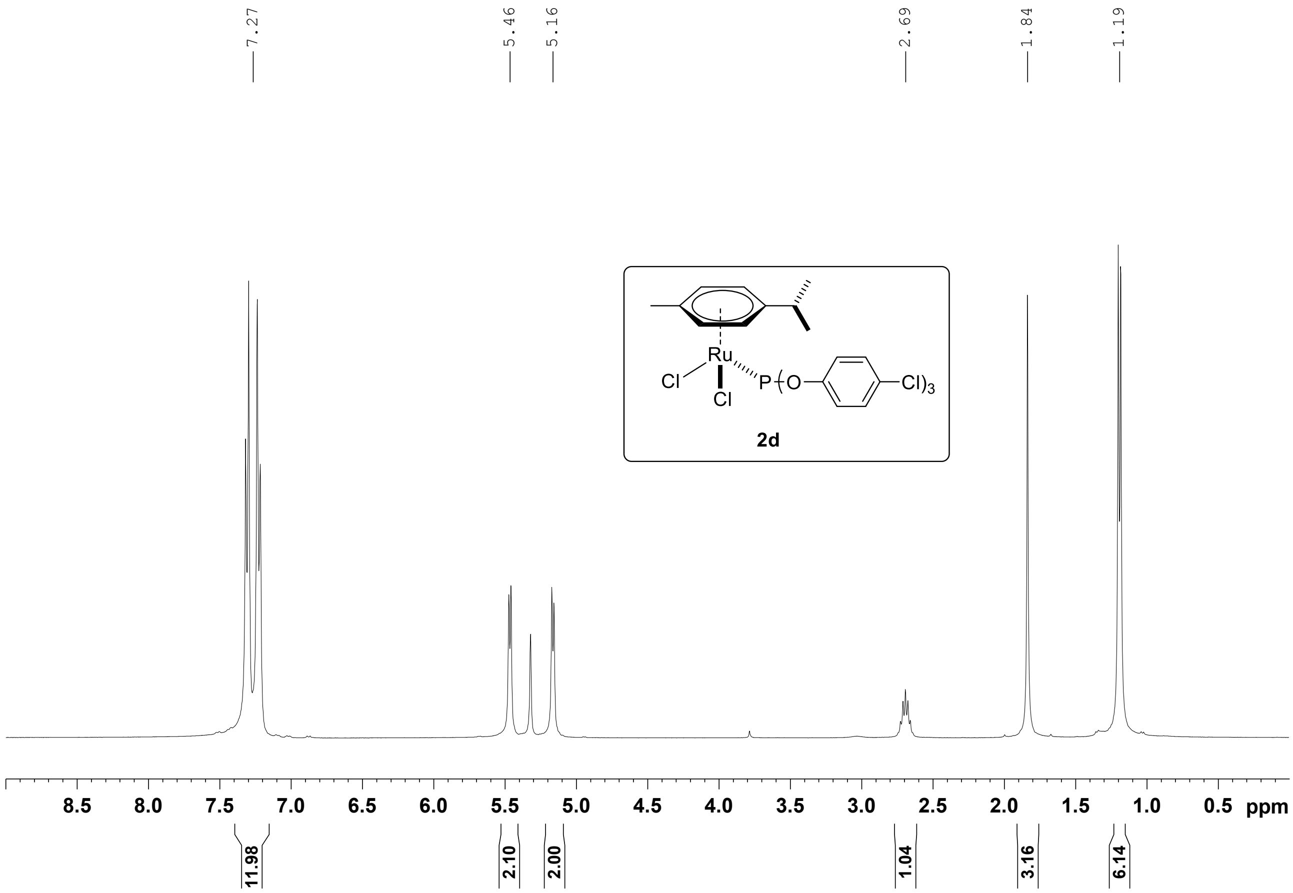
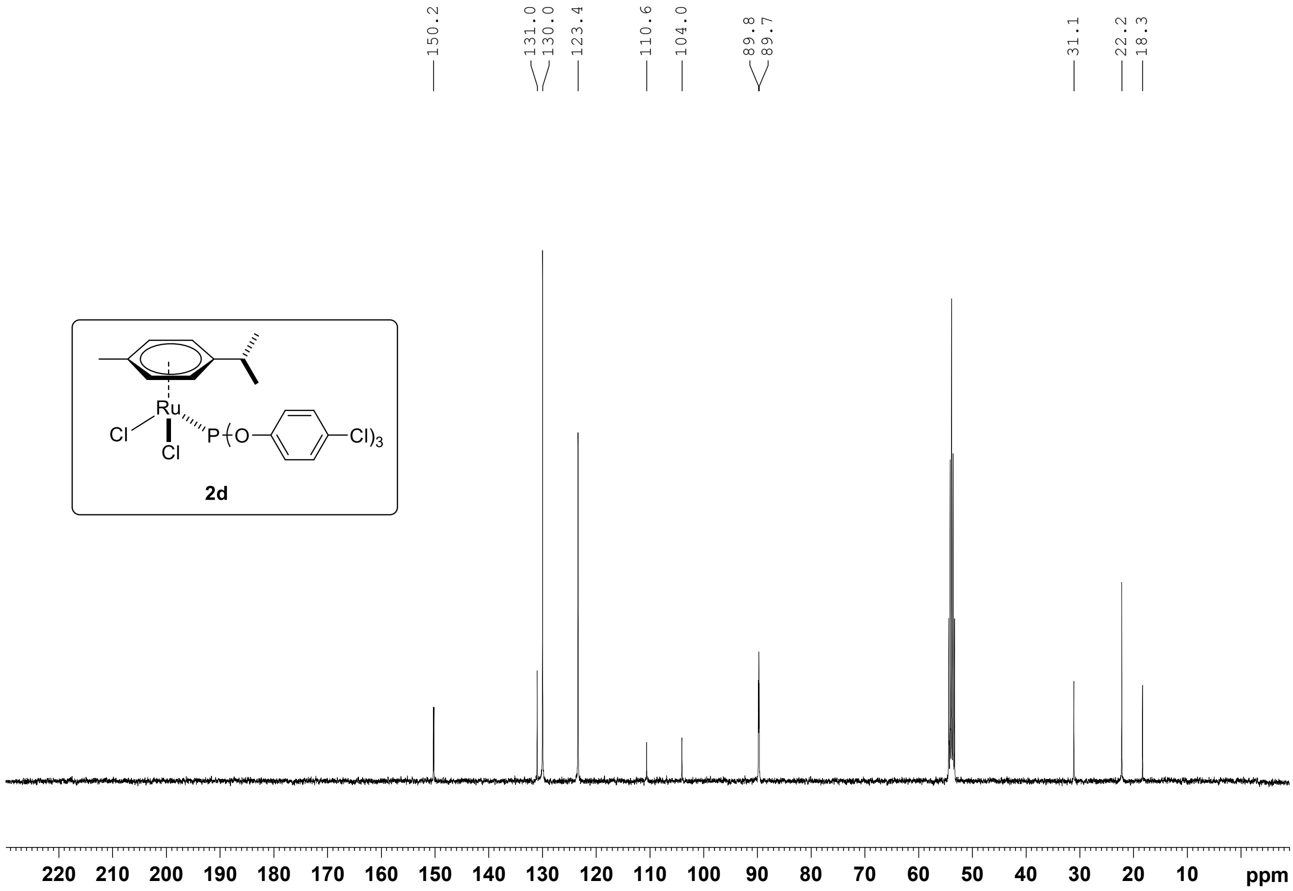
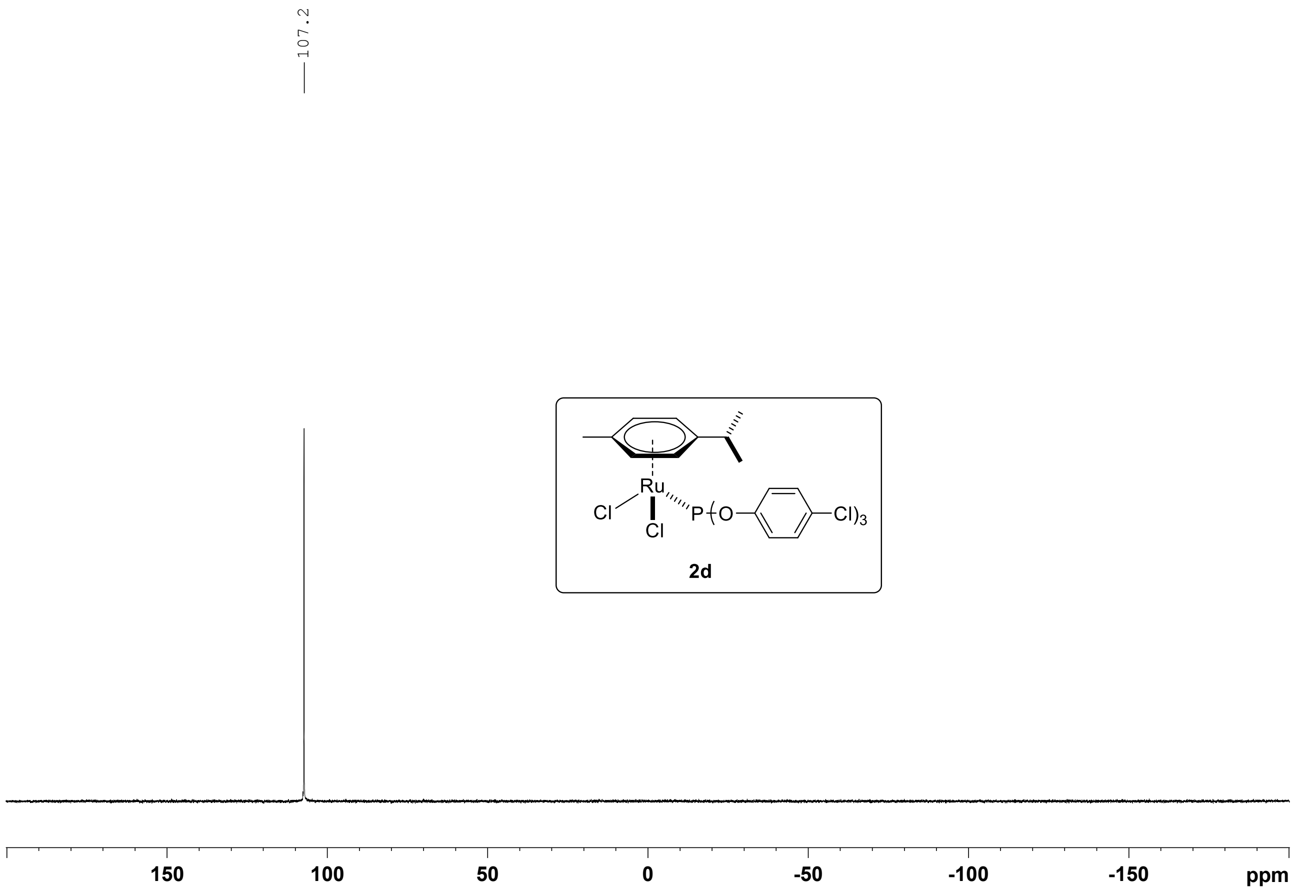
2c
150 100 50 0 -50 -100 -150 ppm

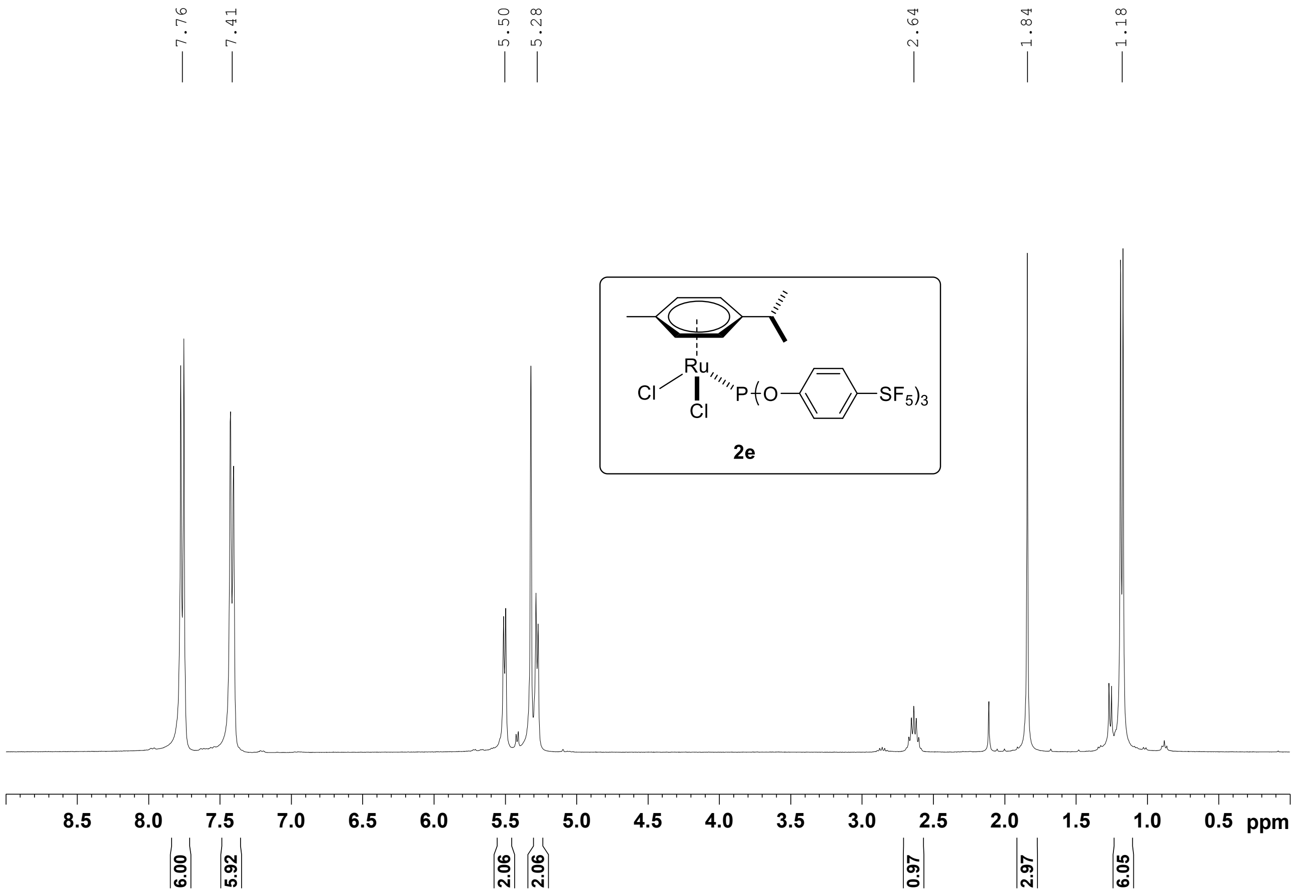
[1]H NMR (400 MHz, CD_2Cl_2, 298K), [13]C-{[1]H} NMR (101 MHz, CD_2Cl_2, 298K) and [31]P-{[1]H} NMR (121 MHz, CD_2Cl_2, 298K) of **2d**

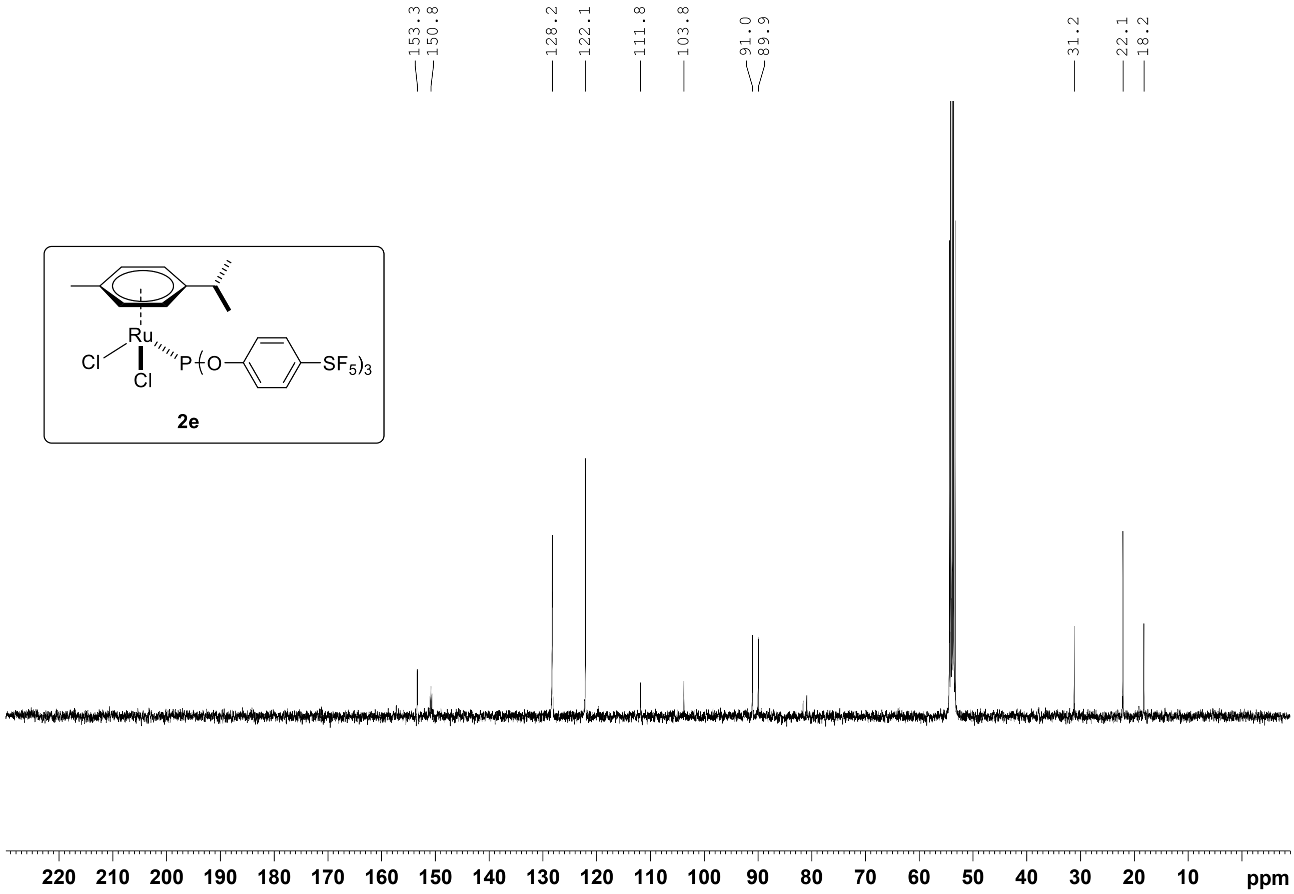


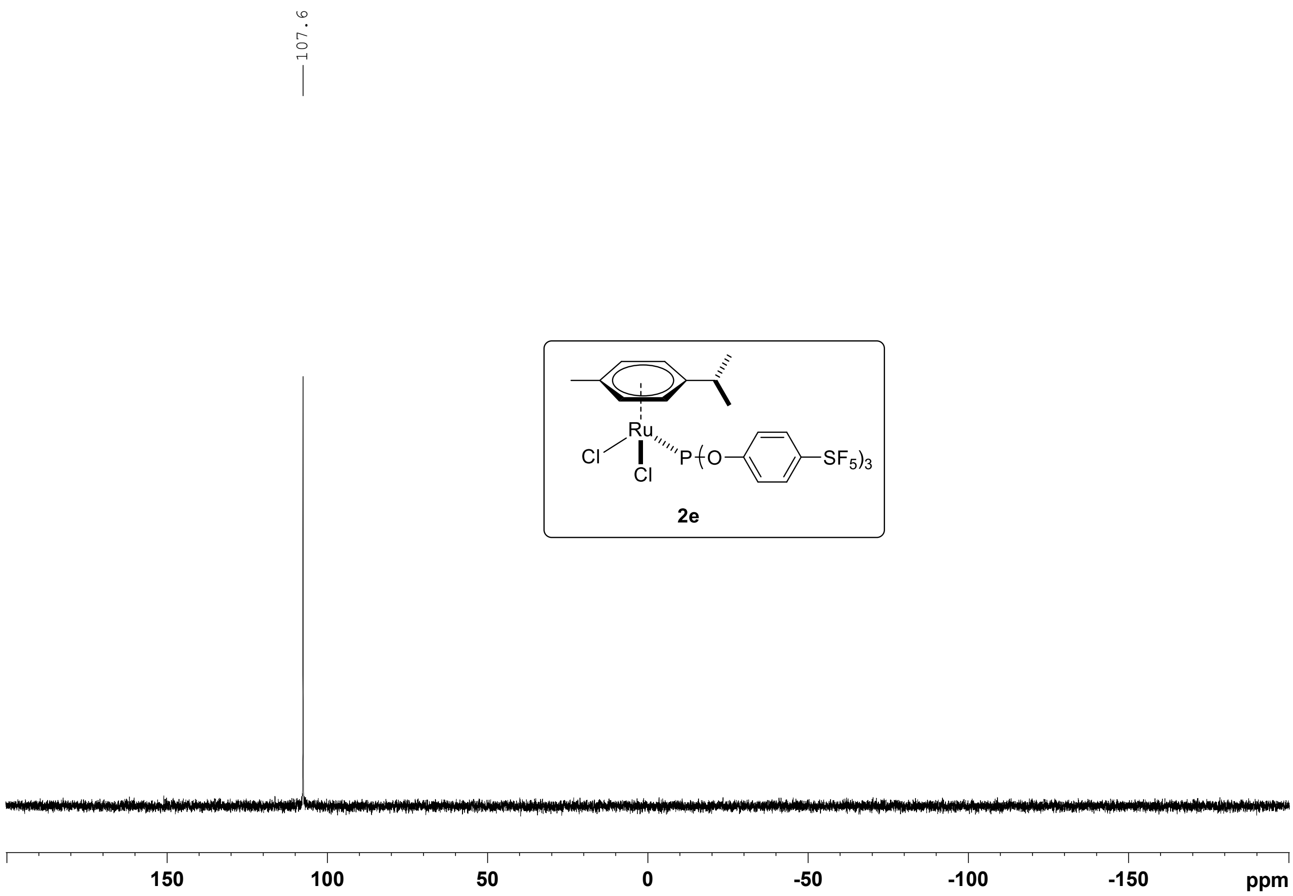

150.2
131.0
130.0
123.4
110.6
104.0
89.8
89.7
31.1
22.2
18.3
Ru
Cl
Cl
P
O
Cl)3
2d
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


107.2
Ru
Cl
Cl
P
O
Cl)3
2d
150 100 50 0 -50 -100 -150 ppm

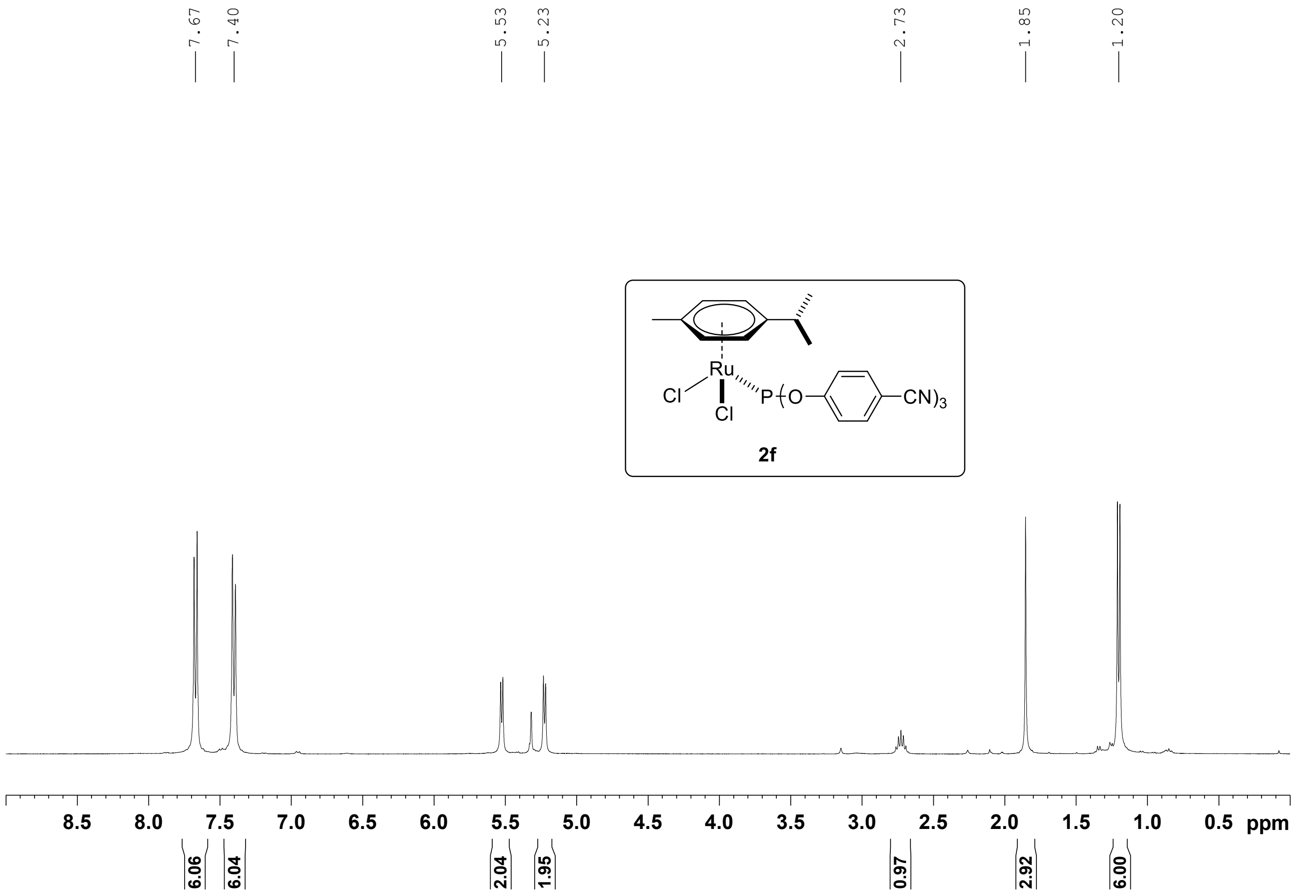
[1]H NMR (400 MHz, CD_2Cl_2, 298K), [13]C-{[1]H} NMR (101 MHz, CD_2Cl_2, 298K) and [31]P-{[1]H} NMR (121 MHz, CD_2Cl_2, 298K) of **2e**

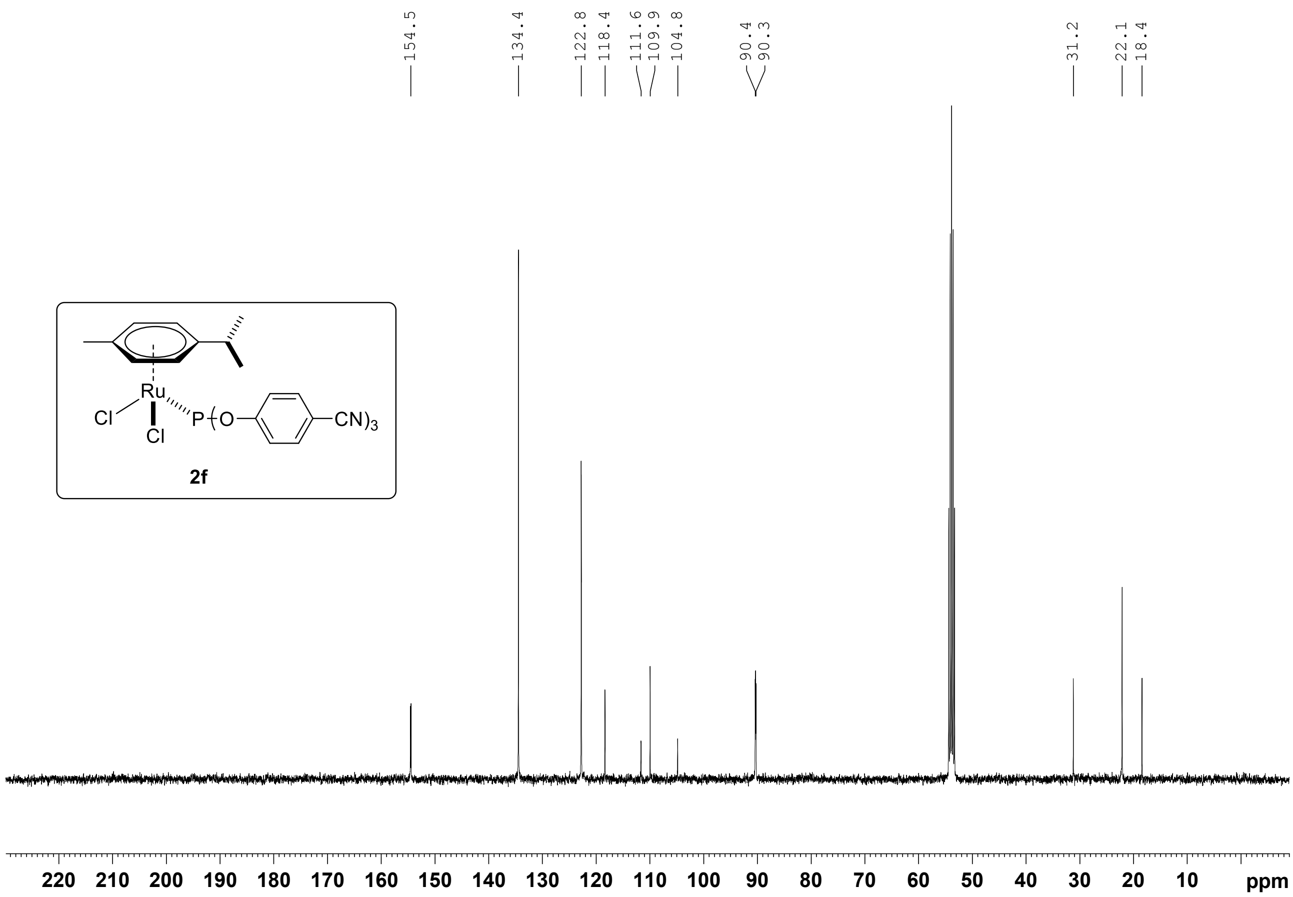


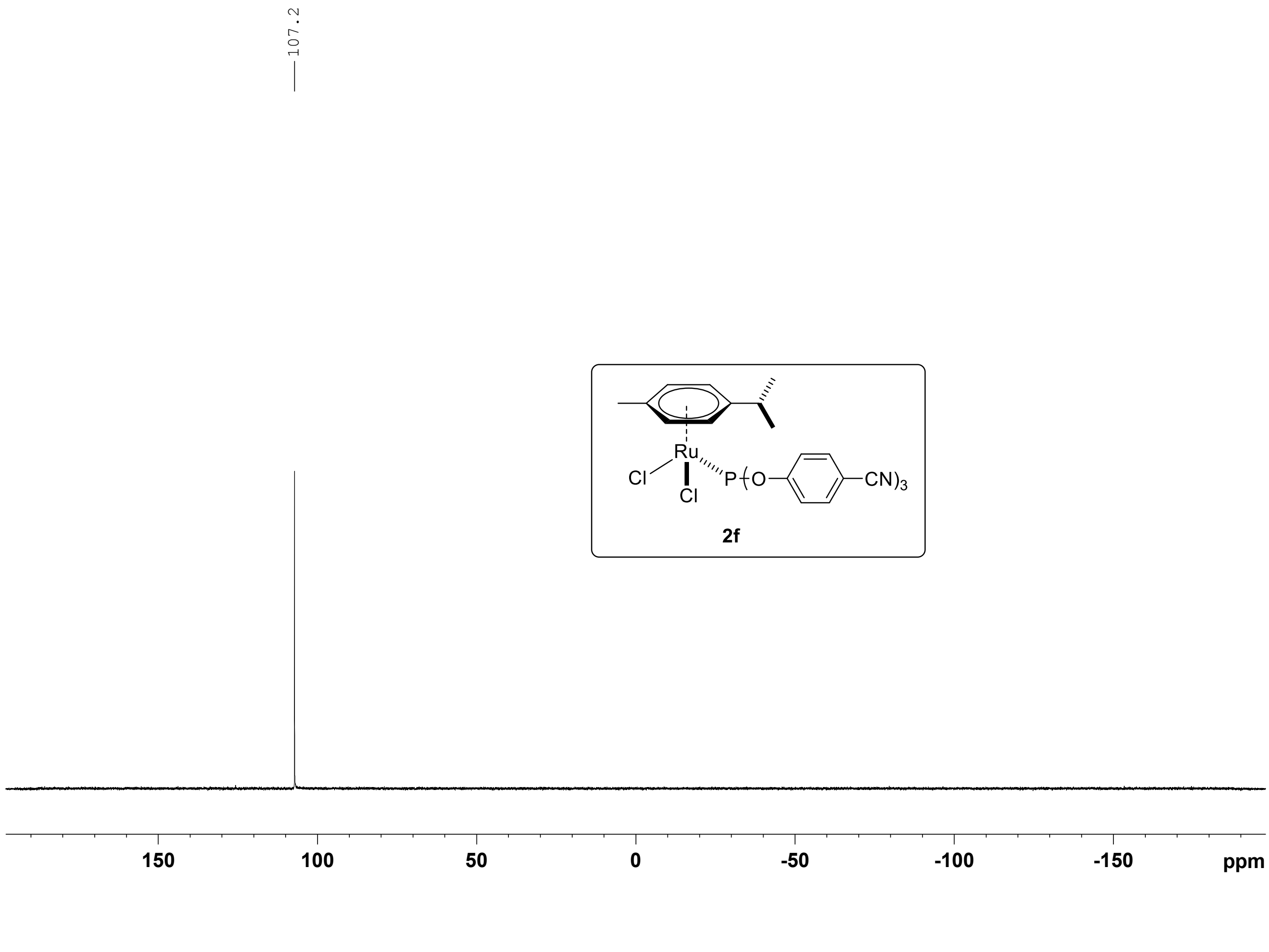

153.3
150.8
128.2
122.1
111.8
103.8
91.0
89.9
31.2
22.1
18.2
Ru
Cl
Cl
P
O
SF5)3
2e
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


107.6
Ru
Cl
Cl
P
O
SF5)3
2e
150 100 50 0 -50 -100 -150 ppm

^{1}H NMR (400 MHz, CD_2Cl_2, 298K), ^{13}C-{^{1}H} NMR (101 MHz, CD_2Cl_2, 298K) and ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 298K) of **2f**

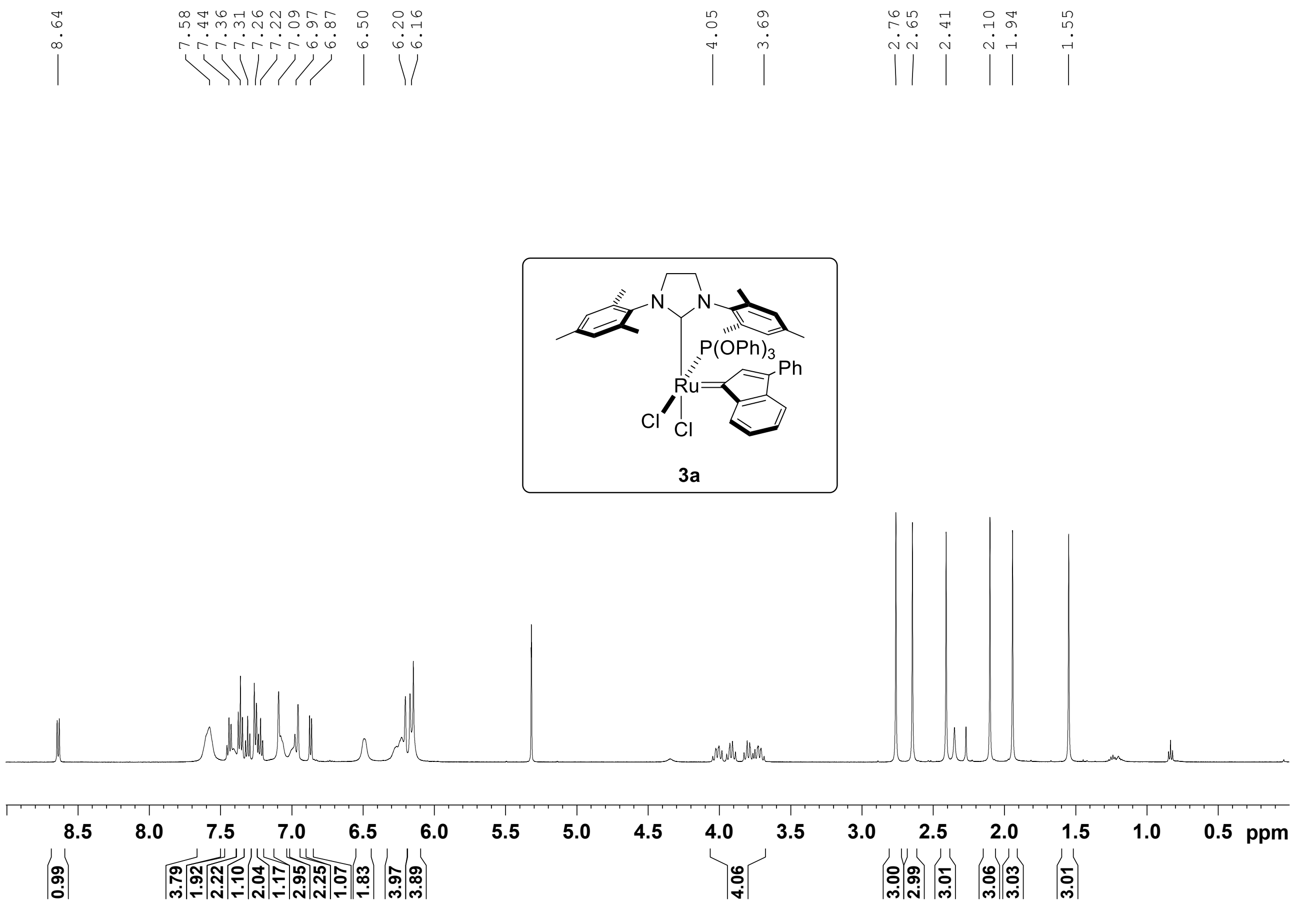


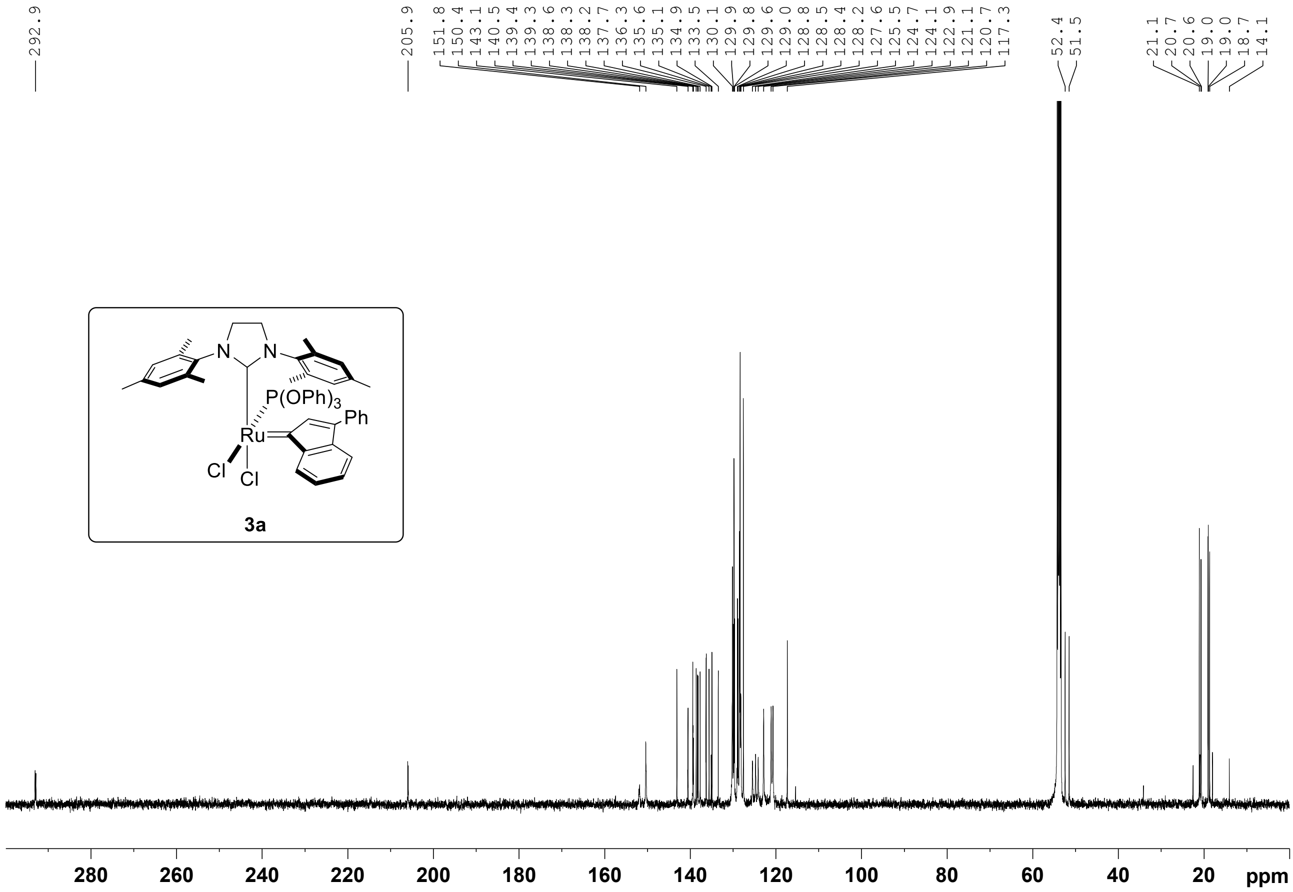

154.5
134.4
122.8
118.4
111.6
109.9
104.8
90.4
90.3
31.2
22.1
18.4
Ru
Cl
Cl
P
O
CN)3
2f
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


107.2
Ru
Cl
Cl
P
O
CN)3
2f
150 100 50 0 -50 -100 -150 ppm

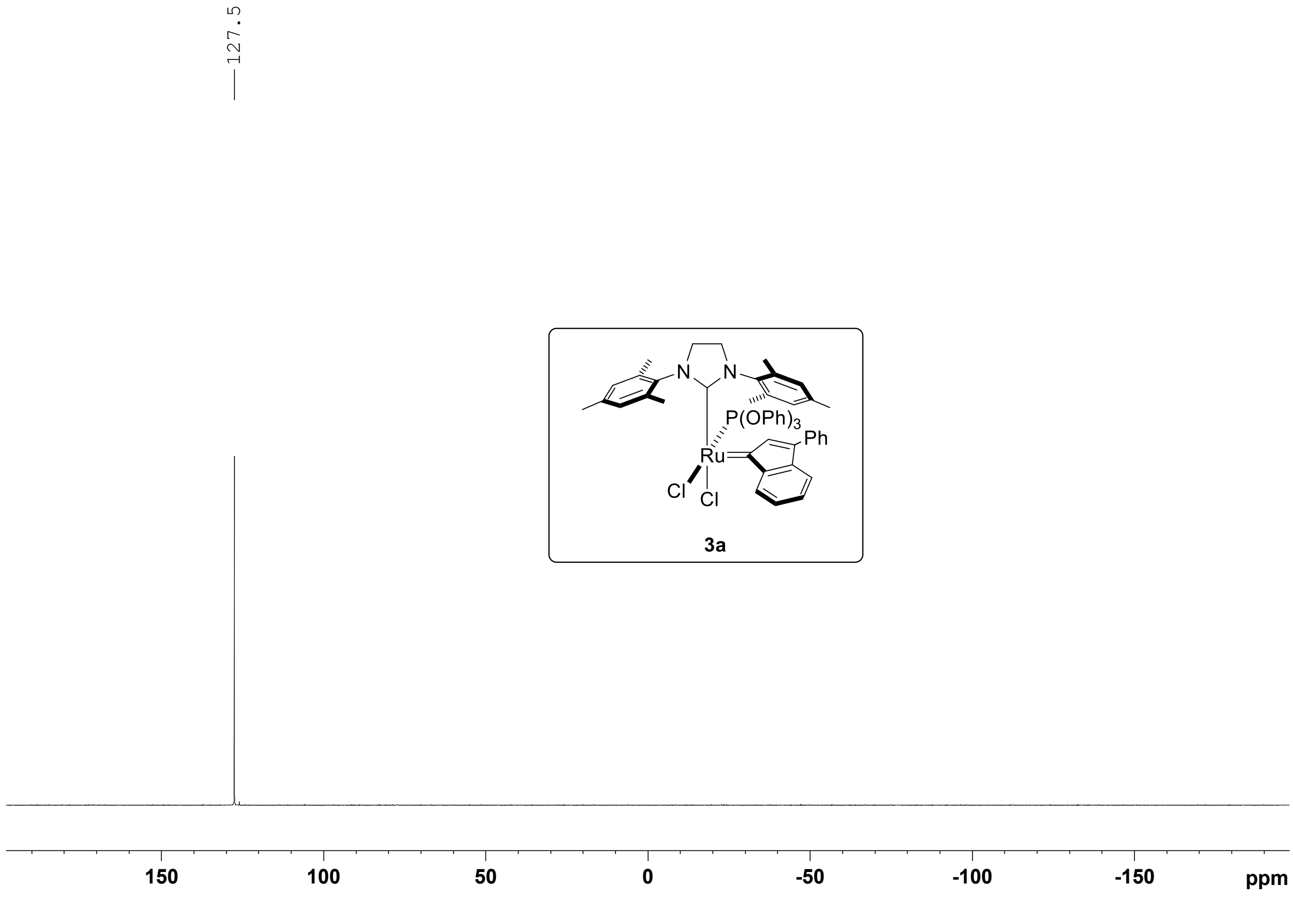
9. NMR Spectra of complexes 3a-f

^{1}H NMR (500 MHz, CD_2Cl_2, 233K), ^{13}C-{^{1}H} NMR (126 MHz, CD_2Cl_2, 233K) and ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 233K) of **3a**



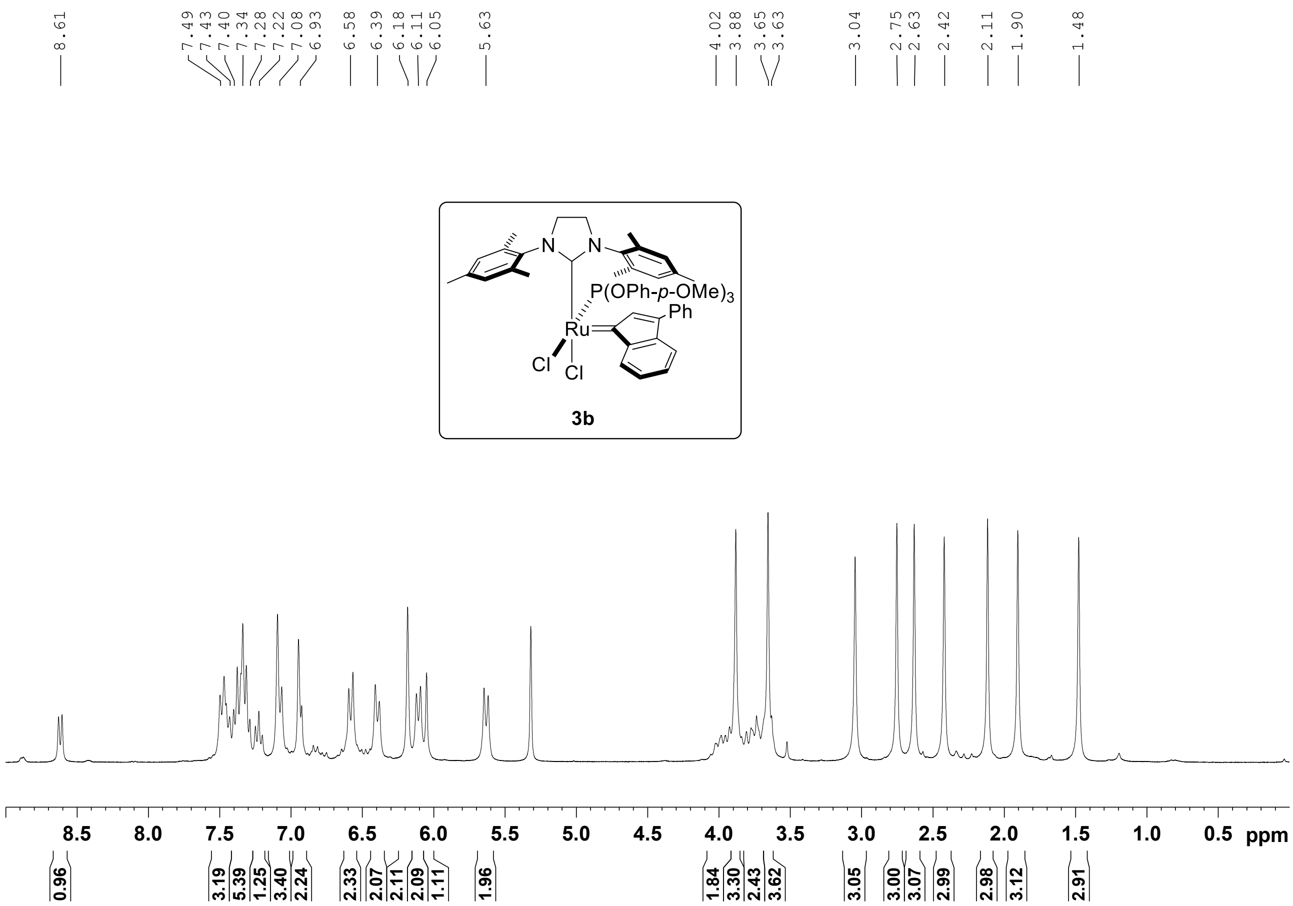


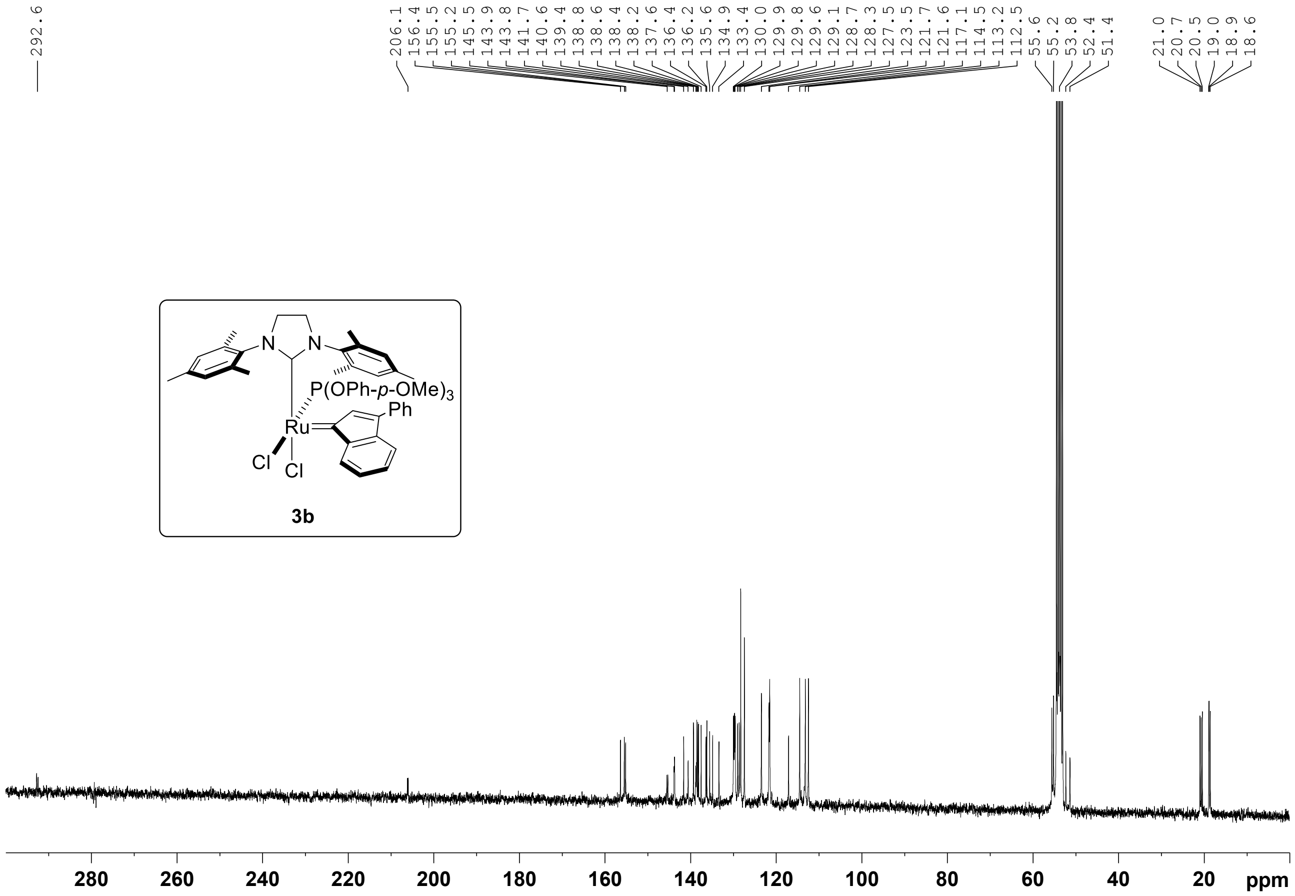
292.9
205.9
151.8 150.4 143.1 140.5 139.4 139.3 138.6 138.3 138.2 137.7 136.3 135.6 135.1 134.9 133.5 130.1 129.9 129.8 129.6 129.0 128.8 128.5 128.4 128.2 127.6 125.5 124.7 124.1 122.9 121.1 120.7 117.3
52.4 51.5
21.1 20.7 20.6 19.0 19.0 18.7 14.1
P(OPh)3
Ph
Ru
Cl
Cl
3a
280 260 240 220 200 180 160 140 120 100 80 60 40 20 ppm

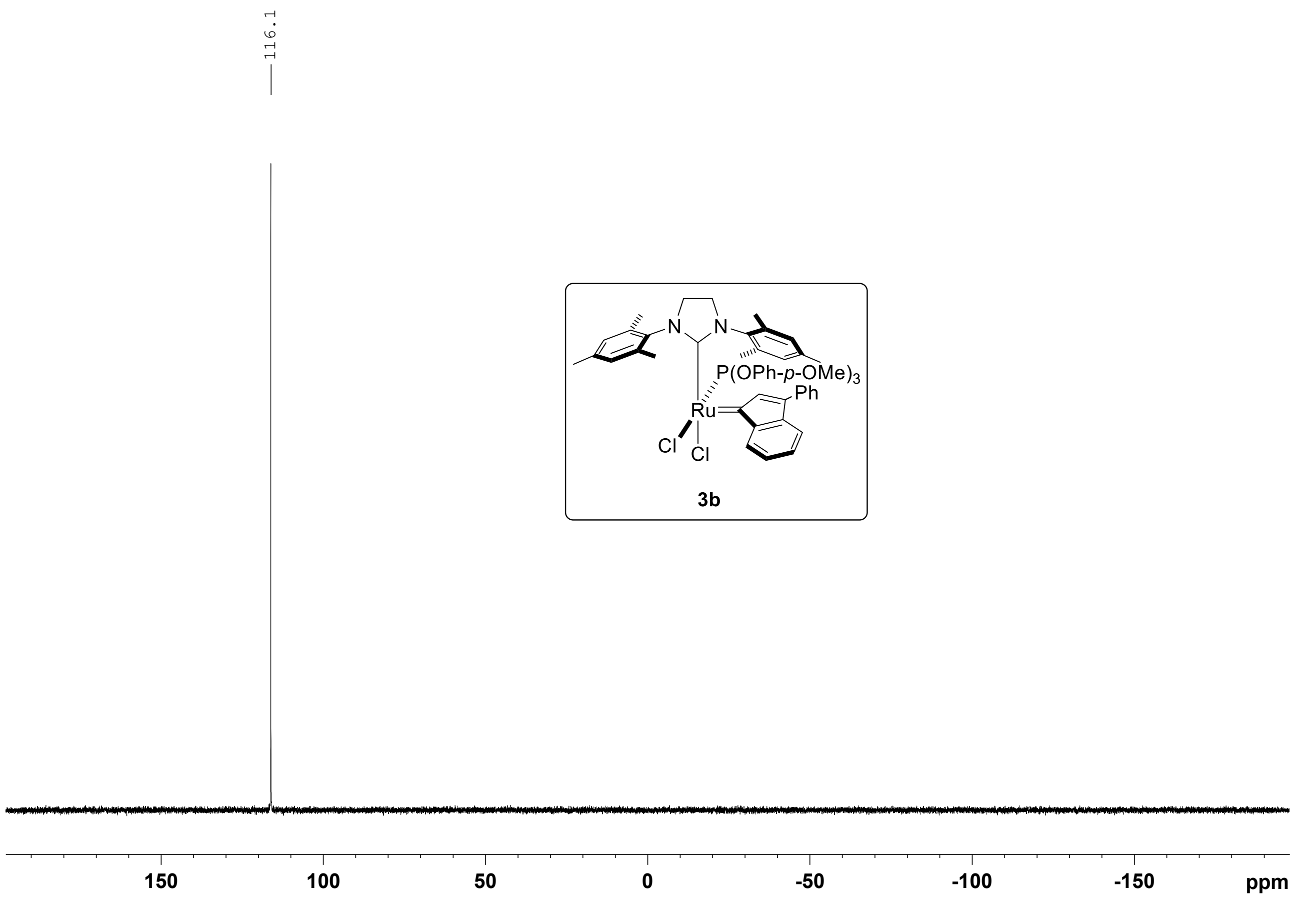


127.5
P(OPh)3
Ph
Ru
Cl
Cl
3a
150 100 50 0 -50 -100 -150 ppm

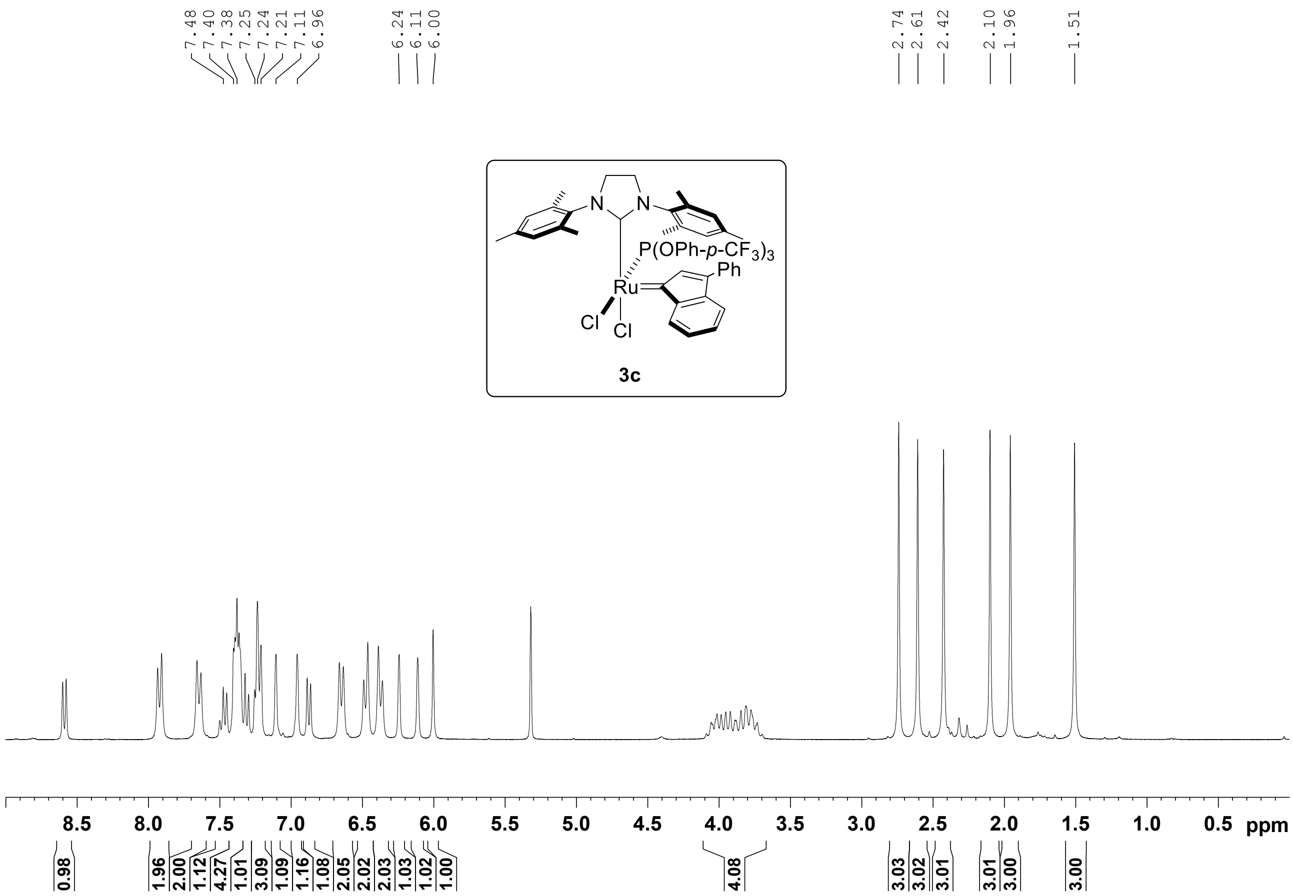
^{1}H NMR (300 MHz, CD_2Cl_2, 233K), ^{13}C-{^{1}H} NMR (75 MHz, CD_2Cl_2, 233K) and ^{31}P-{^{1}H} NMR (162 MHz CD_2Cl_2, 233K) of **3b**

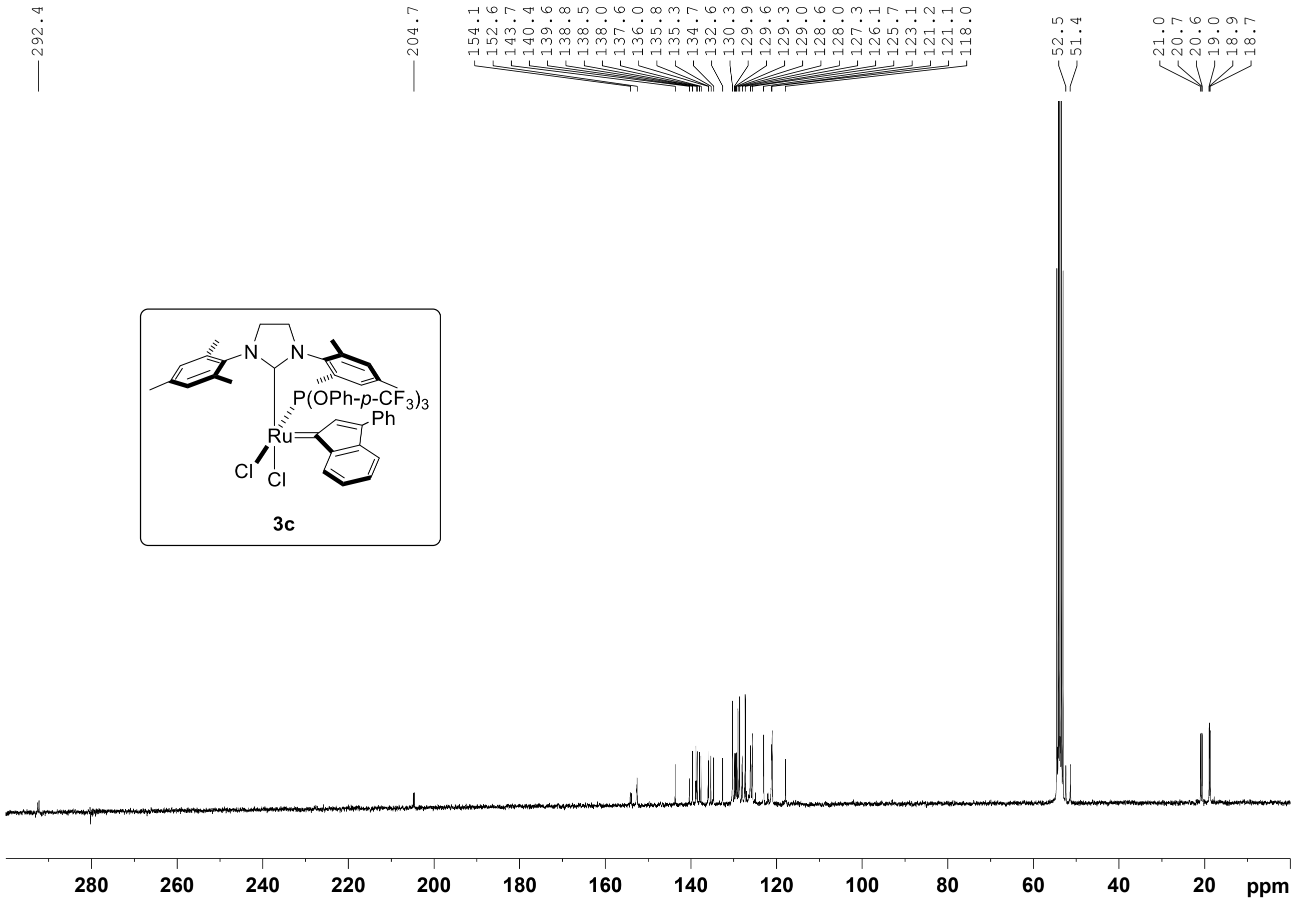


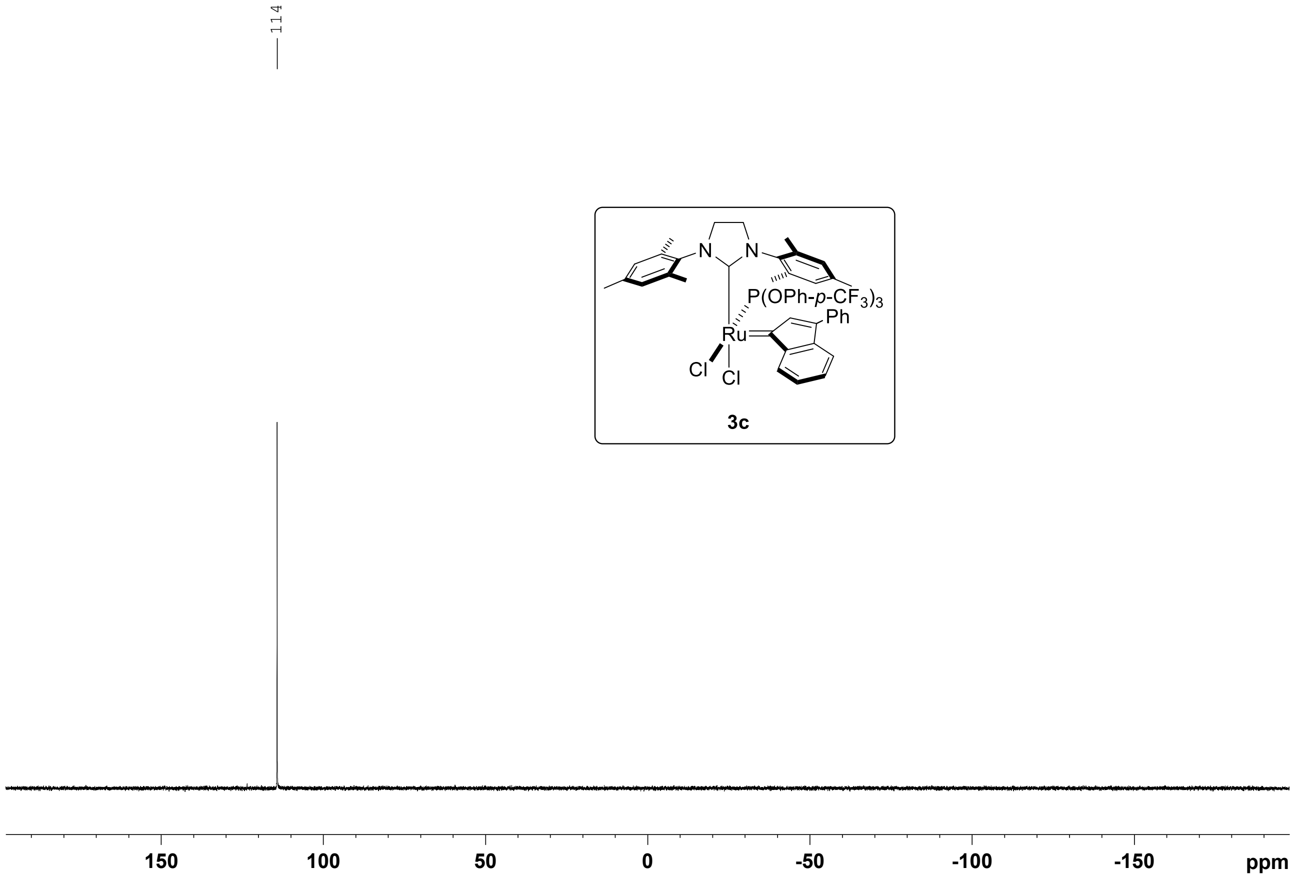

292.6
206.1
156.4
155.5
155.2
145.5
143.9
143.8
141.7
140.6
139.4
138.8
138.6
138.4
138.2
137.6
136.4
136.2
135.6
134.9
133.4
130.0
129.9
129.8
129.6
129.1
128.7
128.3
127.5
123.5
121.7
121.6
117.1
114.5
113.2
112.5
55.6
55.2
53.8
52.4
51.4
21.0
20.7
20.5
19.0
18.9
18.6
N
N
P(OPh-p-OMe)3
Ph
Ru
Cl
Cl
3b
280
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm


116.1
N
N
P(OPh-p-OMe)3
Ph
Ru
Cl
Cl
3b
150
100
50
0
-50
-100
-150
ppm

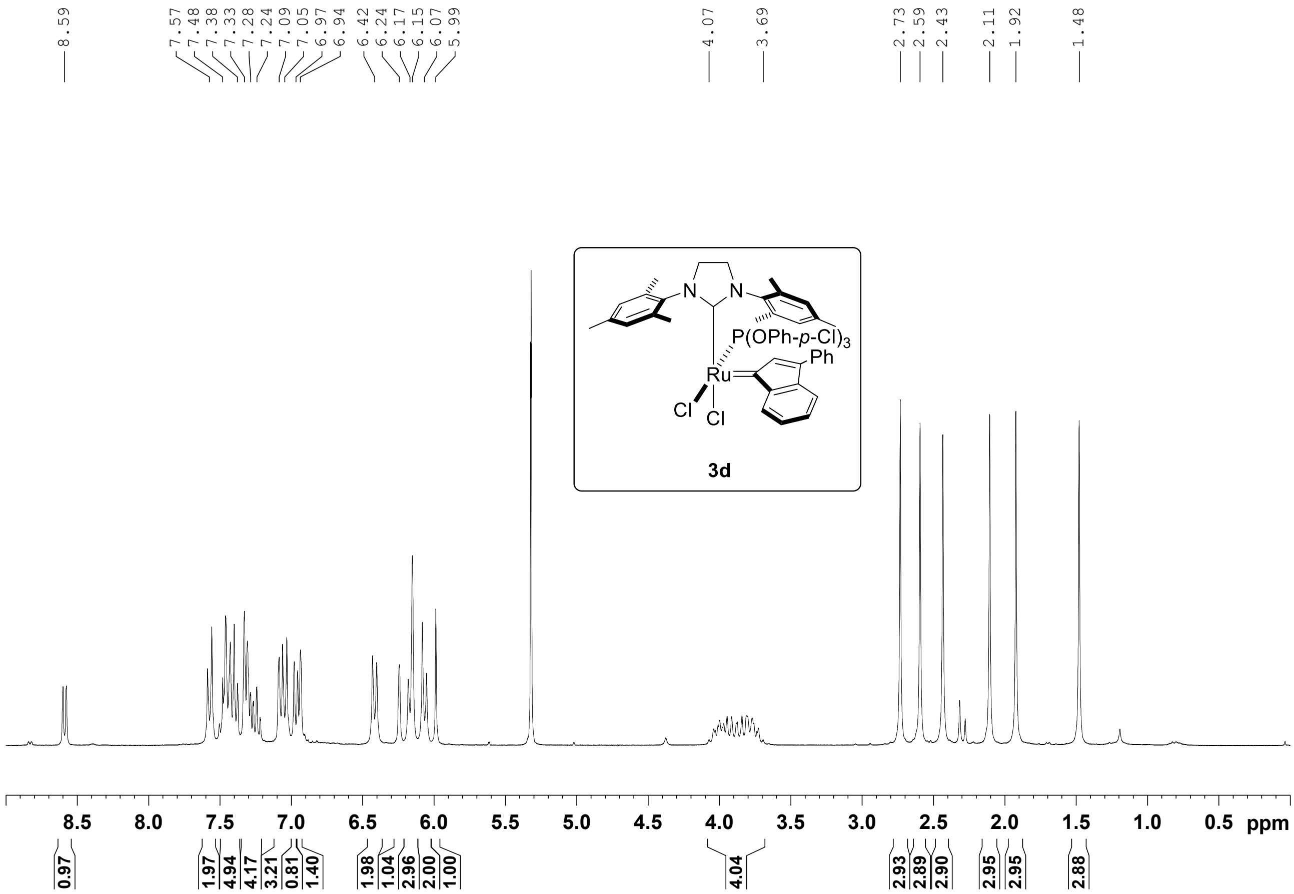
^{1}H NMR (300 MHz, CD_2Cl_2, 233K), ^{13}C-{^{1}H} NMR (75 MHz, CD_2Cl_2, 233K) and ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 233K) of **3c**

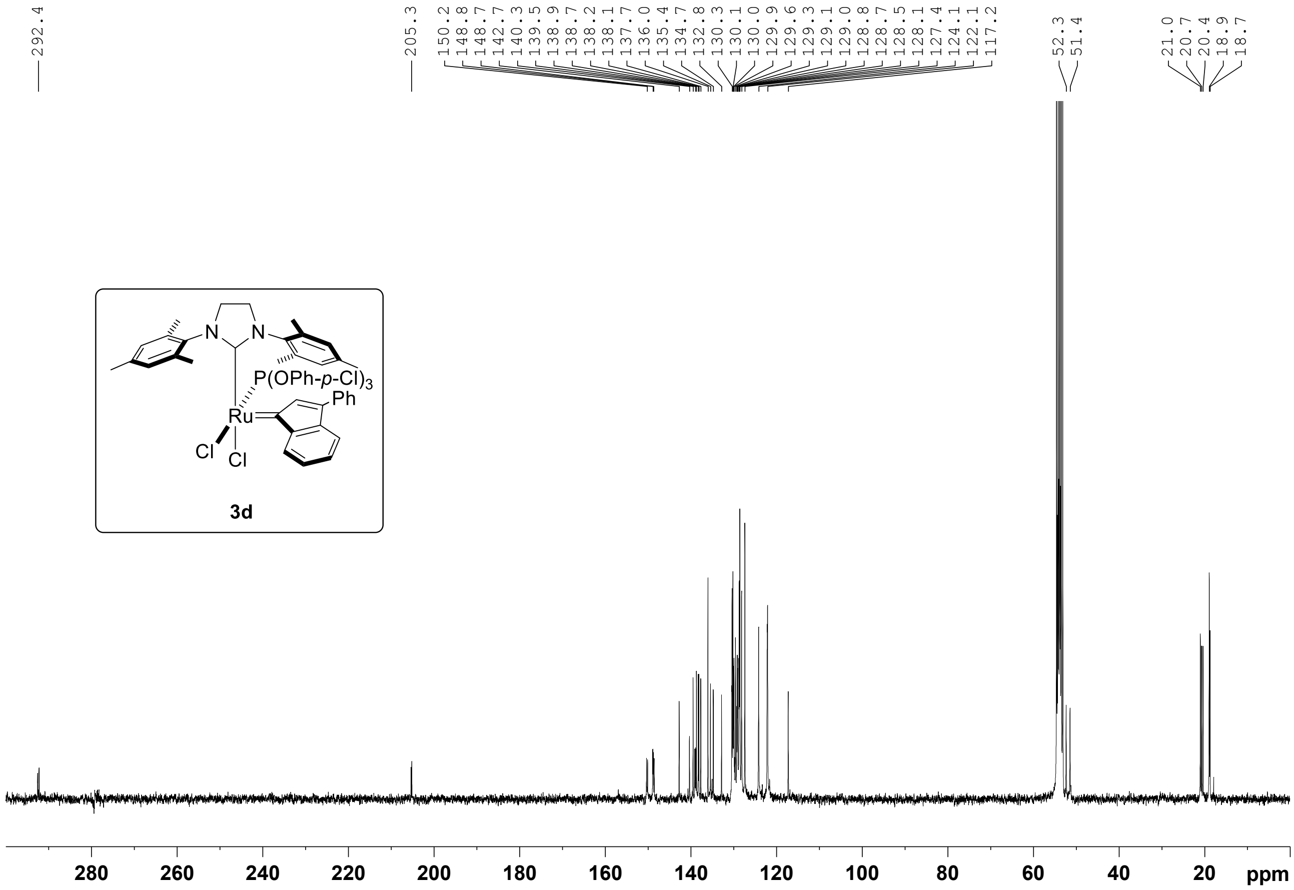


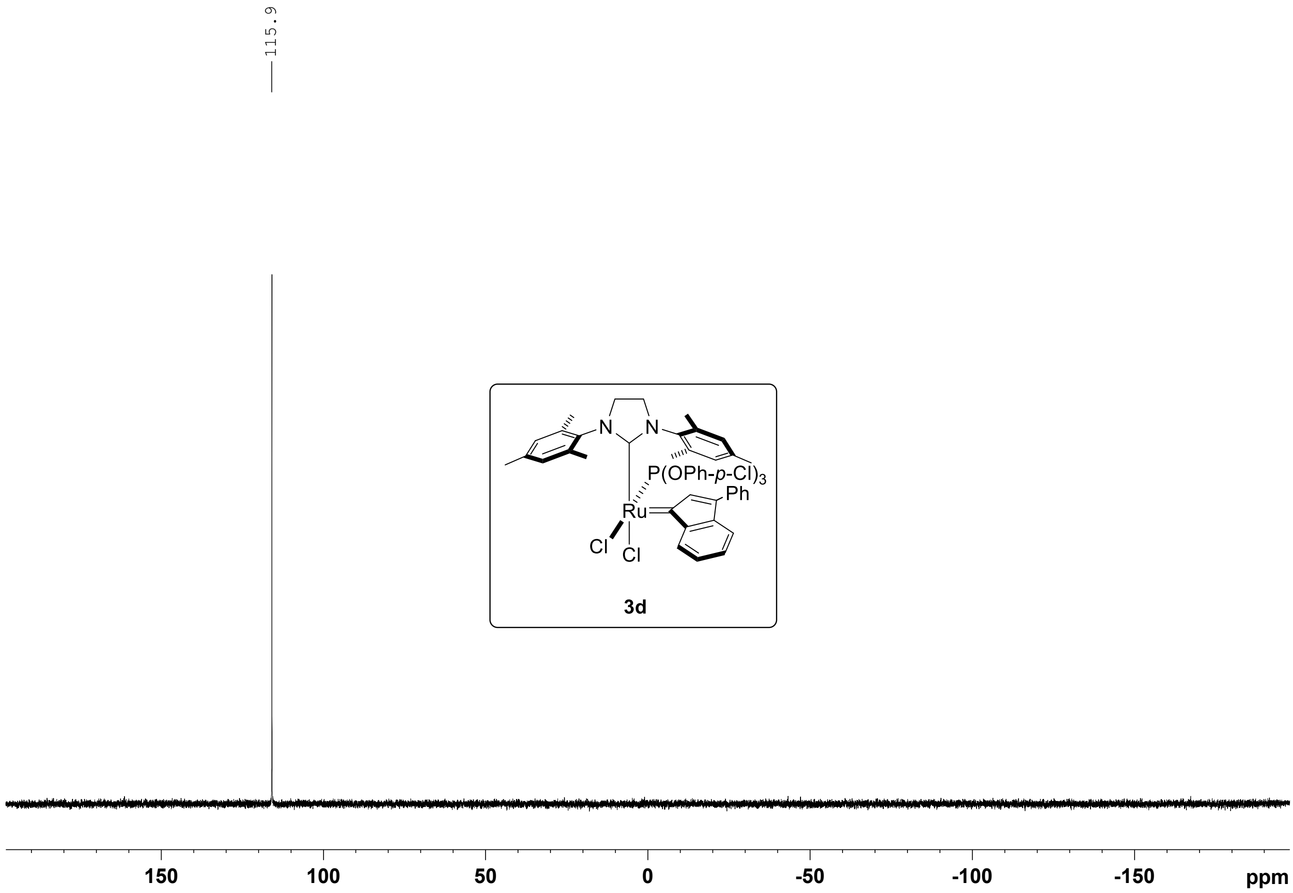

292.4
204.7
154.1 152.6 143.7 140.4 139.6 138.8 138.5 138.0 137.6 136.0 135.8 135.3 134.7 132.6 130.3 129.9 129.6 129.3 129.0 128.6 128.0 127.3 126.1 125.7 123.1 121.2 121.1 118.0
52.5 51.4
21.0 20.7 20.6 19.0 18.9 18.7
N
N
P(OPh-p-CF3)3
Ph
Ru
Cl
Cl
3c
280 260 240 220 200 180 160 140 120 100 80 60 40 20 ppm


114.2
N
N
P(OPh-p-CF3)3
Ph
Ru
Cl
Cl
3c
150 100 50 0 -50 -100 -150 ppm

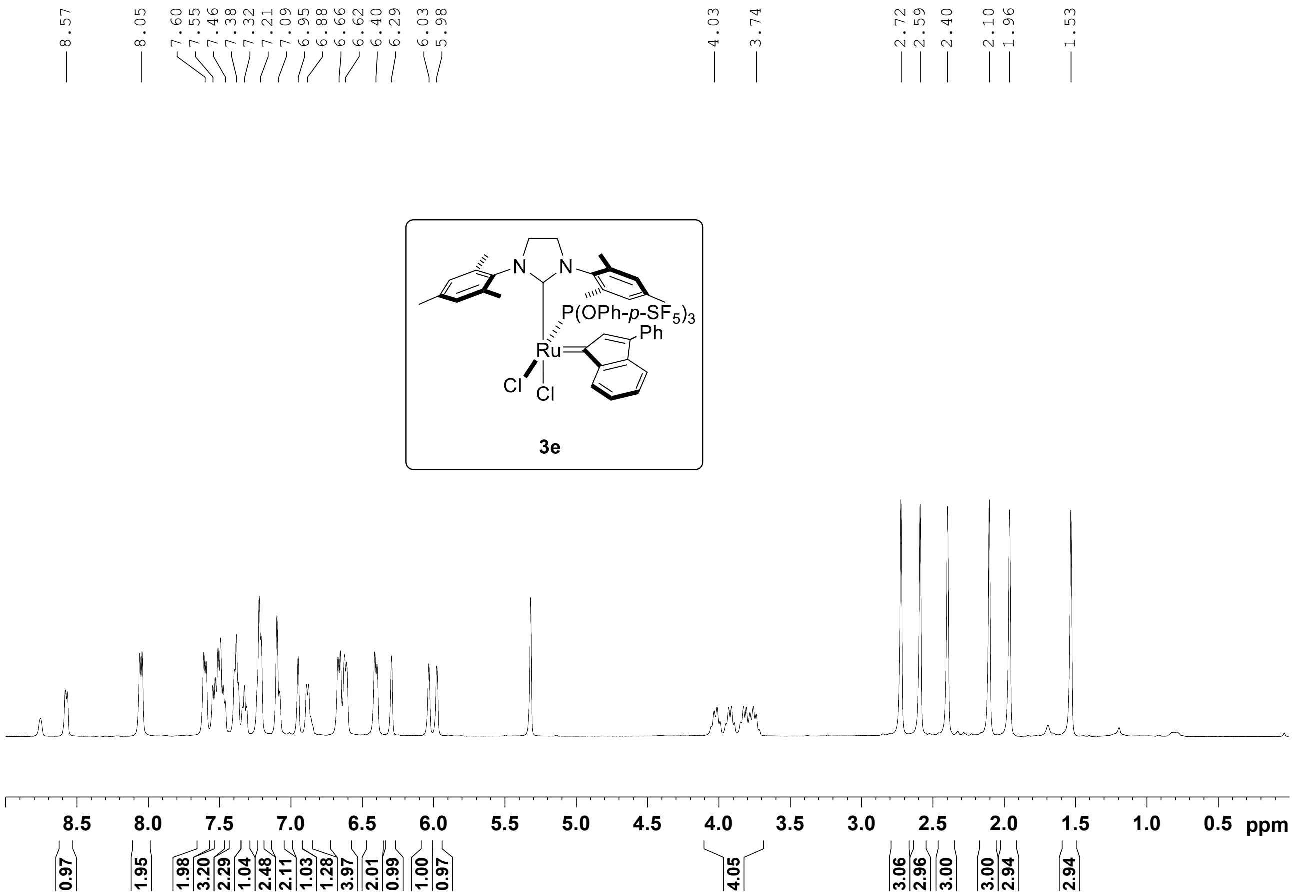
[1]H NMR (300 MHz, CD_2Cl_2, 233K), [13]C-{[1]H} NMR (75 MHz, CD_2Cl_2, 233K) and [31]P-{[1]H} NMR (162 MHz, CD_2Cl_2, 233K) of **3d**

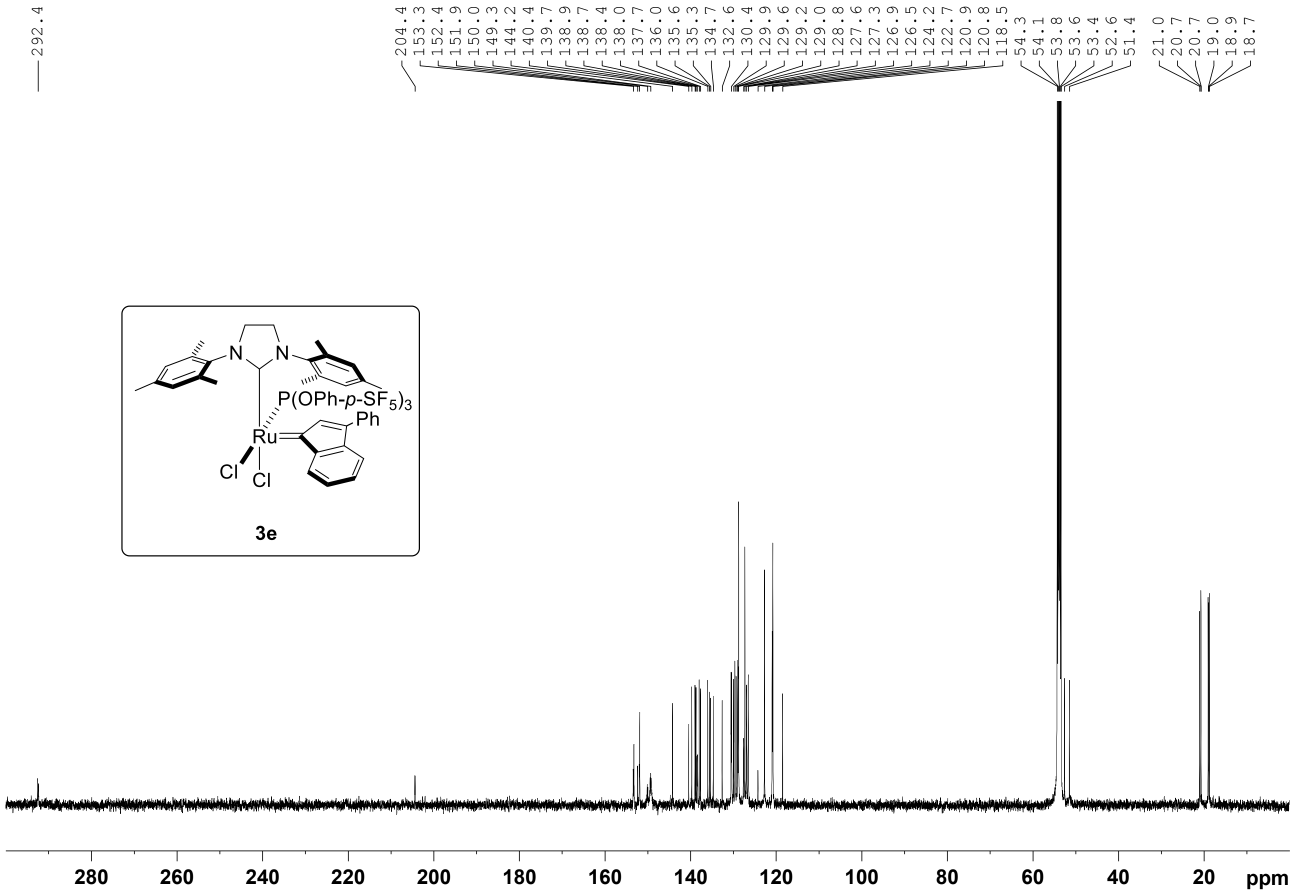


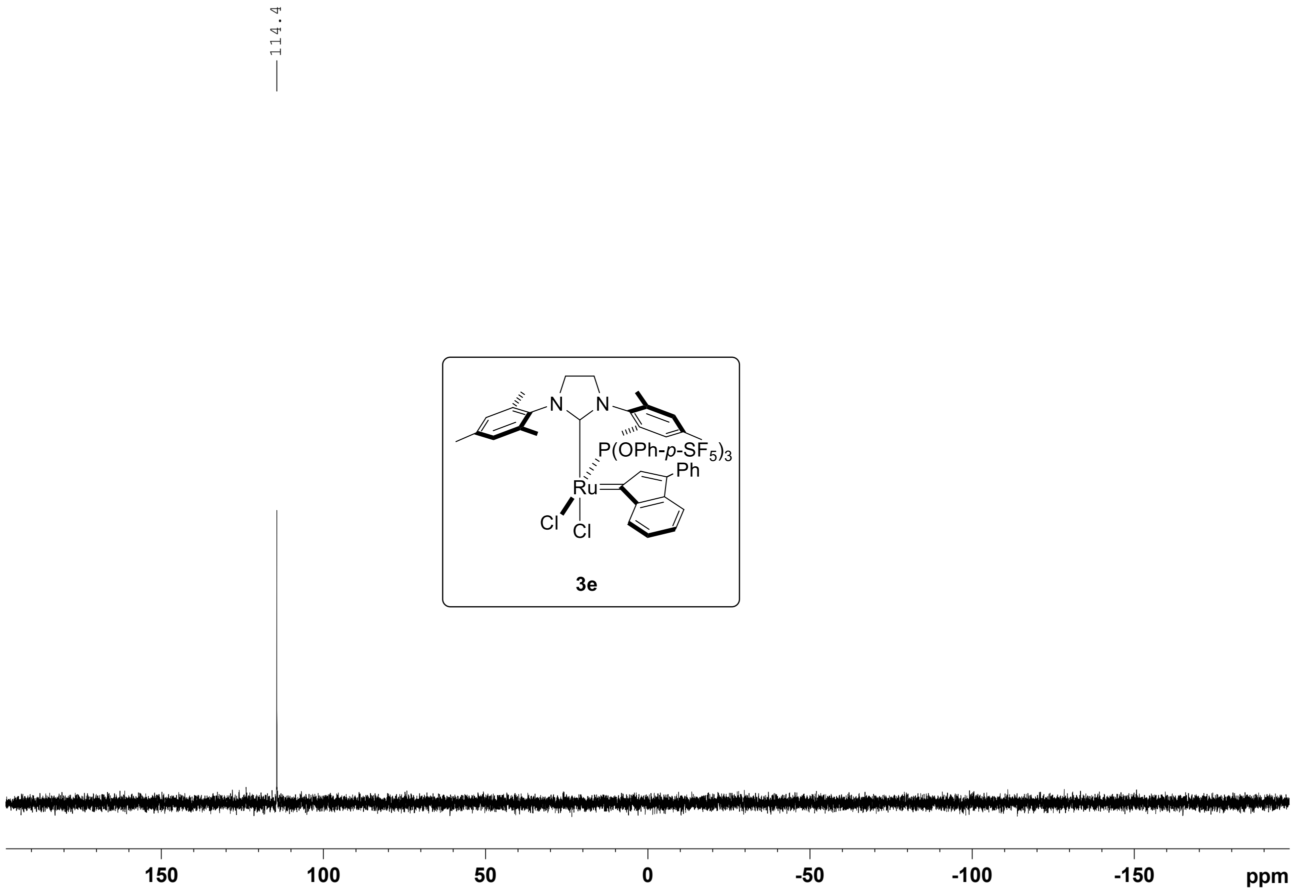

292.4
205.3
150.2 148.8 148.7 142.7 140.3 139.5 138.9 138.7 138.2 138.1 137.7 136.0 135.4 134.7 132.8 130.3 130.1 130.0 129.9 129.6 129.3 129.1 129.0 128.8 128.7 128.5 128.1 127.4 124.1 122.1 117.2
52.3
51.4
21.0 20.7 20.4 18.9 18.7
N
N
P(OPh-p-Cl)3
Ph
Ru
Cl
Cl
3d
280 260 240 220 200 180 160 140 120 100 80 60 40 20 ppm


115.9
N
N
P(OPh-p-Cl)3
Ph
Ru
Cl
Cl
3d
150 100 50 0 -50 -100 -150 ppm

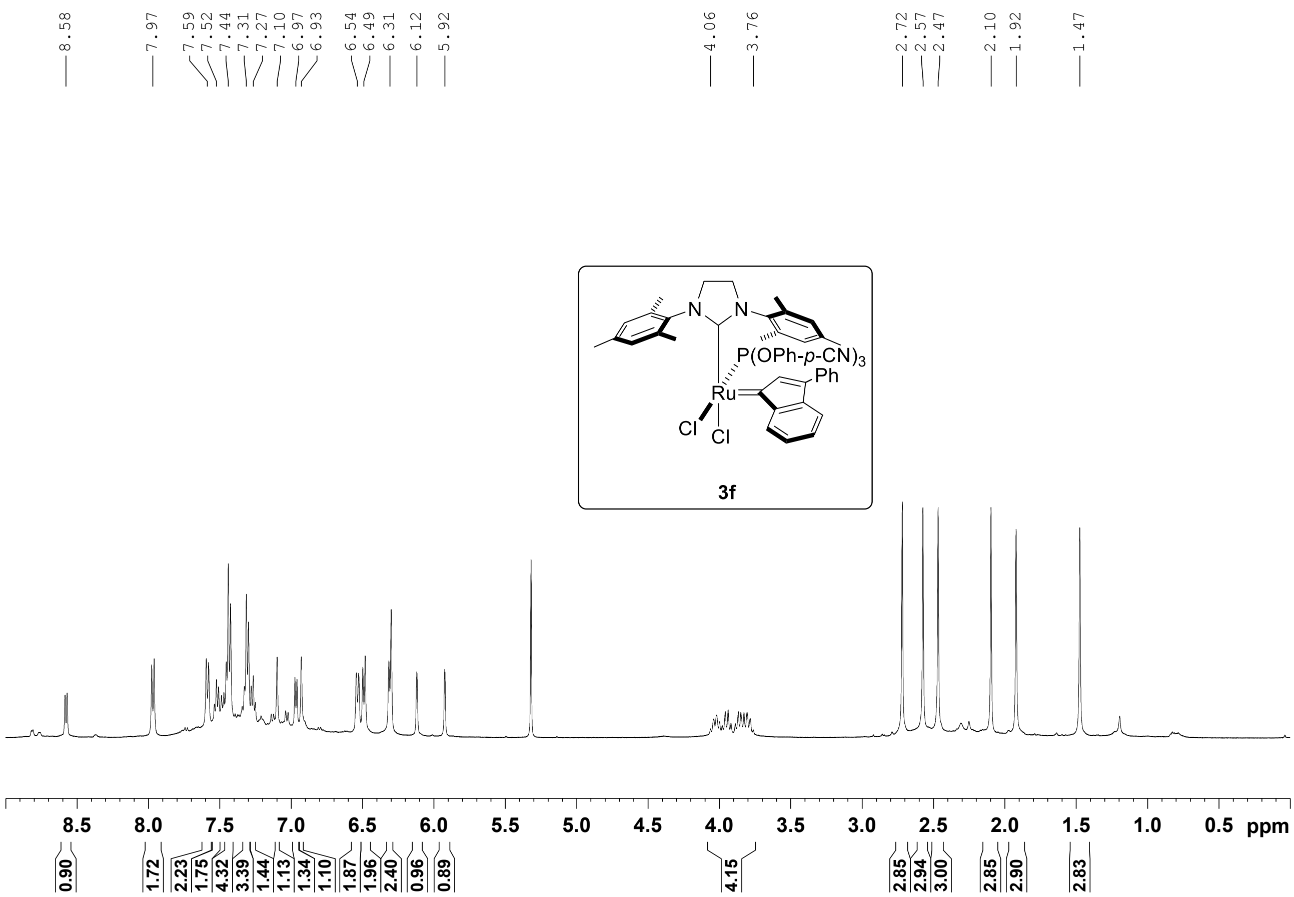
^{1}H NMR (500 MHz, CD_2Cl_2, 233K), ^{13}C-{^{1}H} NMR (126 MHz, CD_2Cl_2, 233K) and ^{31}P-{^{1}H} NMR (162 MHz, CD_2Cl_2, 233K) of **3e**

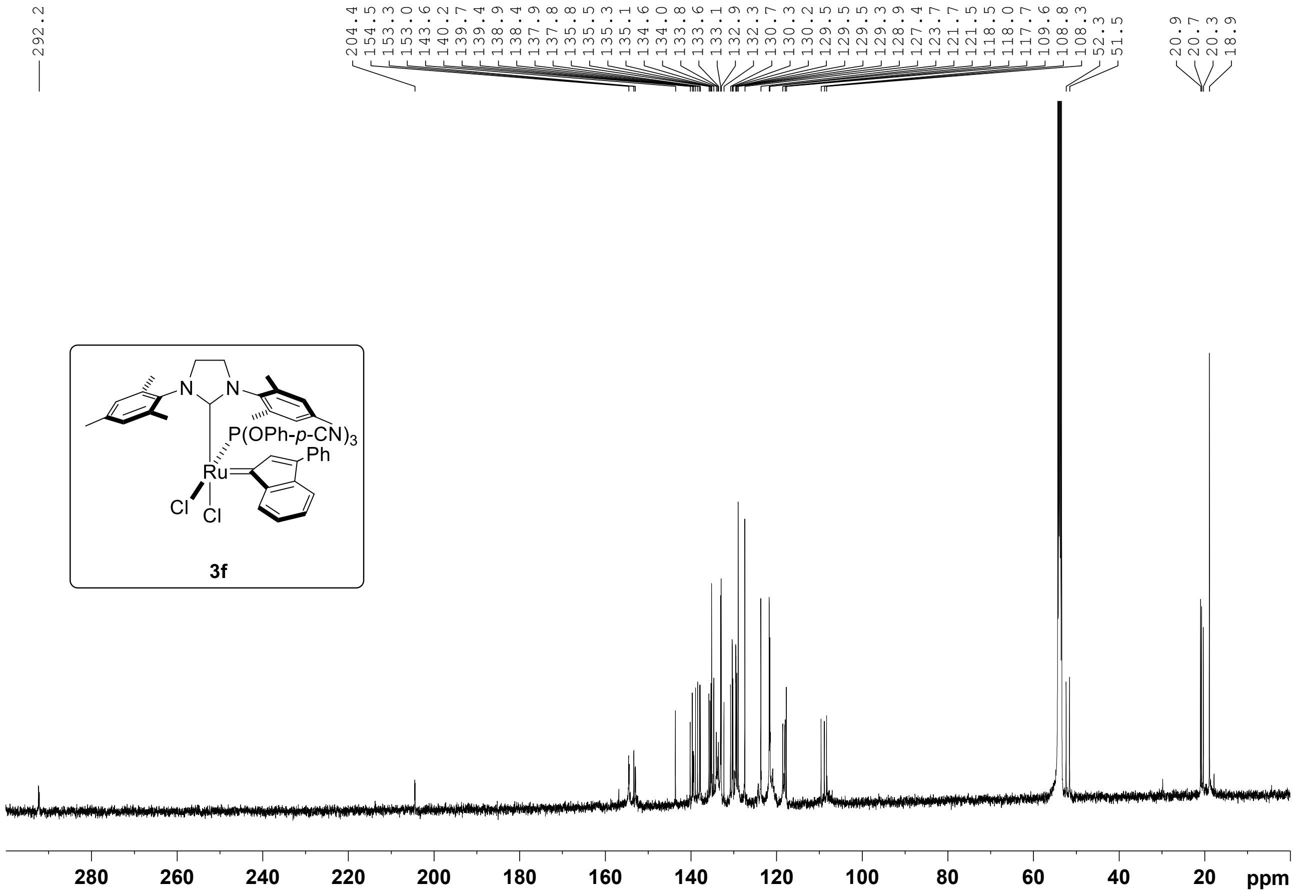


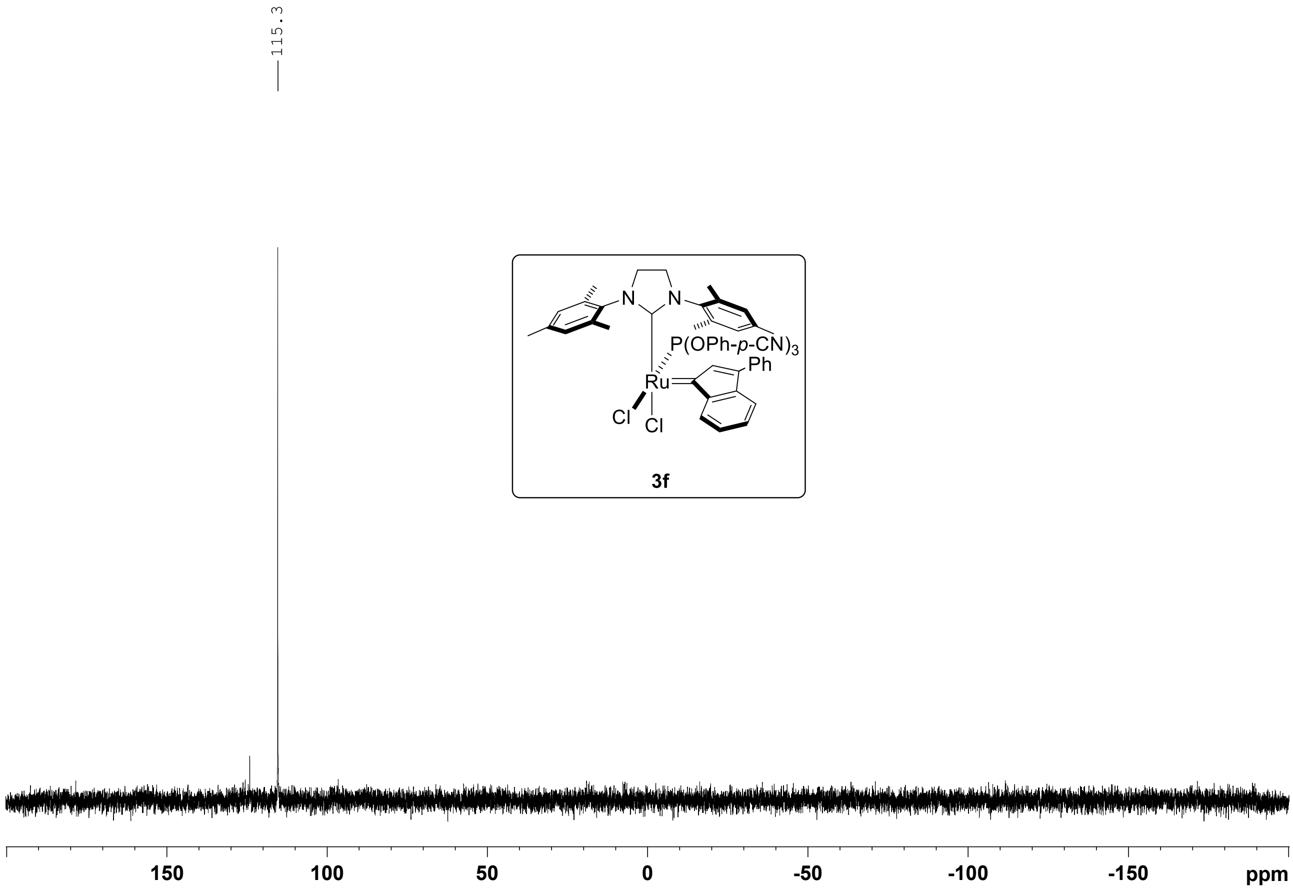

292.4
204.4 153.3 152.4 151.9 150.0 149.3 144.2 140.4 139.7 138.9 138.7 138.4 138.0 137.7 136.0 135.6 135.3 134.7 132.6 130.4 129.9 129.6 129.2 129.0 128.8 127.6 127.3 126.9 126.5 124.2 122.7 120.9 120.8 118.5
54.3 54.1 53.8 53.6 53.4 52.6 51.4
21.0 20.7 20.7 19.0 18.9 18.7
N
N
P(OPh-p-SF5)3
Ph
Ru
Cl
Cl
3e
280 260 240 220 200 180 160 140 120 100 80 60 40 20 ppm


114.4
N
N
P(OPh-p-SF5)3
Ph
Ru
Cl
Cl
3e
150 100 50 0 -50 -100 -150 ppm

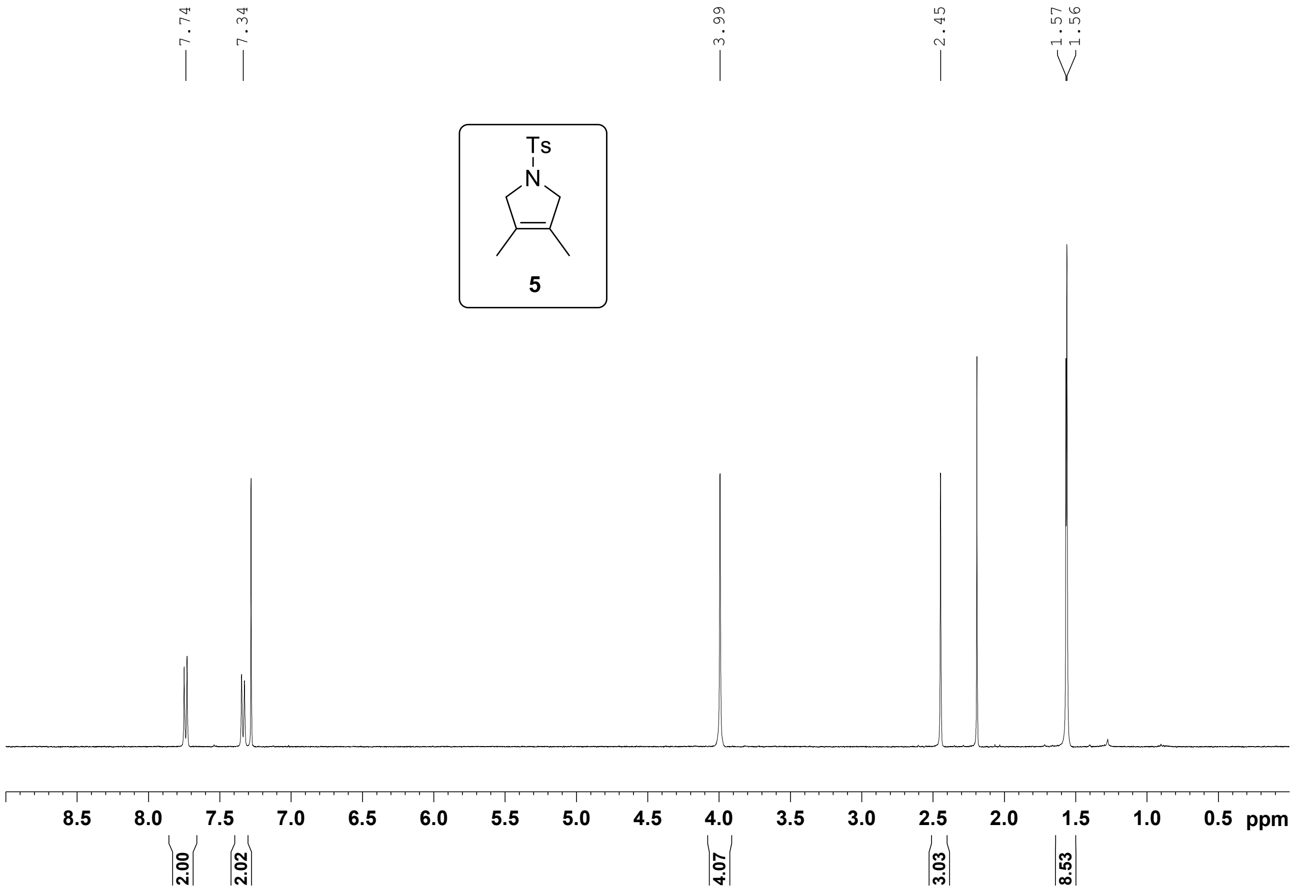
^{1}H NMR (500 MHz, CD_2Cl_2, 233K), ^{13}C-{^{1}H} NMR (126 MHz, CD_2Cl_2, 233K) and ^{31}P-{^{1}H} NMR (121 MHz, CD_2Cl_2, 233K) of **3f**

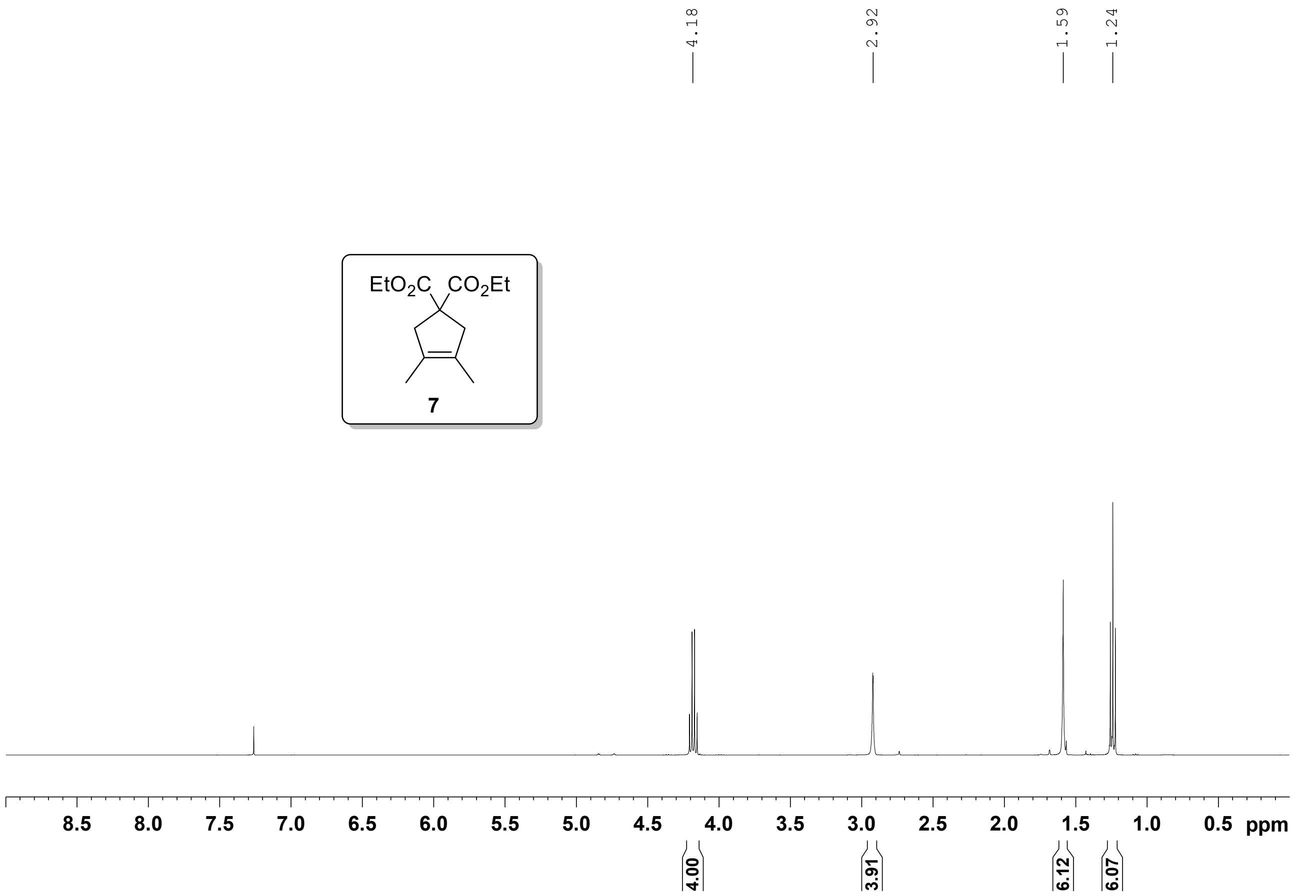


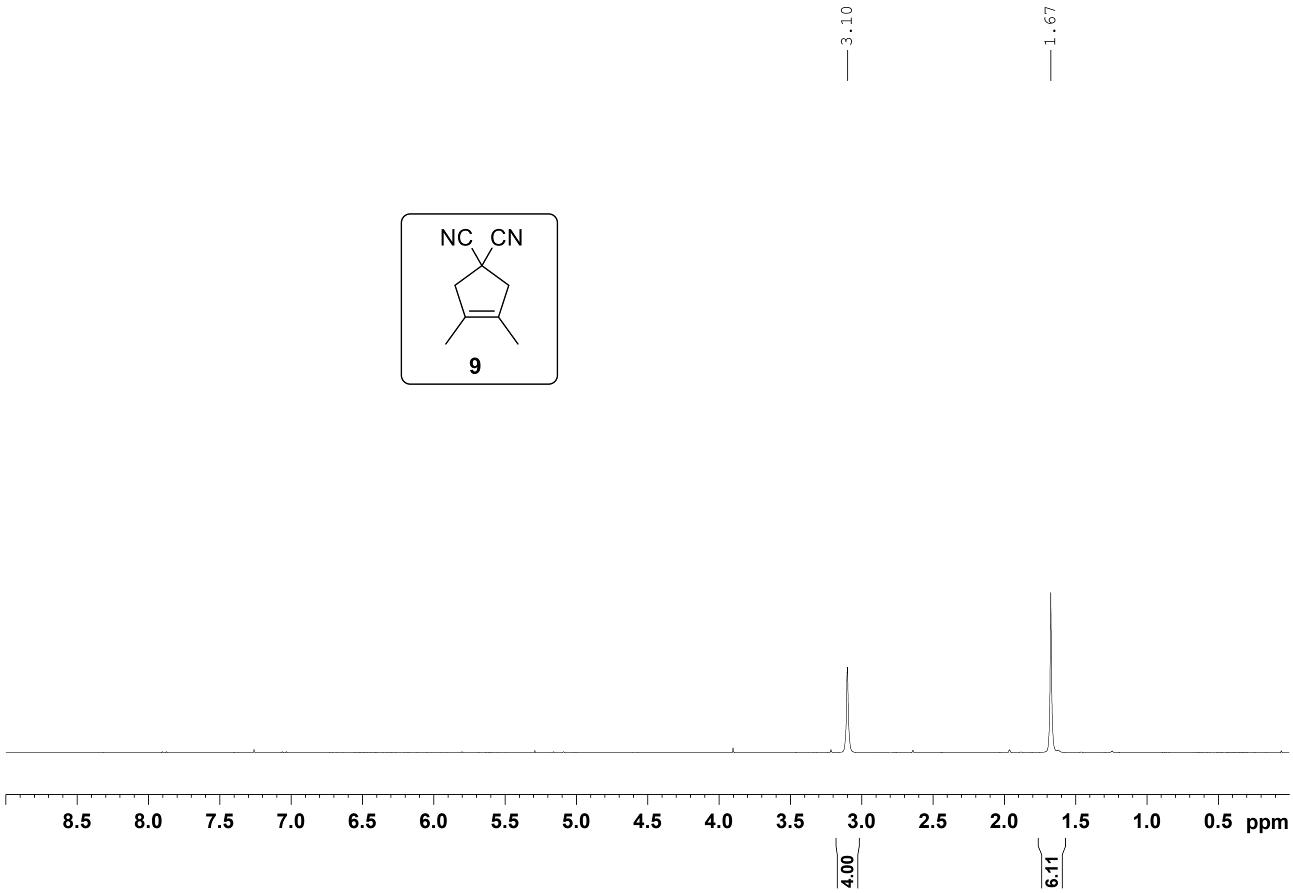

292.2
204.4 154.5 153.3 153.0 143.6 140.2 139.7 139.4 138.9 138.4 137.9 137.8 135.8 135.5 135.3 135.1 134.6 134.0 133.8 133.6 133.1 132.9 132.3 130.7 130.3 130.2 129.5 129.5 129.3 128.9 127.4 123.7 121.7 121.5 118.5 118.0 117.7 109.6 108.8 108.3 52.3 51.5
20.9 20.7 20.3 18.9
N
N
P(OPh-p-CN)3
Ph
Ru
Cl
Cl
3f
280 260 240 220 200 180 160 140 120 100 80 60 40 20 ppm

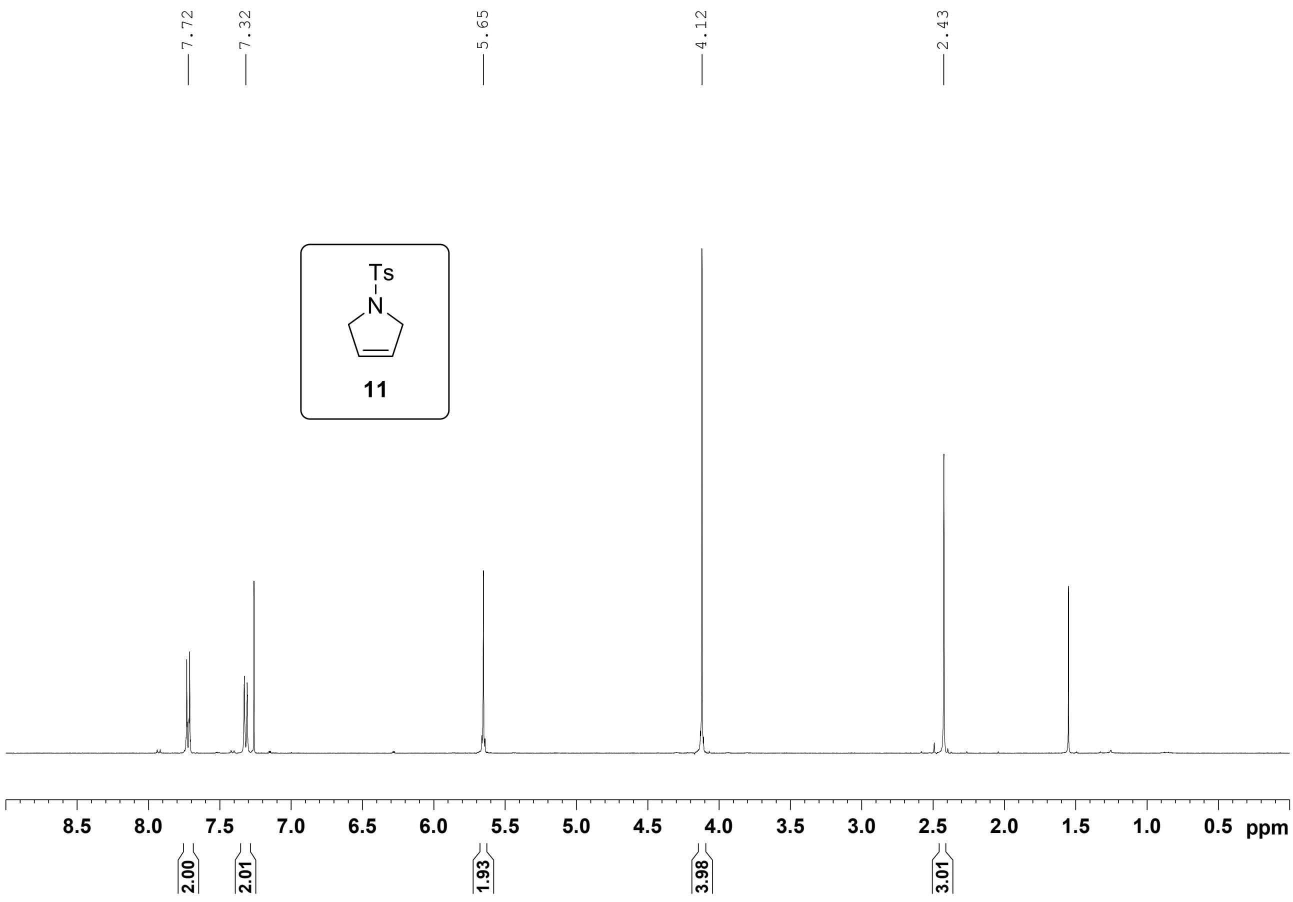

115.3
N
N
P(OPh-p-CN)3
Ph
Ru
Cl
Cl
3f
150 100 50 0 -50 -100 -150 ppm

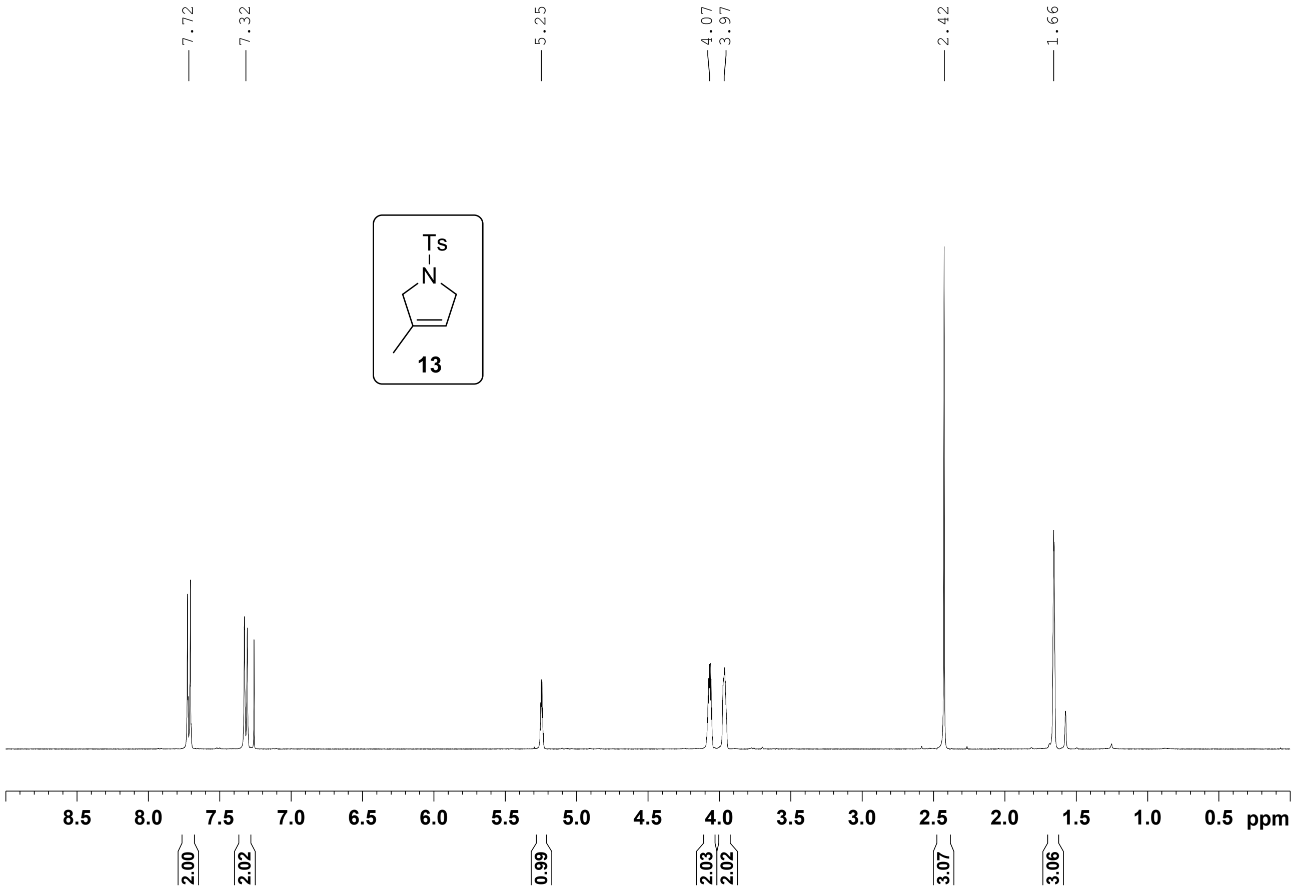
10. ^{1}H NMR spectra of metathesis products

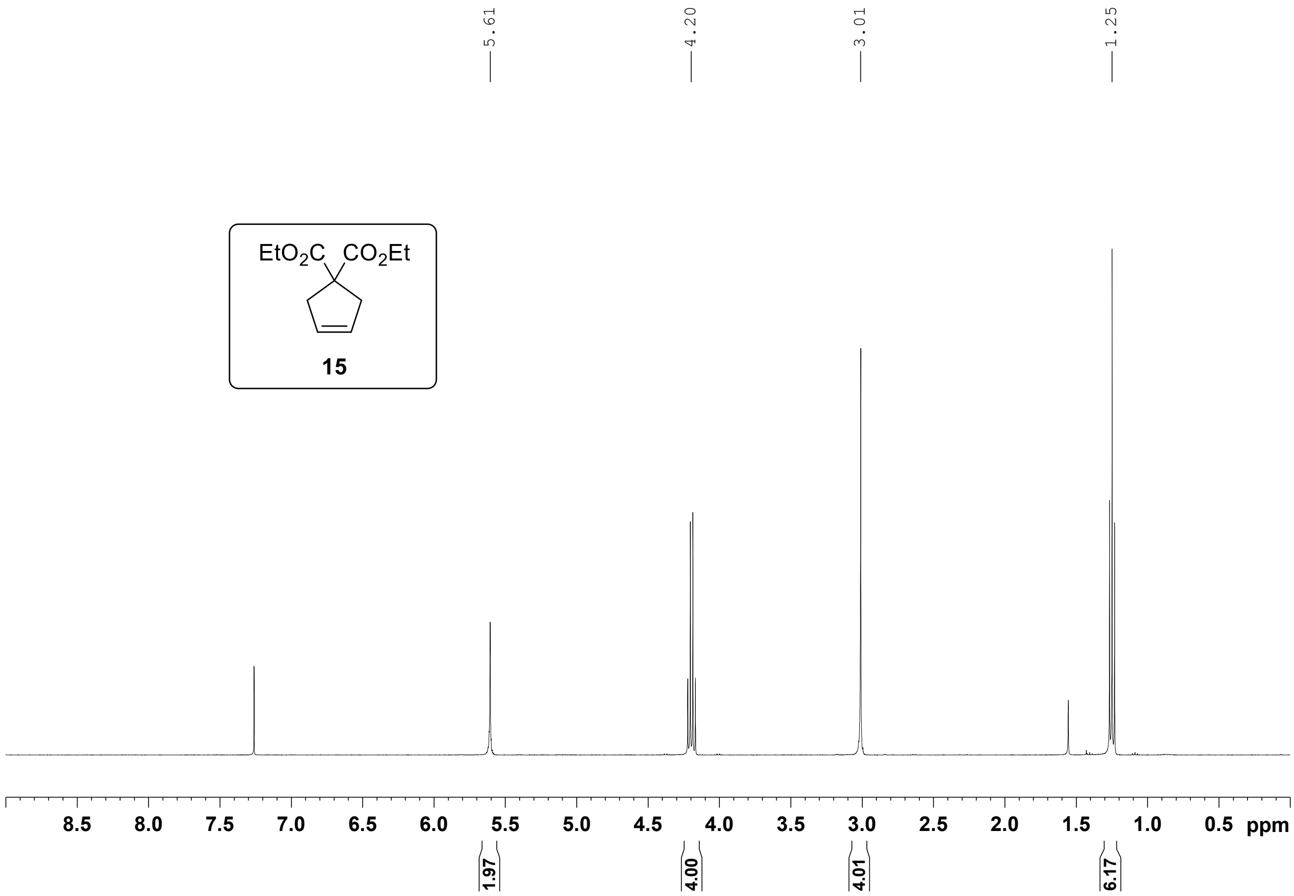


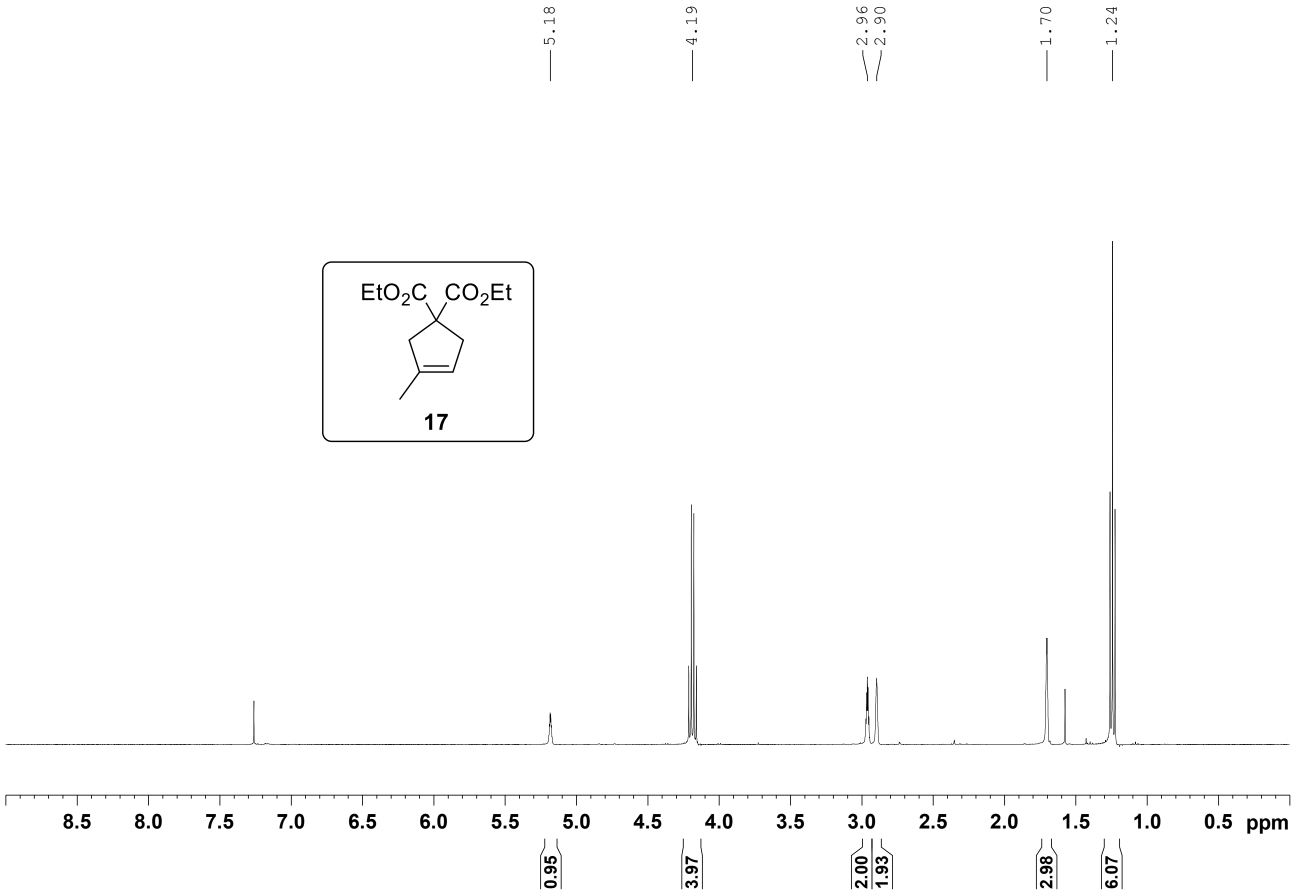


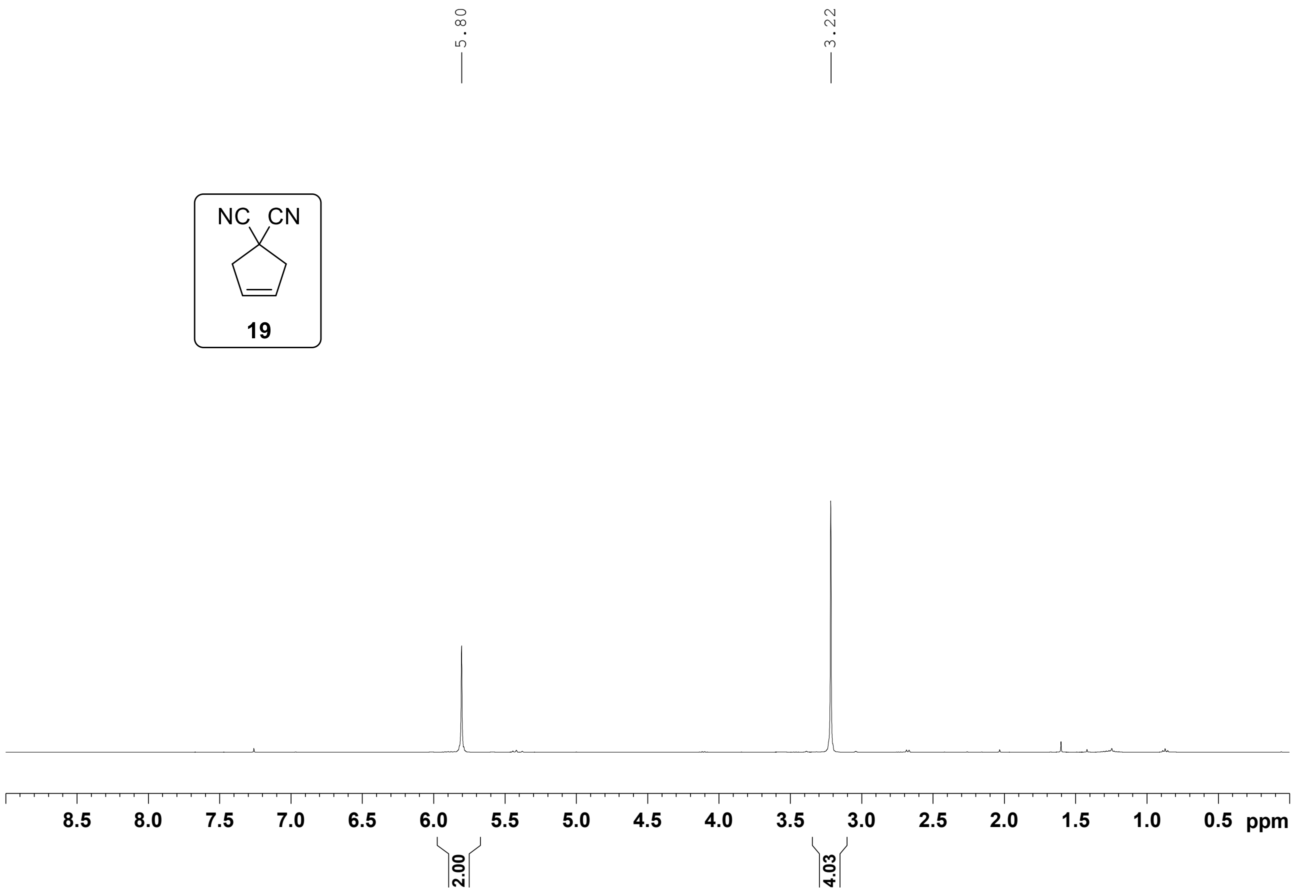

3.10
1.67
NC CN
9
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.00
6.11

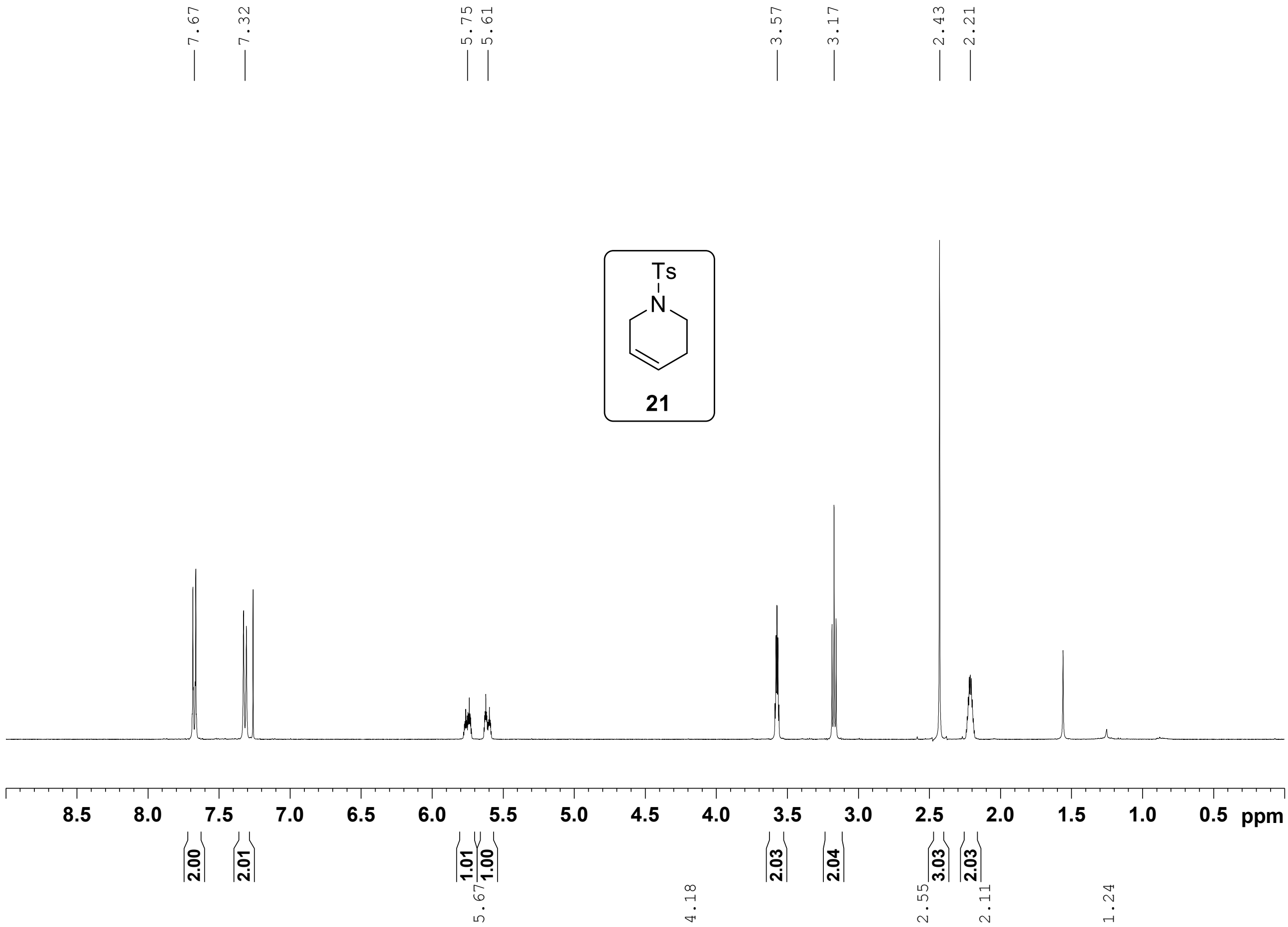

7.72
7.32
5.65
4.12
2.43
Ts
N
11
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.01
1.93
3.98
3.01

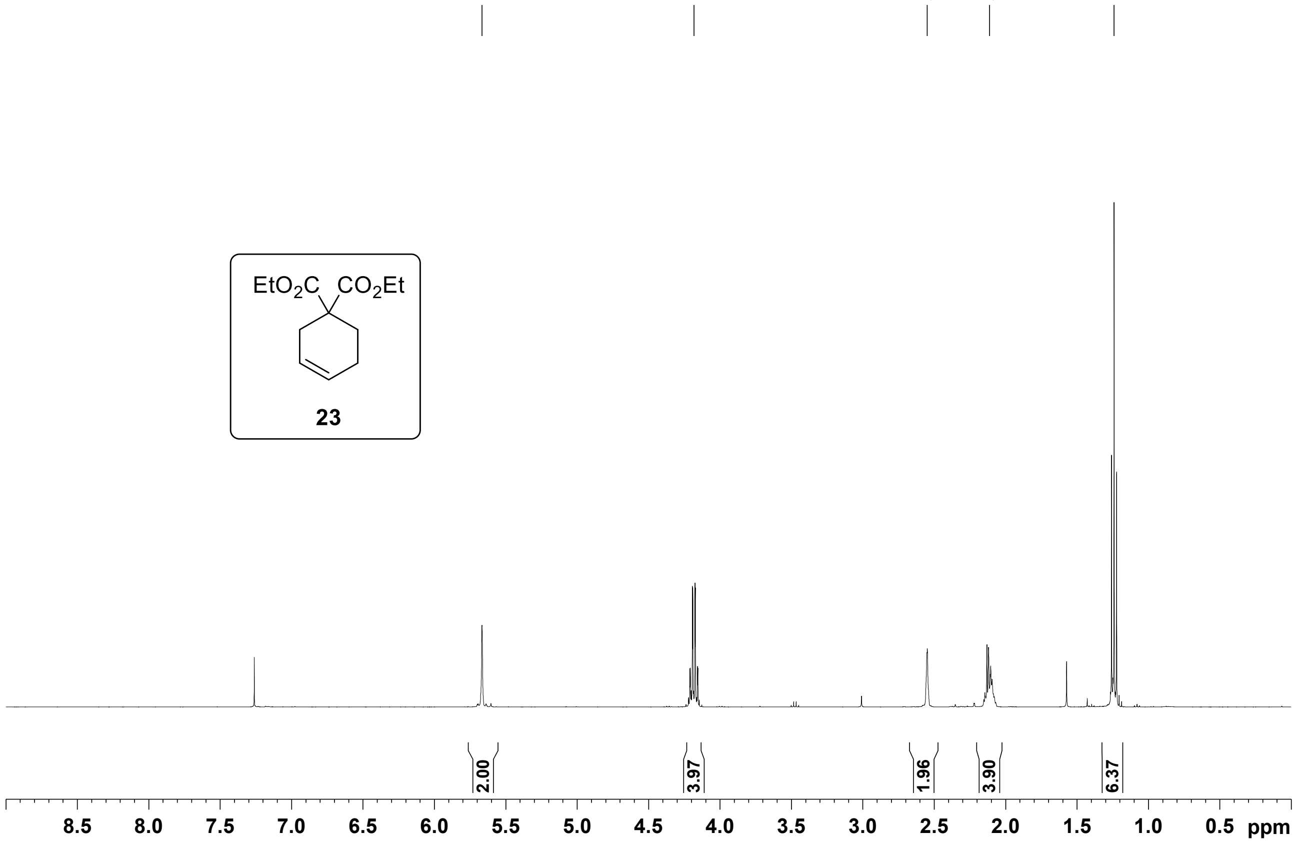

7.72
7.32
5.25
4.07
3.97
2.42
1.66
Ts
N
13
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.02
0.99
2.03
2.02
3.07
3.06

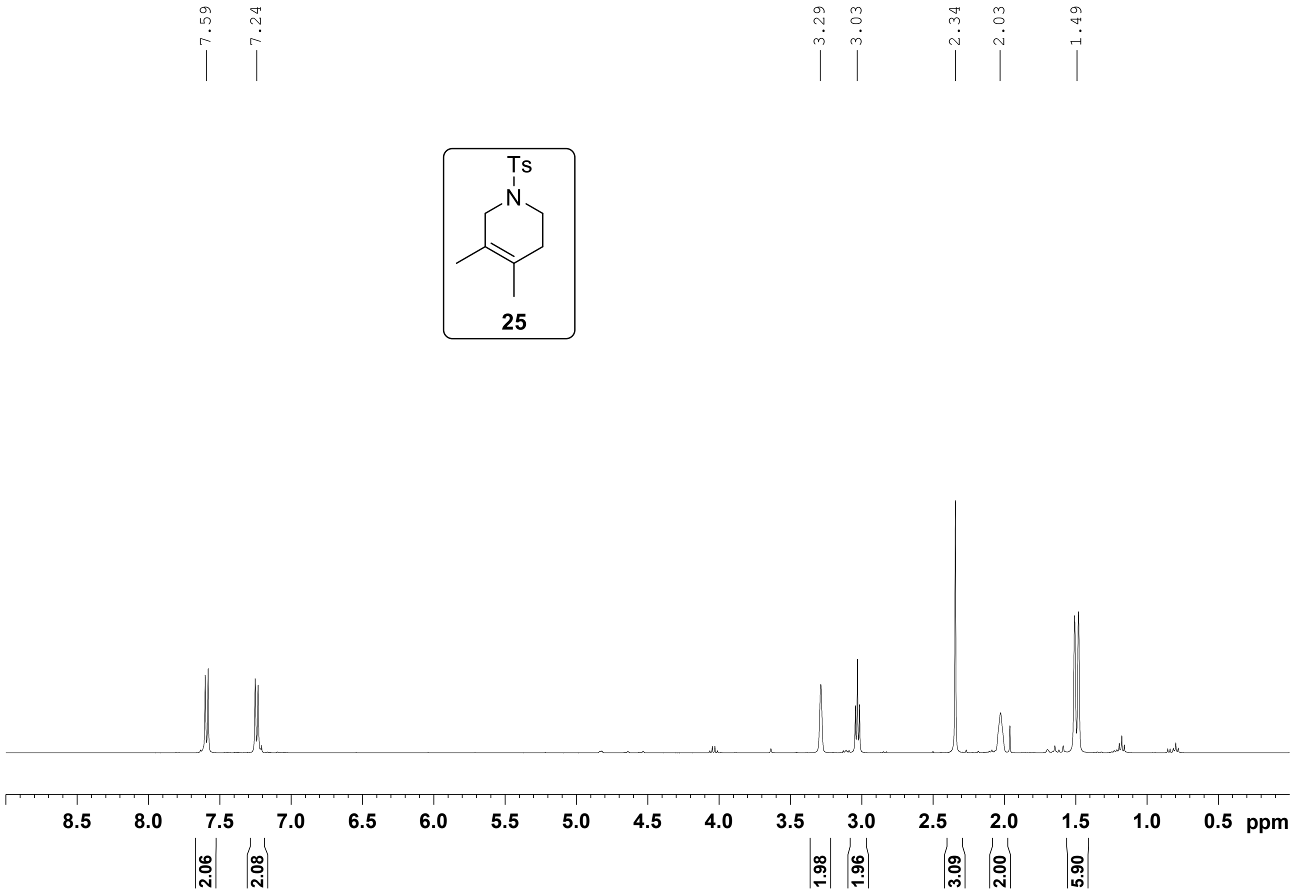

5.61
4.20
3.01
1.25
EtO_2C CO_2Et
15
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.97
4.00
4.01
6.17

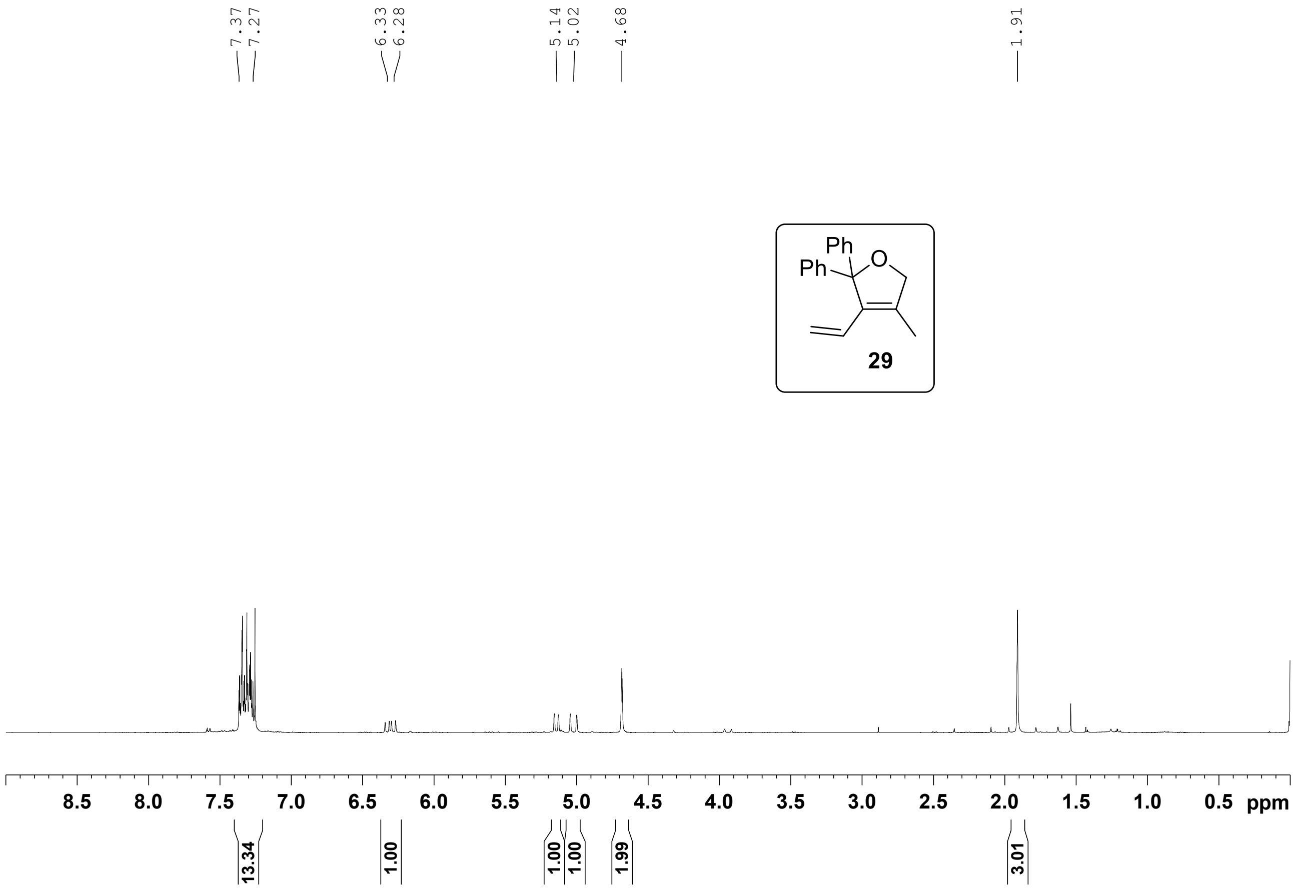

5.18
4.19
2.96
2.90
1.70
1.24
EtO2C CO2Et
17
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.95
3.97
2.00
1.93
2.98
6.07

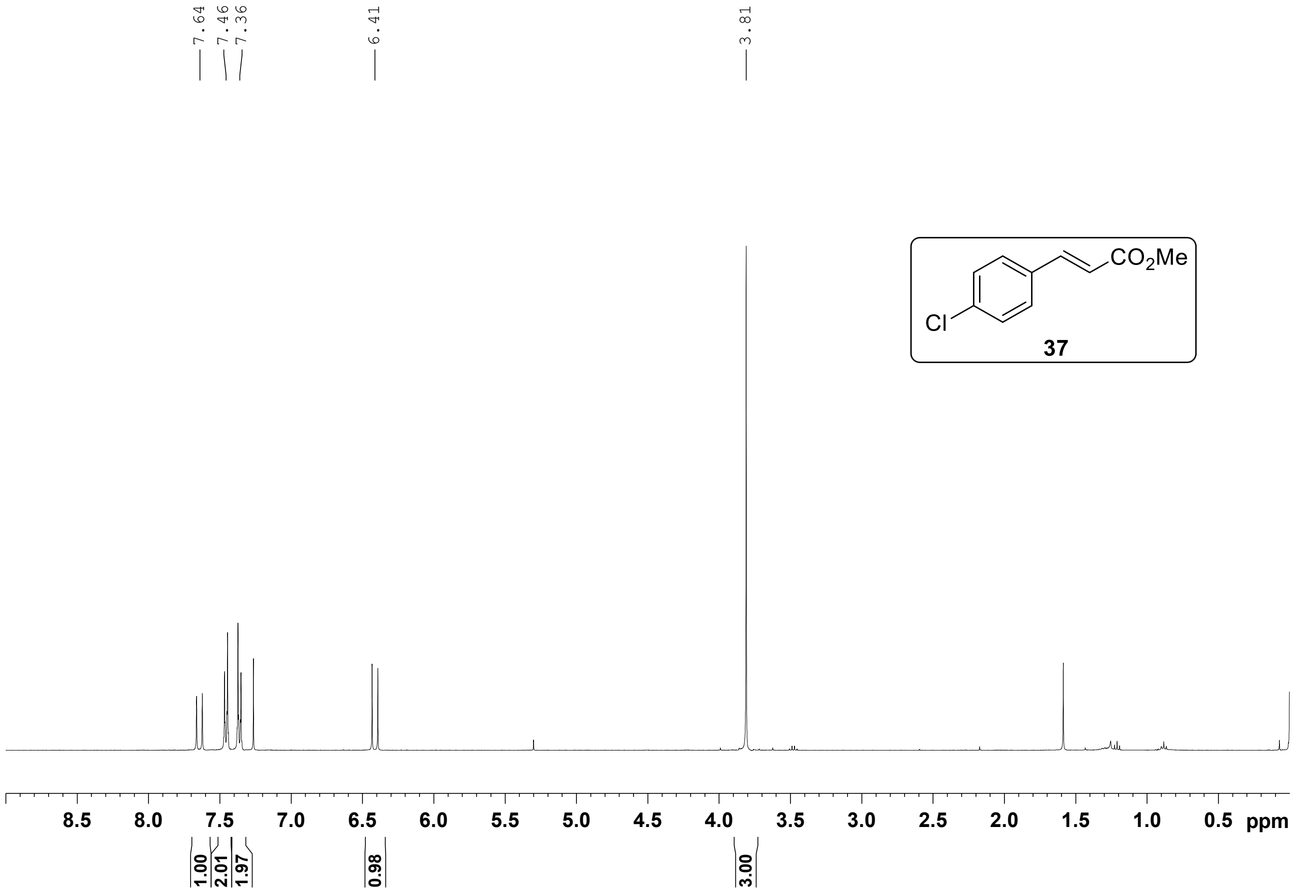

5.80
3.22
NC CN
19
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
4.03

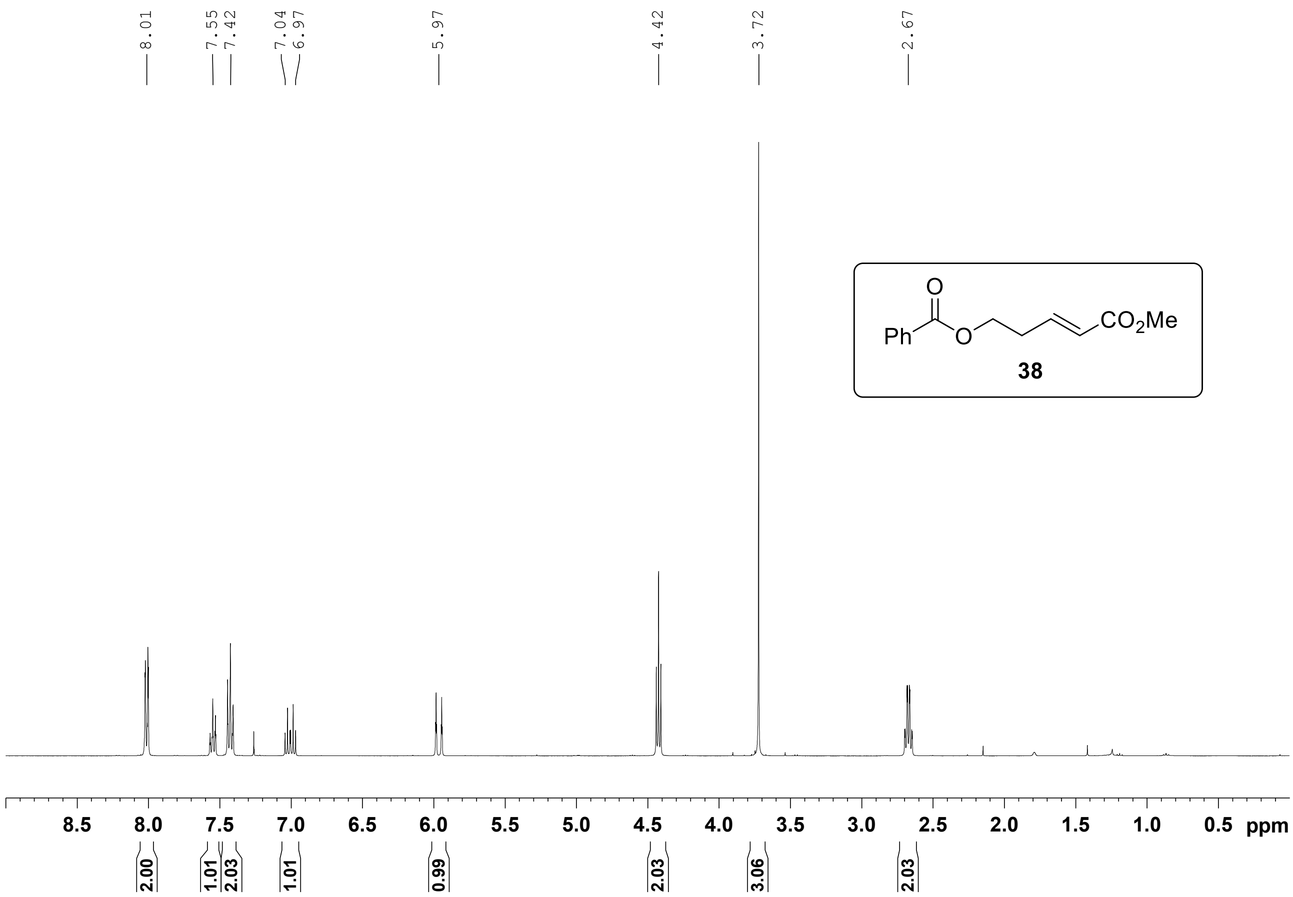

7.67
7.32
5.75
5.61
3.57
3.17
2.43
2.21
Ts
N
21
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.01
1.01
1.00
2.03
2.04
3.03
2.03

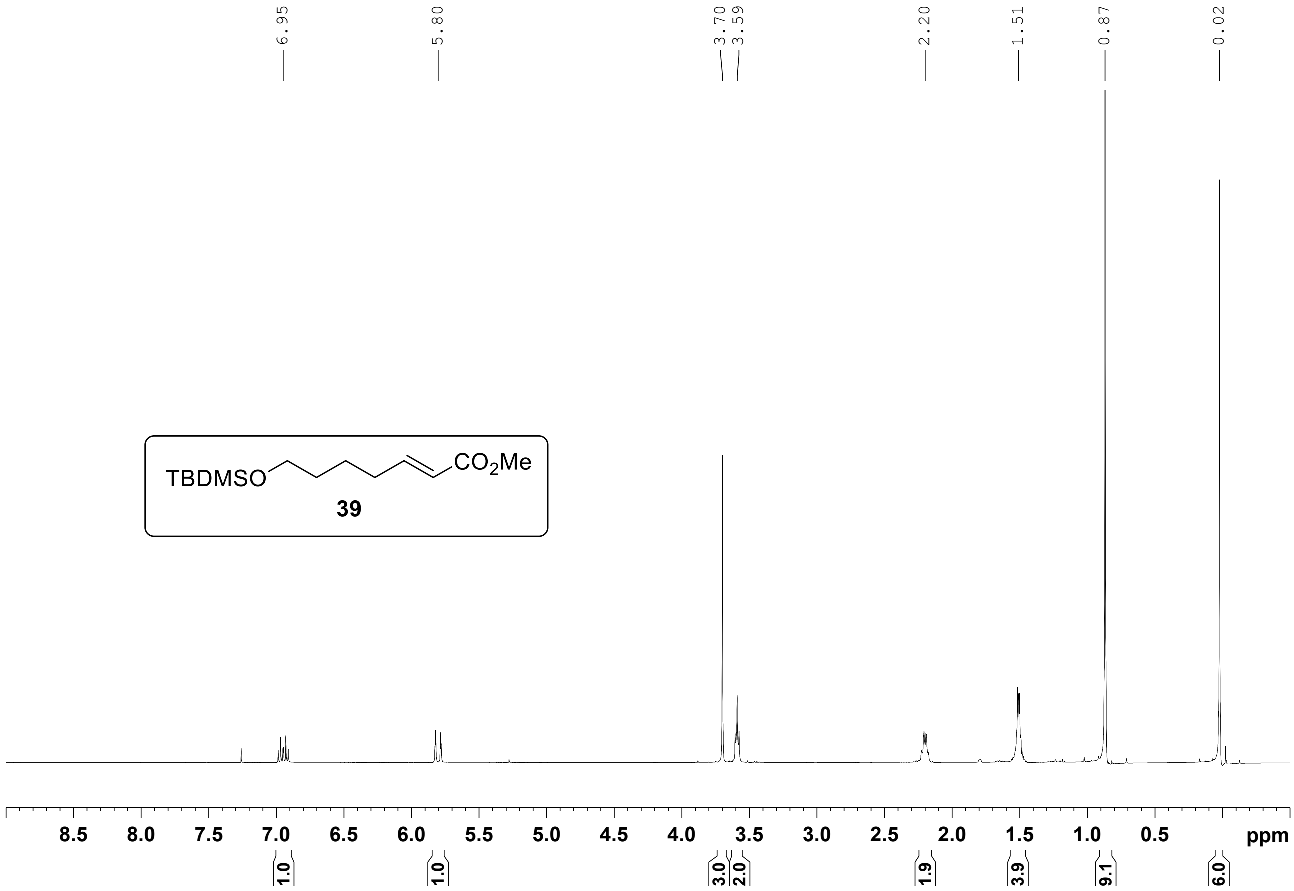

5.67
4.18
2.55
2.11
1.24
EtO2C CO2Et
23
2.00
3.97
1.96
3.90
6.37
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


7.59
7.24
3.29
3.03
2.34
2.03
1.49
Ts
N
25
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.06
2.08
1.98
1.96
3.09
2.00
5.90

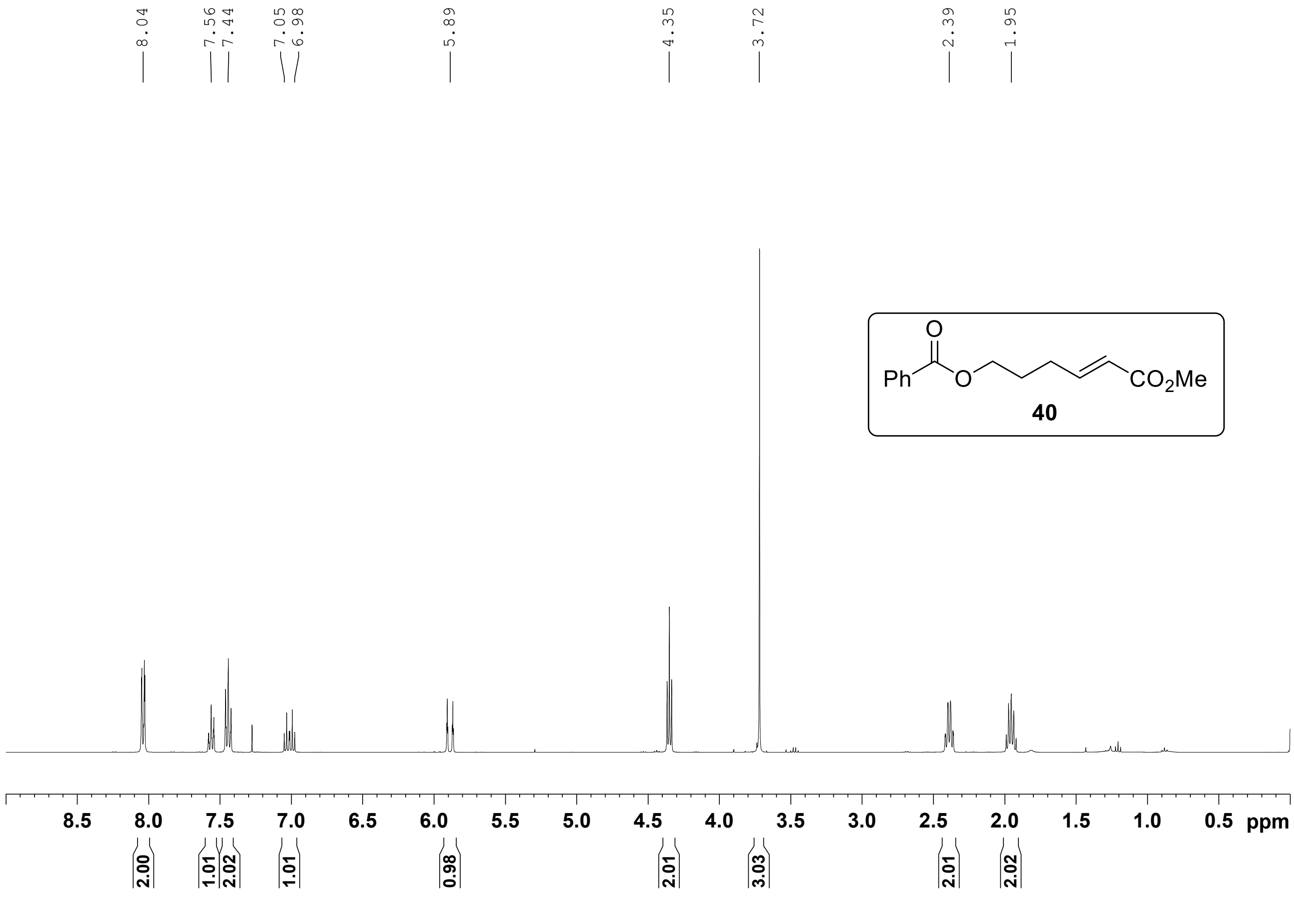

7.37
7.27
6.33
6.28
5.14
5.02
4.68
1.91
Ph
Ph
O
29
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
13.34
1.00
1.00
1.00
1.99
3.01


7.64
7.46
7.36
6.41
3.81
CO2Me
Cl
37
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.01
1.97
0.98
3.00


8.01
7.55
7.42
7.04
6.97
5.97
4.42
3.72
2.67
O
Ph
O
CO2Me
38
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
1.01
2.03
1.01
0.99
2.03
3.06
2.03



6.95
5.80
3.70
3.59
2.20
1.51
0.87
0.02
TBDMSO
CO2Me
39
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.0
1.0
3.0
2.0
1.9
3.9
9.1
6.0



8.04
7.56
7.44
7.05
6.98
5.89
4.35
3.72
2.39
1.95
O
Ph
O
CO2Me
40
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
1.01
2.02
1.01
0.98
2.01
3.03
2.01
2.02

11. Calculation of % V_{Bur} and 3D mapping

11.1. Calculated %V_{Bur} in [$RuCl_2$(Ind)P($(OC_6H_4)_3$)(SIMes)] 3a

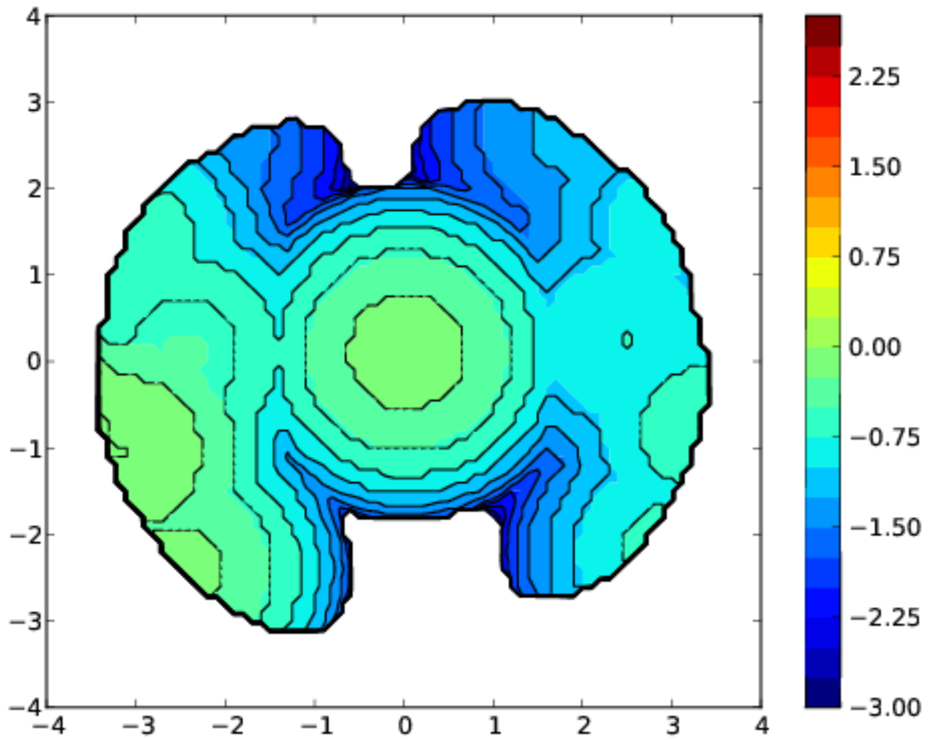
11.1.1. %V_{Bur} and 3D mapping of SIMes in **3a**

V Free	V Buried	V Total	V Exact
125.0	54.5	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
69.650	**30.4**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	28.80	16.07	44.87	64.19	**35.81**
-+	31.61	13.24	44.86	70.48	**29.52**
++	31.43	13.42	44.85	70.08	**29.92**
+-	33.14	11.72	44.86	73.88	**26.12**

Steric Map



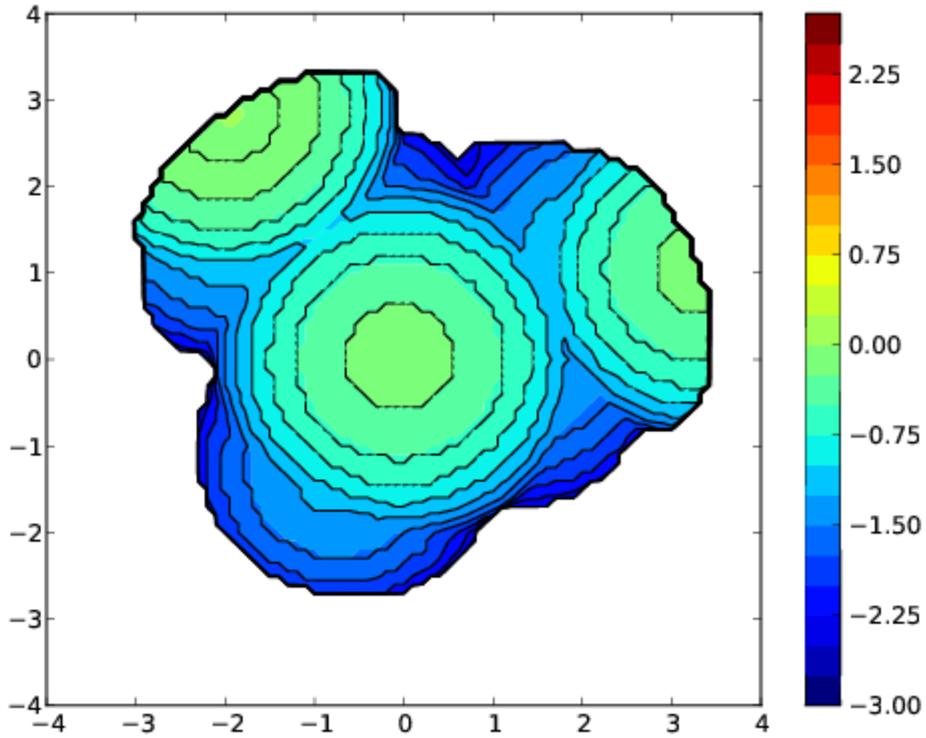
11.1.2. $\%V_{Bur}$ and 3D mapping of $P(OC_6H_4)_3$ in **3a**

V Free	V Buried	V Total	V Exact
133.9	45.6	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
74.612	**25.4**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	34.16	10.71	44.87	76.14	**23.86**
-+	29.99	14.87	44.86	66.85	**33.15**
++	34.32	10.53	44.85	76.53	**23.47**
+-	35.42	9.43	44.86	78.97	**21.03**

Steric Map



11.2. Calculated %V_{Bur} in [$RuCl_2$(Ind)P(O-*p*-$CH_3C_6H_4$)$_3$(SIMes)] 3b

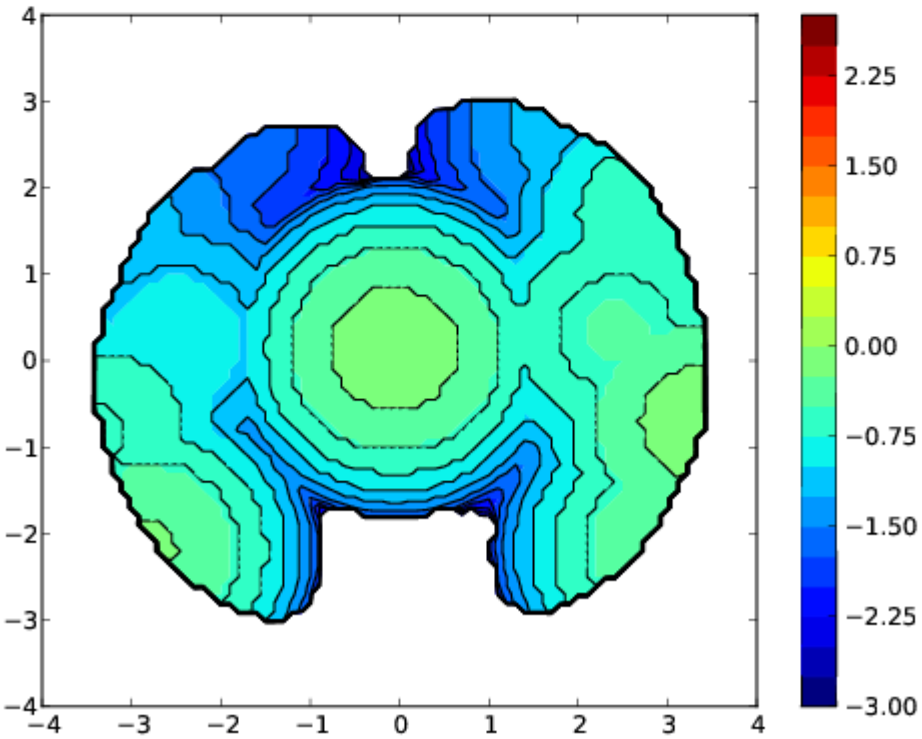
11.2.1. %V_{Bur} and 3D mapping of SIMes in **3b**

V Free	V Buried	V Total	V Exact
125.0	54.5	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
69.651	**30.3**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	30.98	13.89	44.87	69.04	**30.96**
-+	32.79	12.07	44.86	73.10	**26.90**
++	29.97	14.87	44.85	66.84	**33.16**
+-	31.24	13.61	44.86	69.65	**30.35**

Steric Map



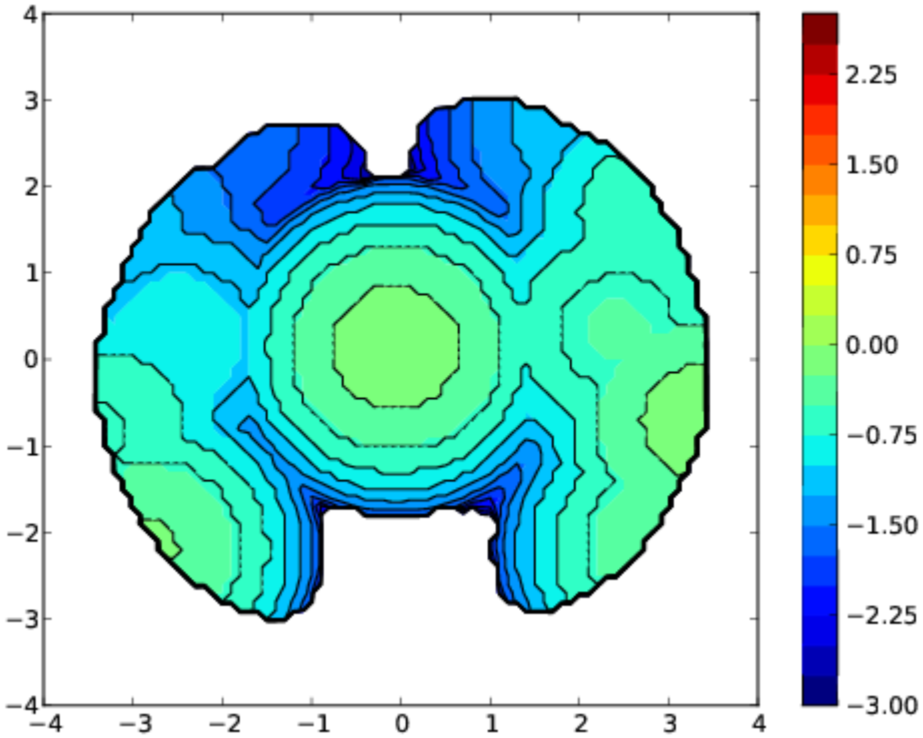
11.2.2. %V_{Bur} and 3D mapping of $P(O\text{-}p\text{-}CH_3C_6H_4)_3$ in **3b**.

V Free	V Buried	V Total	V Exact
130.0	49.5	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
72.408	**27.6**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	34.67	10.21	44.87	77.26	**22.74**
-+	29.05	15.81	44.86	64.75	**35.25**
++	31.05	13.80	44.85	69.23	**30.77**
+-	35.18	9.68	44.86	78.42	**21.58**

Steric Map



11.3. Calculated %V_{Bur} in [$RuCl_2$(Ind)P(O-*p*-$CF_3C_6H_4$)$_3$(SIMes)] 3c

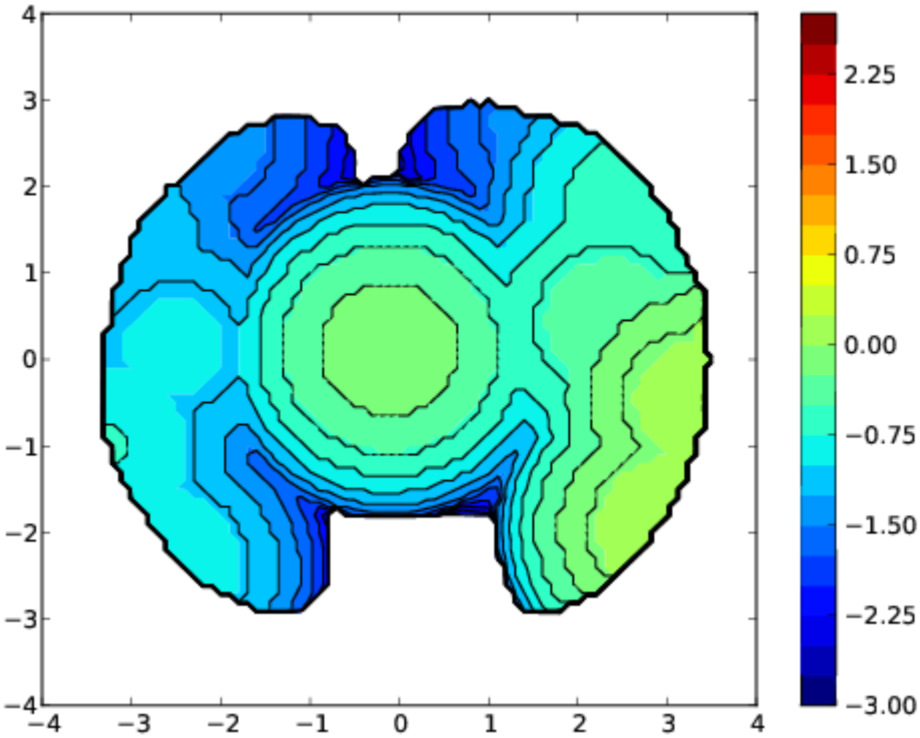
11.3.1. %V_{Bur} and 3D mapping of SIMes in **3c**

V Free	V Buried	V Total	V Exact
123.8	55.7	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
68.969	**31.0**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	32.41	12.46	44.87	72.24	**27.76**
-+	32.63	12.22	44.86	72.75	**27.25**
++	29.30	15.55	44.85	65.34	**34.66**
+-	29.42	15.44	44.86	65.58	**34.42**

Steric Map



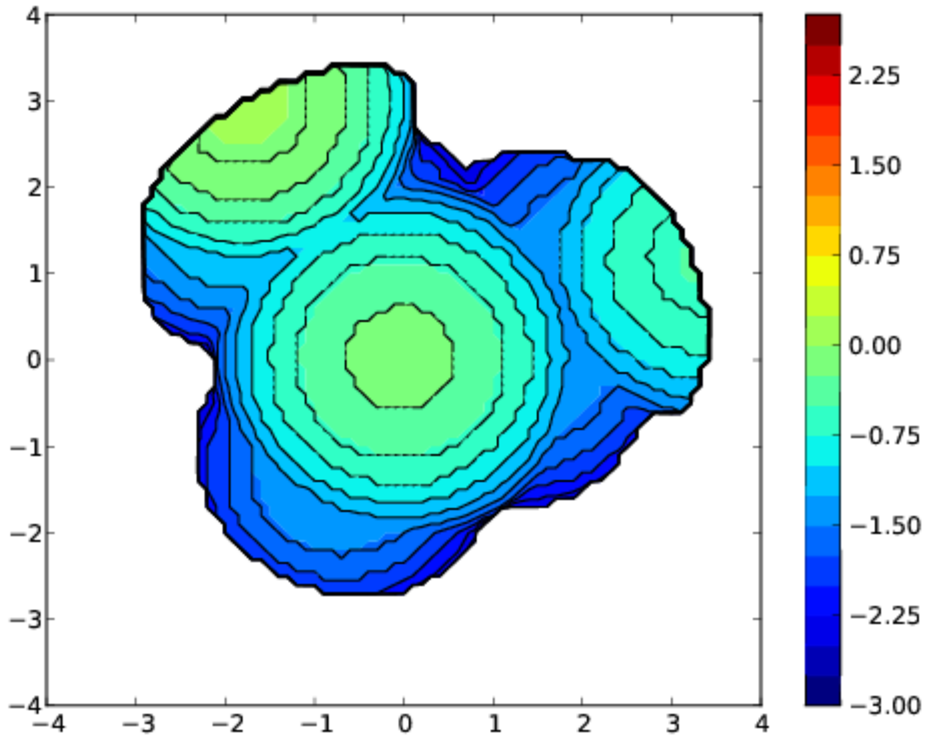
11.3.2. %V_{Bur} and 3D mapping of $P(O\text{-}p\text{-}CF_3C_6H_4)_3$ in **3c**

V Free	V Buried	V Total	V Exact
131.2	48.3	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
73.069	**26.9**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	34.82	10.05	44.87	77.60	**22.40**
-+	28.65	16.20	44.86	63.88	**36.12**
++	32.17	12.68	44.85	71.74	**28.26**
+-	35.48	9.38	44.86	79.09	**20.91**

Steric Map



11.4. Calculated %V_{Bur} in [$RuCl_2$(Ind)P(O-*p*-ClC_6H_4)$_3$(SIMes)] 3d

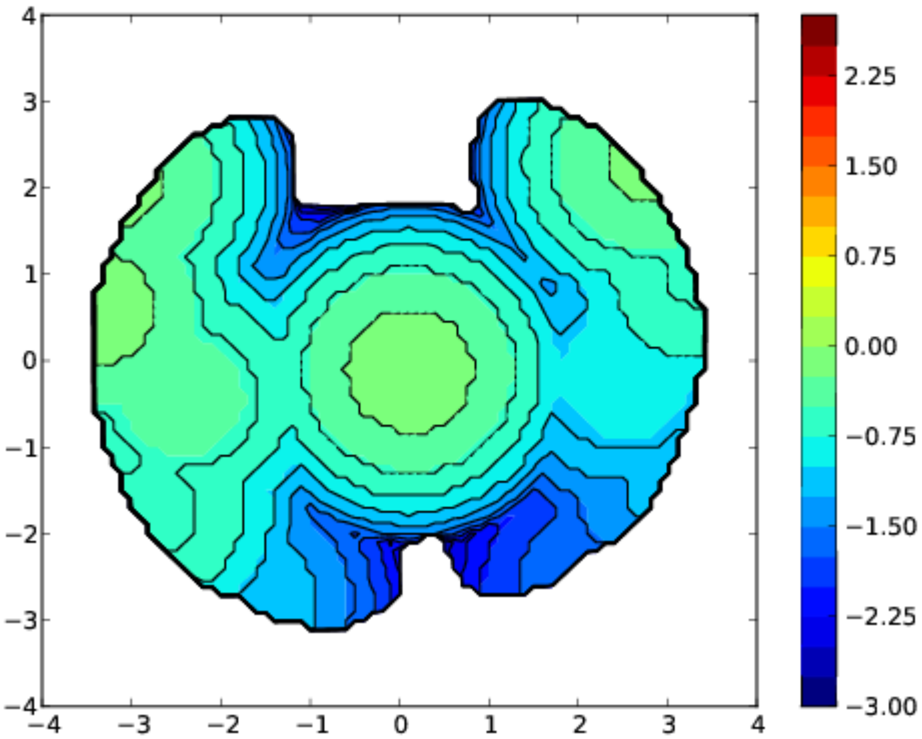
11.4.1. %V_{Bur} and 3D mapping of SIMes in **3d**

V Free	V Buried	V Total	V Exact
124.2	55.4	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
69.166	**30.8**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	29.30	15.57	44.87	65.29	**34.71**
-+	31.35	13.51	44.86	69.89	**30.11**
++	30.55	14.30	44.85	68.12	**31.88**
+-	32.92	11.94	44.86	73.39	**26.61**

Steric Map



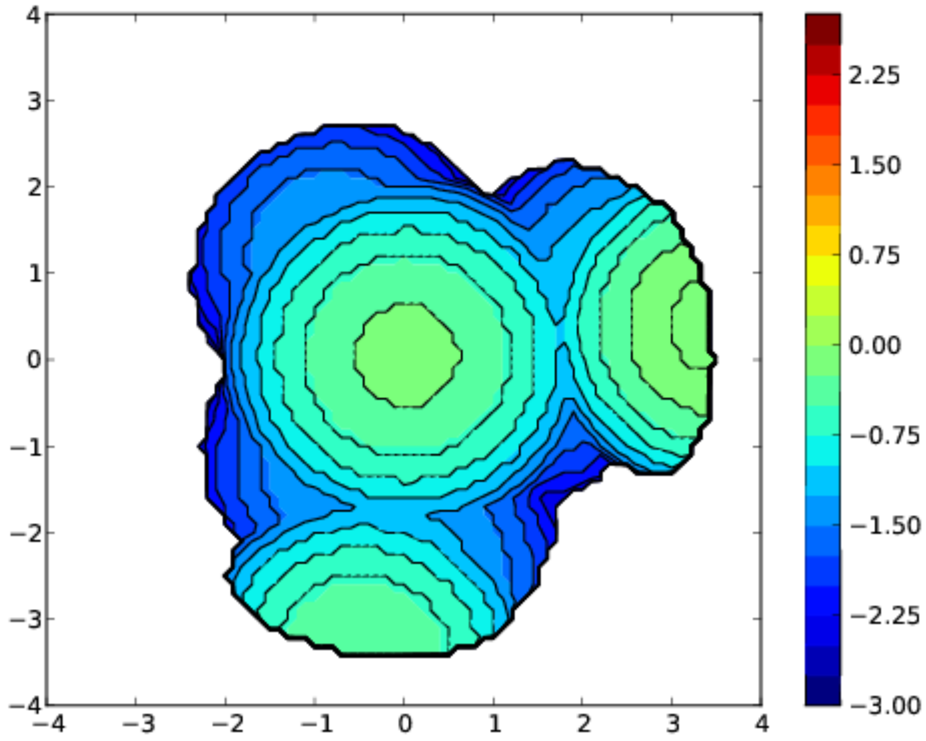
11.4.2. %V_{Bur} and 3D mapping of P(O-*p*-ClC_6H_4)$_3$ of **3d**

V Free	V Buried	V Total	V Exact
131.0	48.5	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
72.984	**27.0**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	32.92	11.95	44.87	73.37	**26.63**
-+	34.79	10.07	44.86	77.56	**22.44**
++	31.47	13.38	44.85	70.17	**29.83**
+-	31.79	13.07	44.86	70.88	**29.12**

Steric Map



11.5. Calculated %V_{Bur} in [$RuCl_2$(Ind)P(O-*p*-$SF_5C_6H_4$)$_3$(SIMes)] 3e

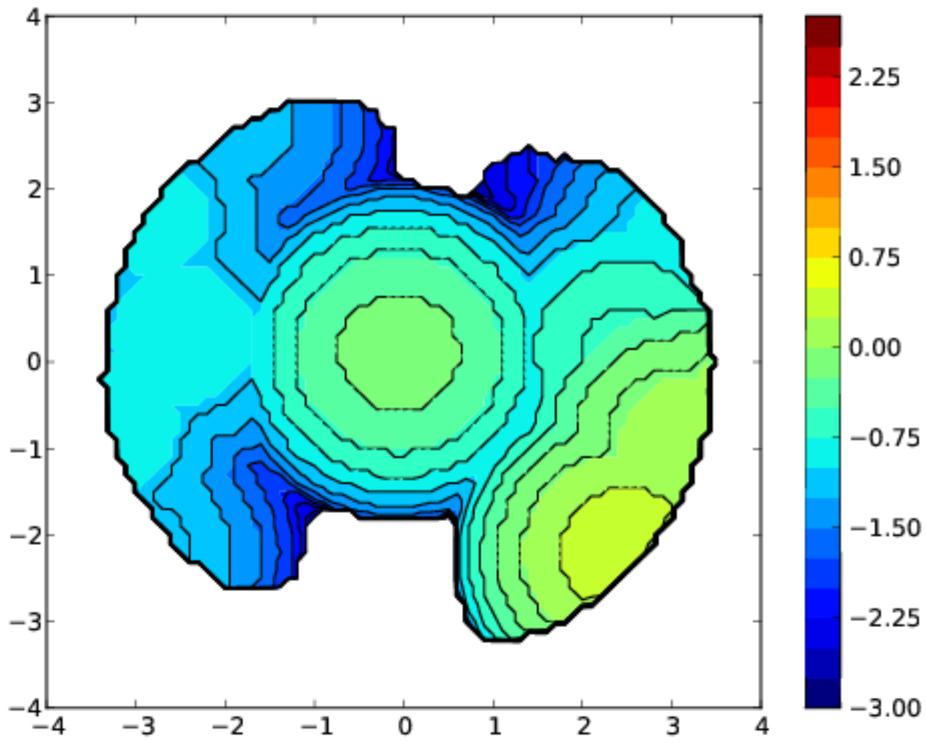
11.5.1. %V_{Bur} and 3D mapping of SIMes in **3e**

V Free	V Buried	V Total	V Exact
123.5	56.0	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
68.808	**31.2**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	33.70	11.17	44.87	75.11	**24.89**
-+	31.50	13.36	44.86	70.22	**29.78**
++	32.01	12.84	44.85	71.37	**28.63**
+-	26.27	18.59	44.86	58.56	**41.44**

Steric Map



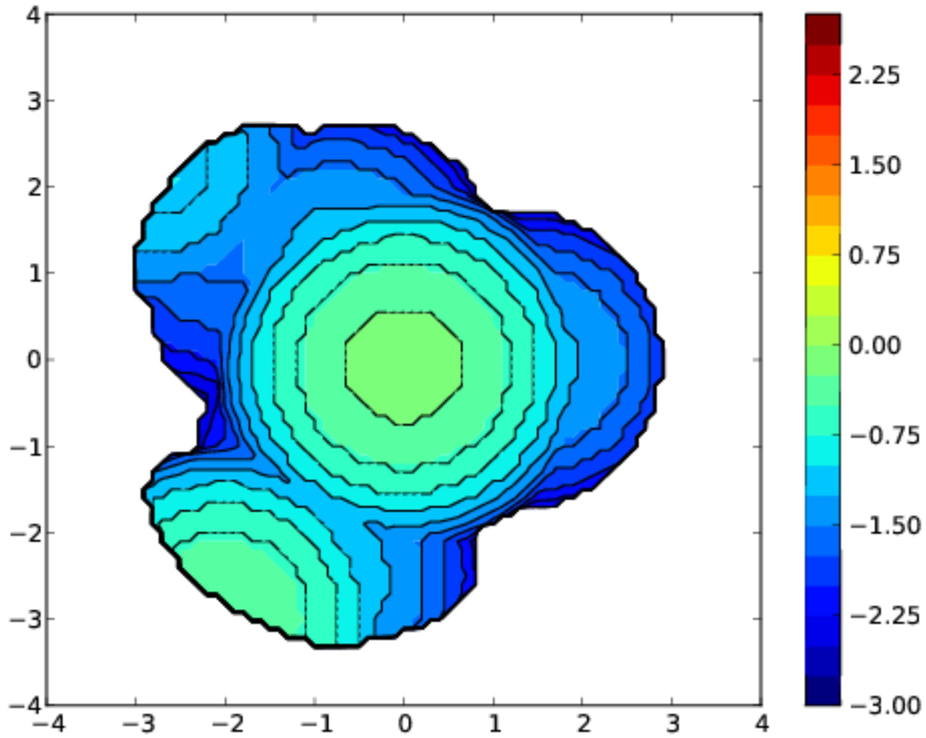
11.5.2. %V_{Bur} and 3D mapping of $P(O\text{-}p\text{-}SF_5C_6H_4)_3$ in **3e**

V Free	V Buried	V Total	V Exact
134.9	44.6	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
75.155	**24.8**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	31.21	13.66	44.87	69.55	**30.45**
-+	33.34	11.51	44.86	74.33	**25.67**
++	35.51	9.34	44.85	79.18	**20.82**
+-	34.81	10.05	44.86	77.59	**22.41**

Steric Map



11.6. Calculated %V_{Bur} in [RuCl$_2$(Ind)P(O-*p*-CNC$_6$H$_4$)$_3$(SIMes)] 3f

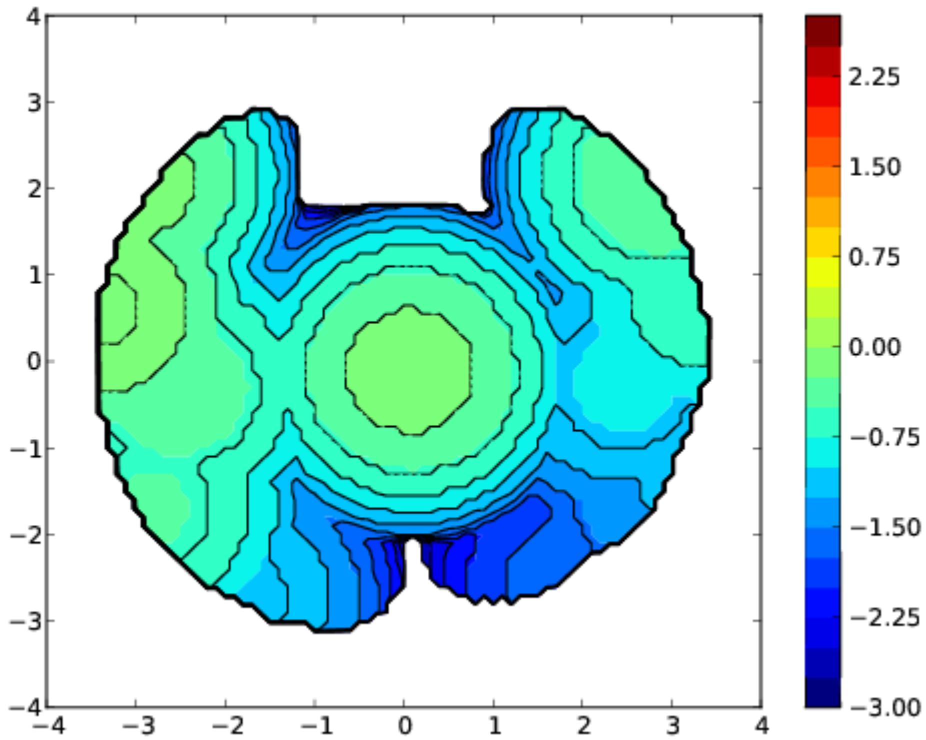
11.6.1. %V_{Bur} and 3D mapping of SIMes in **3f**

V Free	V Buried	V Total	V Exact
123.8	55.7	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
68.949	**31.1**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	29.08	15.79	44.87	64.80	**35.20**
-+	30.74	14.12	44.86	68.53	**31.47**
++	31.04	13.81	44.85	69.21	**30.79**
+-	32.87	11.98	44.86	73.29	**26.71**

Steric Map



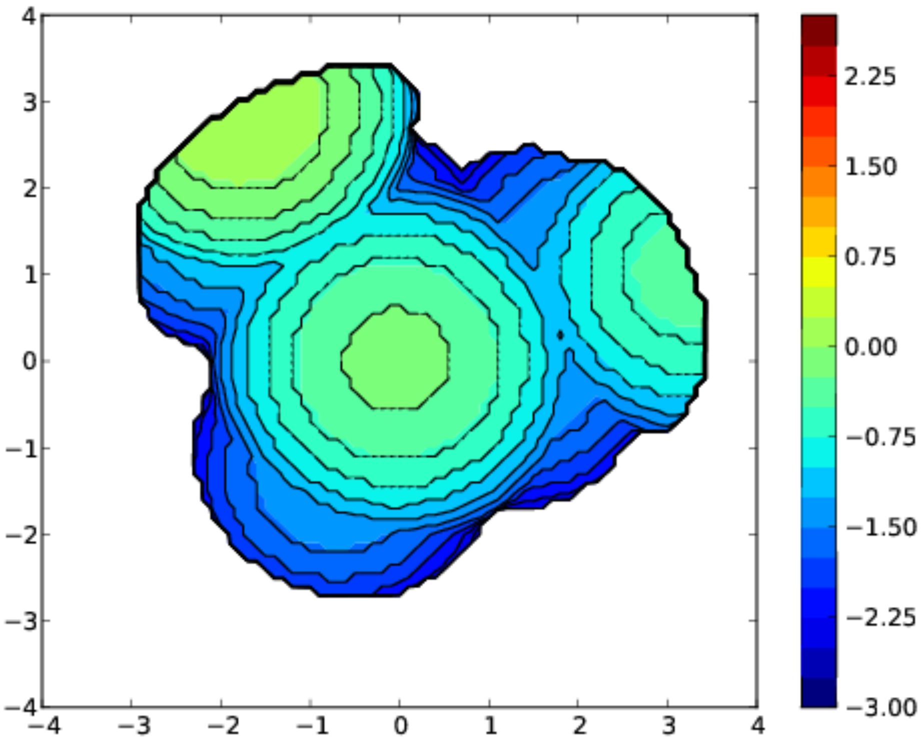
11.6.2. %V_{Bur} and 3D mapping of $P(O\text{-}p\text{-}CNC_6H_4)_3$ in **3f**

V Free	V Buried	V Total	V Exact
129.7	49.8	179.5	179.6

%V_Free	**%V_Bur**	% Tot/Ex
72.265	**27.7**	100.0

xy	V_f	V_b	V_t	%V_f	**%V_b**
--	34.92	9.95	44.87	77.83	**22.17**
-+	27.86	17.00	44.86	62.10	**37.90**
++	31.64	13.20	44.85	70.56	**29.44**
+-	35.26	9.60	44.86	78.61	**21.39**

Steric Map



12. Additional computational data

12.1. Table S1. Selected crystallographic and DFT P-O bond distances (Å) for complexes 3a-f together with mean and standard deviation values.

		P-O1	P-O2	P-O3	Mean P-O	Mean STD P-O
3a	Cis	1.663	1.685	1.665	1.671	0.012
	Trans	1.656	1.653	1.669	1.660	0.008
	Free phosphite	1.660	1.705	1.691	1.686	0.023
	Cis (X-Ray)	1.593(3)	1.610(3)	1.615(3)	1.606	0.009
3b	Cis	1.663	1.687	1.664	1.672	0.014
	Trans	1.671	1.666	1.656	1.664	0.008
	Free phosphite	1.706	1.661	1.692	1.686	0.023
	Cis (X-Ray)	1.603(3)	1.607(3)	1.608(3)	1.606	0.002
3c	Cis	1.672	1.668	1.691	1.677	0.012
	Trans	1.683	1.662	1.669	1.671	0.010
	Free phosphite	1.659	1.692	1.706	1.686	0.024
	Cis (X-Ray)	1.602(3)	1.606(3)	1.616(3)	1.608	0.006
3d	Cis	1.689	1.670	1.667	1.675	0.012
	Trans	1.679	1.668	1.662	1.670	0.009
	Free phosphite	1.660	1.707	1.692	1.686	0.024
	Cis (X-Ray)	1.598(10)	1.614(10)	1.628(10)	1.613	0.012
3e	Cis	1.672	1.689	1.677	1.679	0.009
	Trans	1.687	1.670	1.669	1.675	0.010
	Free phosphite	1.660	1.707	1.692	1.686	0.024
	Cis (X-Ray)	1.607(4)	1.611(5)	1.611(4)	1.610	0.02
3f	Cis	1.677	1.673	1.689	1.679	0.008
	Trans	1.689	1.671	1.667	1.675	0.012
	Free phosphite	1.659	1.708	1.692	1.686	0.025
	Cis (X-Ray)	1.594(5)	1.609(5)	1.609(5)	1.604	0.007

12.2. Table S2. xyz coordinate data sets and absolute gas phase energies (in a.u.) for DFT optimized complexes.

cis-3a	*cis*-3b	*cis*-3c
-3778.55733368	-4121.87630339	-4788.94181911
Ru 0.605141 -0.966541 -0.927739	Ru 0.335572 -1.485863 -0.852847	Ru 0.150038 -1.838129 -0.767109
Cl 1.489616 -0.083860 -2.964640	Cl 1.297761 -0.775856 -2.920029	Cl 1.270142 -1.130985 -2.760841
Cl 0.734194 -3.112136 -2.049455	Cl 0.181708 -3.665739 -1.911768	Cl -0.105131 -3.950033 -1.917761
C 0.739493 -2.186210 0.736798	C 0.325346 -2.665834 0.842872	C 0.031981 -3.086460 0.876437
N 1.954352 -2.667362 1.157782	N 1.474189 -3.298248 1.251097	N 1.143125 -3.780416 1.280942
C 1.830092 -3.781479 2.123270	C 1.205469 -4.494591 2.077262	C 0.810641 -4.981166 2.078679
H 2.418542 -4.656666 1.778845	H 1.451755 -5.412485 1.500758	H 1.086631 -5.896940 1.513942
H 2.230268 -3.474050 3.114094	H 1.836196 -4.485007 2.990557	H 1.383534 -4.982865 3.029994
C 0.319638 -4.047393 2.144185	C -0.295229 -4.373336 2.373070	C -0.706601 -4.848882 2.282359
H -0.110633 -4.067209 3.166870	H -0.513964 -4.129762 3.436529	H -0.994893 -4.689035 3.344234
H 0.047272 -5.000909 1.641932	H -0.860737 -5.291944 2.115645	H -1.269061 -5.730014 1.910762
N -0.231240 -2.909379 1.371698	N -0.720139 -3.256699 1.496127	N -1.054903 -3.656682 1.472755
C 3.271299 -2.091906 0.988120	C 2.851748 -2.894240 1.086282	C 2.538835 -3.427381 1.147074
C 4.179613 -2.630848 0.034052	C 3.700865 -3.537741 0.146495	C 3.372622 -4.074742 0.196079
C 5.479647 -2.084526 -0.025513	C 5.057462 -3.145591 0.102470	C 4.745779 -3.741400 0.183030
H 6.180917 -2.493443 -0.772288	H 5.713846 -3.627667 -0.641654	H 5.391211 -4.229007 -0.566928
C 5.916220 -1.066226 0.842420	C 5.600892 -2.192508 0.982054	C 5.318952 -2.846464 1.104042
C 5.018863 -0.619390 1.830504	C 4.749280 -1.642472 1.961133	C 4.477019 -2.290407 2.088826
H 5.349365 0.142035 2.556825	H 5.159516 -0.930217 2.696775	H 4.907937 -1.624463 2.855341
C 3.711048 -1.127845 1.938905	C 3.388454 -1.985277 2.043210	C 3.101219 -2.574591 2.140756
C 3.826621 -3.785504 -0.868779	C 3.239678 -4.677689 -0.728563	C 2.876618 -5.165083 -0.721807
H 3.072375 -3.498016 -1.630984	H 2.168652 -4.599408 -0.998577	H 1.817098 -5.027865 -1.011648
H 4.729997 -4.166326 -1.383973	H 3.824750 -4.714090 -1.669037	H 3.480661 -5.204017 -1.649938
H 3.375236 -4.627829 -0.303633	H 3.403231 -5.649265 -0.209473	H 2.981301 -6.157690 -0.228092
C 7.298224 -0.468384 0.715595	C 7.046346 -1.763611 0.878623	C 6.785954 -2.488293 1.043684
H 7.276169 0.426966 0.055655	H 7.136237 -0.838596 0.267151	H 6.934438 -1.528728 0.501079
H 7.695360 -0.139418 1.697546	H 7.479829 -1.539001 1.874832	H 7.217147 -2.356456 2.057260
H 8.017578 -1.186352 0.272242	H 7.672103 -2.540280 0.394404	H 7.376621 -3.261644 0.512975
C 2.846732 -0.705812 3.104303	C 2.538185 -1.444562 3.167715	C 2.260943 -2.033561 3.273064
H 3.201211 0.249857 3.536355	H 3.118311 -0.745178 3.800366	H 2.864467 -1.385024 3.937254
H 1.786188 -0.576753 2.822696	H 1.648001 -0.905871 2.791305	H 1.400320 -1.442653 2.906367
H 2.890849 -1.460487 3.921731	H 2.171898 -2.261693 3.827538	H 1.849310 -2.854131 3.900624
C -1.654548 -2.704818 1.467089	C -2.104635 -2.869638 1.602590	C -2.415971 -3.193871 1.581332
C -2.131469 -1.898380 2.539847	C -2.467154 -1.965261 2.640269	C -2.735836 -2.334528 2.671012
C -3.518338 -1.808210 2.746792	C -3.831901 -1.706065 2.856364	C -4.082937 -1.998629 2.886754
H -3.890609 -1.199293 3.588072	H -4.117258 -1.020239 3.671932	H -4.336643 -1.351076 3.743160
C -4.443235 -2.475417 1.915033	C -4.840719 -2.295411 2.065821	C -5.114935 -2.467404 2.045615
C -3.935399 -3.280641 0.881651	C -4.446154 -3.198080 1.063296	C -4.763078 -3.325778 0.990044
H -4.637767 -3.828783 0.231703	H -5.217287 -3.686491 0.444565	H -5.554368 -3.719030 0.330360
C -2.550857 -3.441325 0.653585	C -3.093658 -3.529248 0.830190	C -3.431506 -3.732525 0.752985

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H	2.995502	2.494169	2.209262	H	3.100384	1.697302	2.264153	H	2.938373	1.147152	2.557803
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C	-0.336718	2.936975	2.914031
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C	-1.405462	-0.928702	-0.834093	C	-1.945981	-1.556724	-0.668177	C	-1.320931	-0.906628	-0.846906
C	-2.157242	-0.031124	0.037910	C	-2.551238	-0.533157	0.175467	C	-2.125371	-0.039559	0.006546
H	-1.735031	0.441804	0.931332	H	-2.103702	-0.175739	1.109526	H	-1.741466	0.461714	0.902532
C	-3.439560	0.187290	-0.441292	C	-3.722863	-0.045199	-0.382735	C	-3.409842	0.115671	-0.494691
C	-3.596905	-0.620401	-1.679381	C	-3.959317	-0.789845	-1.647346	C	-3.509870	-0.709131	-1.728215
C	-4.694320	-0.813780	-2.526180	C	-5.008695	-0.730803	-2.570099	C	-4.583163	-0.964923	-2.589307
H	-5.668451	-0.350460	-2.309316	H	-5.863582	-0.055657	-2.416524	H	-5.583141	-0.550622	-2.392915
C	-4.543255	-1.628505	-3.675003	C	-4.964040	-1.562786	-3.715894	C	-4.373949	-1.781775	-3.727949
H	-5.402164	-1.780174	-4.348226	H	-5.783575	-1.517044	-4.450578	H	-5.213588	-1.980034	-4.413012
C	-3.310325	-2.228304	-3.963368	C	-3.883280	-2.429462	-3.923093	C	-3.109518	-2.323962	-3.991404
H	-3.195524	-2.843809	-4.869535	H	-3.849458	-3.061393	-4.824489	H	-2.950814	-2.940915	-4.889792
C	-2.203404	-2.057405	-3.096745	C	-2.827464	-2.508382	-2.981918	C	-2.026267	-2.091837	-3.108961
H	-1.237163	-2.533476	-3.316704	H	-1.982784	-3.194311	-3.139950	H	-1.034593	-2.523242	-3.306413
C	-2.354374	-1.284508	-1.939560	C	-2.878050	-1.711806	-1.832050	C	-2.233475	-1.315877	-1.963175
C	-4.425706	1.111099	0.139852	C	-4.543018	1.048057	0.159431	C	-4.445169	0.999904	0.060513
C	-4.453040	1.352132	1.539551	C	-4.659915	1.233108	1.563309	C	-4.498442	1.264092	1.455514
H	-3.766909	0.788157	2.188691	H	-4.180669	0.506124	2.236025	H	-3.797081	0.740064	2.121953
C	-5.360297	2.261566	2.101359	C	-5.408605	2.293702	2.092714	C	-5.451150	2.142002	1.991164
H	-5.370084	2.420667	3.191789	H	-5.498721	2.408464	3.184945	H	-5.481395	2.319429	3.078307
C	-6.260917	2.965171	1.279233	C	-6.050124	3.205806	1.233109	C	-6.371907	2.791035	1.146563
H	-6.973583	3.679968	1.720446	H	-6.637159	4.040355	1.648230	H	-7.119092	3.482514	1.567135
C	-6.237477	2.751927	-0.110258	C	-5.929794	3.048392	-0.158582	C	-6.326503	2.553385	-0.238516
H	-6.918152	3.314884	-0.768313	H	-6.401805	3.771767	-0.841198	H	-7.023692	3.072933	-0.914382
C	-5.336328	1.835592	-0.674084	C	-5.190804	1.981299	-0.692256	C	-5.380578	1.666406	-0.775246
H	-5.297821	1.723824	-1.766720	H	-5.065815	1.906198	-1.781248	H	-5.333402	1.530071	-1.864830
P	1.024721	0.543578	0.050680	P	0.653297	-0.529378	0.314344	P	1.041822	0.665607	0.054251
O	0.610247	0.829499	1.662750	O	0.243350	-0.137106	1.905219	O	0.642009	0.941061	1.671443
C	0.830388	2.002803	2.380688	C	0.605542	1.014430	2.587944	C	0.755601	2.123080	2.384911
C	2.128485	2.429812	2.722869	C	1.932436	1.232704	3.007548	C	1.991693	2.775343	2.576169
H	2.997569	1.862376	2.364732	H	2.711576	0.505935	2.741649	H	2.895926	2.371568	2.103332
C	2.299207	3.576438	3.515380	C	2.244719	2.374389	3.761938	C	2.050420	3.930241	3.366294
H	3.308459	3.919529	3.786761	H	3.277602	2.549121	4.091536	H	3.012693	4.441870	3.517974

C	1.174054	4.286803	3.970318	C	1.224678	3.278990	4.092731	C	0.882184	4.445152	3.980747
C	-0.124327	3.859449	3.638923	C	-0.101955	3.068837	3.686800	C	-0.353111	3.778330	3.785189
H	-0.996744	4.420993	4.003989	H	-0.891451	3.783772	3.954002	H	-1.264704	4.171469	4.259423
C	-0.292853	2.716633	2.841307	C	-0.409052	1.930754	2.927175	C	-0.413958	2.628136	2.990521
H	-1.302415	2.369792	2.575064	H	-1.441884	1.748288	2.595483	H	-1.369719	2.108037	2.831419
O	2.657331	0.847099	0.196239	O	2.312654	-0.495041	0.518209	O	2.665167	1.050903	0.170917
C	3.522551	1.372228	-0.763540	C	3.277570	-0.128280	-0.412135	C	3.501970	1.542818	-0.824757
C	4.404331	0.505831	-1.431571	C	4.007380	-1.133639	-1.069501	C	4.429812	0.670039	-1.421271
H	4.341187	-0.575610	-1.246322	H	3.753372	-2.188153	-0.893713	H	4.417606	-0.395022	-1.151336
C	5.351068	1.031184	-2.324053	C	5.045430	-0.778040	-1.941859	C	5.349969	1.172095	-2.347835
H	6.043535	0.365424	-2.859530	H	5.615627	-1.556680	-2.465277	H	6.075840	0.497241	-2.825128
C	5.403416	2.419967	-2.542045	C	5.332711	0.581105	-2.143999	C	5.346734	2.549086	-2.685957
C	4.519828	3.287683	-1.876453	C	3.572644	1.231327	-0.619141	C	4.402141	3.413300	-2.079345
H	4.573729	4.370975	-2.058519	H	2.989072	2.001032	-0.095856	H	4.397016	4.482197	-2.339790
C	3.575161	2.760492	-0.981196	O	0.550322	0.997800	-0.370512	C	3.481920	2.912540	-1.149997
H	2.876191	3.420868	-0.449576	C	-0.368764	1.634709	-1.186033	H	2.745036	3.573295	-0.673575
O	0.645080	2.017121	-0.636286	C	-0.866678	2.873822	-0.735866	O	0.588131	2.139719	-0.604930
C	-0.489069	2.454571	-1.313015	H	-0.568141	3.249176	0.253952	C	-0.551867	2.541132	-1.282314
C	-1.260359	3.466215	-0.710635	C	-1.721075	3.624313	-1.555065	C	-1.347282	3.535611	-0.677869
H	-0.981369	3.835284	0.287431	H	-2.106853	4.592539	-1.210399	H	-1.074564	3.910734	0.319566
C	-2.366996	3.998045	-1.389404	C	-2.072715	3.113862	-2.814594	C	-2.465587	4.033474	-1.353913
H	-2.980546	4.786621	-0.930516	C	-1.580537	1.882440	-3.272627	H	-3.094746	4.806595	-0.888932
C	-2.692978	3.504777	-2.665061	H	-1.853094	1.496068	-4.263655	C	-2.799231	3.534746	-2.638481
C	-1.914747	2.505879	-3.274491	C	-0.714085	1.140563	-2.455955	C	-1.978612	2.546363	-3.237445
H	-2.177711	2.136709	-4.276488	H	-0.286668	0.188090	-2.805929	H	-2.228922	2.163299	-4.237891
C	-0.800023	1.983443	-2.599943	C	4.609024	1.591695	-1.493918	C	-0.851792	2.054702	-2.567717
H	-0.166563	1.208147	-3.058643	H	4.845535	2.650928	-1.660627	H	-0.198923	1.293919	-3.023452
Cl	-4.101260	4.141872	-3.504741	S	6.688978	1.045079	-3.288438	C	0.948433	5.625548	4.796696
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				F	5.773735	2.207412	-4.003813	N	7.083345	3.487489	-4.396623
				F	6.194015	-0.041420	-4.417326	N	1.000930	6.590308	5.465642
				F	7.280238	2.162726	-2.234501	N	-4.947674	4.390290	-3.852456
				F	7.699441	-0.085573	-2.646557				
				F	7.902323	1.458091	-4.307869				
				F	2.574779	3.904442	6.112180				
				F	2.945388	5.101135	4.155261				
				F	0.708657	5.731940	4.116520				
				F	0.337459	4.533308	6.072361				
				F	1.987248	6.099270	5.964546				
				F	-4.174584	4.489623	-2.629293				
				F	-4.140119	2.770285	-4.202573				
				F	-4.195922	4.952387	-4.855182				

	F -2.330535 5.467037 -3.653815	
	F -2.300182 3.757114 -5.232893	

***trans*-3a**	***trans*-3b**	***trans*-3c**
-3778.55082506	**-4121.86825329**	**-4788.93387769**
Ru -0.297565 -0.660750 -0.146978	Ru -0.300121 1.204422 0.133792	Ru 0.788778 -1.469183 0.043458
Cl -0.100201 -0.310282 -2.553939	Cl -0.614269 1.311098 -2.247998	Cl 1.179837 -1.293326 -2.318993
Cl -1.115403 -1.143961 2.075623	Cl 0.233200 1.556471 2.469753	Cl 0.232195 -2.122136 2.301110
C -0.103015 -2.682035 -0.676580	C -1.424826 2.957182 0.433981	C 2.111185 -3.099596 0.156138
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C -0.821831 -4.676003 -1.729656	C -1.567400 5.273374 0.935866	C 2.580269 -5.427496 0.134244
H -1.342227 -5.551115 -1.288693	H -1.030634 5.668914 1.824432	H 2.136433 -6.202102 0.792327
H -1.129606 -4.596846 -2.795012	H -1.681413 6.106302 0.210253	H 2.857426 -5.914526 -0.826754
C 0.704425 -4.723178 -1.559853	C -2.899249 4.597342 1.301936	C 3.753141 -4.682135 0.790624
H 1.241731 -4.884930 -2.516127	H -3.758181 4.970507 0.702279	H 4.729786 -4.881362 0.303433
H 1.039389 -5.509089 -0.846465	H -3.162560 4.711937 2.373632	H 3.860528 -4.915890 1.871875
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C -3.105159 -3.638821 0.522423	C 1.648688 4.635422 0.415424	C -0.755367 -5.072144 0.042515
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H -4.878894 -3.769312 1.754446	H 3.768853 5.045986 0.285397	H -2.833916 -5.670397 0.000484
C -5.323104 -2.785218 -0.132059	C 2.861552 5.092723 -1.687159	C -2.109347 -5.279953 -2.010668
C -4.783518 -2.404242 -1.374847	C 1.639652 5.010073 -2.383452	C -0.967833 -4.955559 -2.768617
H -5.441531 -1.941800 -2.129438	H 1.623624 5.191453 -3.471179	H -1.036573 -4.941089 -3.869346
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H -6.881730 -1.485436 0.625783	H 4.585313 4.402268 -2.810237	H -3.949705 -4.585741 -2.930725
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H -1.955443 -1.766334 -3.089369	H -1.212838 3.652092 -2.658380	H 2.276211 -3.872461 -2.572119
H -2.836260 -3.207429 -3.704203	H -1.669540 5.257745 -2.002473	H 1.913575 -5.472018 -3.317708
C 2.384330 -3.086774 -0.679783	C -3.770811 2.274579 1.079768	C 4.387282 -2.268142 0.894541
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H	1.875864	-1.774289	-3.117536
H	3.581084	-1.883093	-3.697745
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C	6.566827	-2.490026	0.299018
H	7.197945	-2.387702	-0.606363
H	6.683936	-1.558381	0.894611
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C	1.396417	0.098519	0.238151
C	2.143714	0.963958	-0.683303
H	1.744572	1.295555	-1.648064
C	3.392160	1.271606	-0.176151
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H	5.515873	1.112616	1.873425
C	4.365770	-0.032278	3.336104
H	5.182558	-0.039745	4.075809
C	3.146646	-0.656110	3.629834
H	2.998307	-1.141855	4.607410
C	2.100132	-0.678812	2.675947
H	1.141321	-1.168050	2.898148
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C	4.530084	2.022367	-2.277766
H	3.883164	1.330080	-2.838433
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C	6.313486	3.681666	-2.242138
H	7.052959	4.299779	-2.775685
C	6.202570	3.760689	-0.842731
H	6.847445	4.452006	-0.276760
C	5.267033	2.968114	-0.159416
H	5.167904	3.065567	0.931837
P	-1.306821	1.408737	-0.025384
O	-0.722195	2.550559	-1.073165
C	-1.436175	3.607957	-1.637232
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H	-5.556833	0.451247	3.354784
C	-4.102813	1.679588	2.321107
C	-4.254689	2.786363	-1.375328
H	-3.284922	2.399350	-1.758619
H	-5.032755	2.588289	-2.138477
H	-4.142577	3.889495	-1.295554
C	-7.445955	-0.008981	1.406205
H	-8.311711	0.541776	0.981797
H	-7.359919	-0.961347	0.838537
H	-7.684431	-0.266492	2.457312
C	-3.231650	1.857866	3.540949
H	-3.360166	2.871916	3.982562
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H	-2.154074	1.741016	3.300332
C	-1.469989	-0.258671	0.404006
C	-2.627446	-0.545155	-0.444632
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C	-3.176828	-1.779026	-0.130580
C	-2.453848	-2.310239	1.056489
C	-2.688510	-3.428430	1.862954
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H	-2.008819	-4.554723	3.602962
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H	-0.112310	-2.999504	4.110889
C	-0.552911	-1.651434	2.457301
H	0.256972	-0.950423	2.702204
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C	-5.213221	-1.735804	-1.597066
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C	-6.197894	-2.382872	-2.356368
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C	-6.220739	-3.788215	-2.440080
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H	-5.237845	-5.635179	-1.832821
C	-4.256897	-3.890404	-0.996918
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C	4.598758	-1.801917	2.214943
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H	4.023379	-2.115232	-1.951309
H	5.790393	-2.023670	-2.270548
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C	7.741274	0.367442	1.683623
H	8.685045	-0.020006	1.245615
H	7.558541	1.364101	1.225526
H	7.903689	0.522810	2.768609
C	3.715217	-2.233365	3.360291
H	3.976531	-3.259751	3.703701
H	3.843498	-1.561110	4.231233
H	2.641794	-2.242044	3.078923
C	1.807916	0.064148	0.497188
C	2.958199	0.533499	-0.268588
H	3.339107	0.013561	-1.153446
C	3.320723	1.814456	0.127387
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C	2.549459	3.264953	2.185234
H	3.294352	4.064034	2.051728
C	1.645098	3.317672	3.276010
H	1.681099	4.173898	3.968448
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H	0.019301	2.339296	4.333949
C	0.668900	1.175757	2.608409
H	-0.034541	0.350566	2.791110
C	1.552646	1.119735	1.526012
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H	5.569125	1.069134	-1.205324
C	6.281627	2.984328	-1.945866
H	7.149617	2.544297	-2.462673
C	6.067553	4.375308	-1.989290
H	6.762405	5.026393	-2.543154
C	4.954966	4.926167	-1.329773
H	4.757338	6.007823	-1.382333
C	4.072997	4.099321	-0.617984
H	3.184349	4.541706	-0.146099
P	-1.205965	-0.306075	-0.112087
O	-1.978414	-0.794926	-1.509044
C	-3.279799	-0.464871	-1.856232
C	-4.342747	-1.296455	-1.455705

H	-1.865788	4.607844	0.246295
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H	-3.040213	6.529493	-0.869016
C	-2.744373	5.750967	-2.882182
H	-3.256246	6.594826	-3.370842
C	-2.207616	4.705169	-3.656251
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C	-1.554206	3.626626	-3.038210
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H	-5.697394	0.216285	2.981612
C	-6.492456	1.725441	1.625173
H	-7.446663	1.827727	2.165606
C	-6.245281	2.495243	0.474273
H	-7.006094	3.202270	0.106502
C	-5.025274	2.375732	-0.212474
H	-4.808204	2.972355	-1.110739
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H	0.833003	3.456078	0.937869
C	1.562940	3.520003	2.997193
H	2.496617	4.036524	2.724689
C	1.300182	3.195332	4.338705
H	2.029154	3.452590	5.122829
C	0.102209	2.537172	4.674848
H	-0.109248	2.275740	5.723963
C	-0.827073	2.198857	3.679418
H	-1.762269	1.670886	3.913066
H	4.682845	1.555409	-0.611606
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H	6.997757	0.880090	-1.269846
C	6.329566	-0.826823	-2.472310
C	5.202635	-1.552931	-2.923657
H	5.367232	-2.423218	-3.576940
C	3.910819	-1.164923	-2.550276
H	3.031585	-1.720881	-2.908697
O	2.763163	-0.023990	1.075369
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C	3.036364	-0.711092	3.364477
H	2.408301	0.144490	3.656333
C	3.603438	-1.565243	4.316691
H	3.440504	-1.403928	5.393289
C	4.402680	-2.660480	3.913271
C	4.065925	-2.017878	1.580749
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H	0.154132	-1.129937	-2.437393
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H	-1.234310	-2.712381	-3.731188
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H	1.226277	-4.297944	0.336397
O	-1.544688	-5.384543	-3.091694
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H	6.633612	-4.247461	4.026058
H	6.002719	-5.037734	5.523047
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H	8.825150	-0.607229	-1.365183
H	9.570250	-1.125027	-2.927539
H	8.717023	0.463753	-2.820275
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H	-2.751199	-5.915161	-4.636898
H	-3.000266	-4.218995	-4.068374
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C	-5.648398	-0.992530	-1.867241
H	-6.484150	-1.640430	-1.563359
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H	-3.282459	-0.012024	5.396375
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C	-4.584622	1.736699	2.743174
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H	-4.096253	1.382371	0.646946
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C	-0.762222	2.355607	-0.733310
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H	-0.455302	5.753740	-0.423882
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C	2.219806	-0.285990	0.540628
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H	3.798302	-0.045158	-1.052053
C	3.637459	1.576561	0.437332
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C	-0.740192	-2.802221	3.269287
H	-0.089354	-2.999803	4.135379
C	-0.513691	-1.650657	2.475628
H	0.283170	-0.939333	2.735295
C	-1.340243	-1.405974	1.375045
C	-4.163137	-2.456824	-0.900339
C	-5.154138	-1.718225	-1.600716
H	-5.175781	-0.623931	-1.490465
C	-6.110101	-2.366120	-2.393954
H	-6.875417	-1.773545	-2.920409
C	-6.093873	-3.768381	-2.522298
H	-6.839236	-4.276426	-3.154390
C	-5.113510	-4.515979	-1.846482
H	-5.071837	-5.609780	-1.964704
C	-4.165088	-3.871071	-1.038278
H	-3.380976	-4.465558	-0.547879
P	1.637790	-0.222898	-0.055623
O	2.531710	0.262642	-1.380893
C	3.790363	-0.200751	-1.721916
C	4.936464	0.422073	-1.188902

H	4.690606	1.480559	-0.537850
C	6.117512	0.241476	-1.630176
H	7.008158	0.761556	-1.247961
C	6.265216	-0.835995	-2.522835
C	5.140288	-1.515969	-3.023469
H	5.272516	-2.354349	-3.723000
C	3.855001	-1.113558	-2.626214
H	2.961660	-1.625481	-3.013954
O	2.761556	0.072766	1.074039
C	3.240984	-0.774950	2.062579
C	2.977021	-0.453074	3.406362
H	2.335524	0.414926	3.623045
C	3.525151	-1.239342	4.431927
H	3.328835	-0.998344	5.487117
C	4.332168	-2.343719	4.103120
C	4.602440	-2.663442	2.760276
H	5.243403	-3.524635	2.520486
C	4.056724	-1.874138	1.735168
H	4.267027	-2.101475	0.680693
O	1.675890	-1.783842	-0.167873
C	0.879262	-2.659223	-0.884455
C	0.111772	-2.274867	-2.000540
H	0.065202	-1.221229	-2.327756
C	-0.633808	-3.247385	-2.689902
H	-1.248289	-2.957290	-3.554515
C	-0.596483	-4.587448	-2.271251
C	0.176470	-4.972762	-1.160242
H	0.196831	-6.025406	-0.842066
C	0.910375	-4.003747	-0.463371
H	1.516049	-4.273709	0.414011
Cl	-1.531220	-5.800249	-3.135374
Cl	7.872283	-1.335710	-3.019882
Cl	5.014267	-3.332349	5.384160

H	-3.664691	-2.530105	-0.890419
C	-5.197693	-1.349336	-1.894197
H	-6.024919	-2.001698	-1.584376
C	-5.437367	-0.212142	-2.681356
C	-4.394279	0.632373	-3.090963
H	-4.595913	1.515478	-3.711647
C	-3.080986	0.332500	-2.698985
H	-2.243570	0.971832	-3.015090
O	-1.959594	-1.188650	0.881952
C	-2.470169	-0.603398	2.025242
C	-2.220939	-1.225048	3.263075
H	-1.570661	-2.112529	3.285377
C	-2.772829	-0.689709	4.435322
H	-2.574341	-1.165970	5.404759
C	-3.567564	0.464428	4.349419
C	-3.293591	0.536353	1.946191
H	-3.500225	0.995289	0.970018
O	-1.066299	0.933837	-0.034506
C	-0.426684	1.998813	-0.628805
C	0.367269	1.878507	-1.786157
H	0.584298	0.891266	-2.232072
C	0.921692	3.032992	-2.362266
H	1.545287	2.941638	-3.261534
C	0.674488	4.284076	-1.779355
C	-0.106010	4.411225	-0.618316
H	-0.287918	5.394957	-0.166079
C	-0.654448	3.260413	-0.040641
H	-1.265932	3.325704	0.870757
C	-3.842636	1.078196	3.118058
H	-4.480297	1.970658	3.065197
S	-4.243809	1.199477	5.886396
S	-7.156104	0.178002	-3.190385
S	1.388250	5.788189	-2.542712
F	-3.832006	2.721557	5.414209
F	-2.796430	1.054972	6.660256
F	-5.732178	1.396658	5.216615
F	-4.698502	-0.270623	6.466614
F	-4.841700	1.856836	7.261339
F	-7.446628	-1.381861	-3.623977
F	-7.738657	-0.135097	-1.684626
F	-6.978294	1.762778	-2.788876
F	-6.689006	0.516881	-4.730103
F	-8.689247	0.526532	-3.644184

H	4.815750	1.239982	-0.464834
C	6.206406	-0.006358	-1.593516
H	7.107958	0.473410	-1.184131
C	6.340604	-1.059526	-2.533438
C	5.178135	-1.674557	-3.062539
H	5.279372	-2.488546	-3.795777
C	3.907804	-1.246962	-2.657649
H	2.997877	-1.708301	-3.068848
O	2.841421	-0.095281	1.090000
C	3.276917	-0.948768	2.086286
C	3.015061	-0.601100	3.425735
H	2.407455	0.294823	3.625104
C	3.518551	-1.400866	4.458033
H	3.319670	-1.137351	5.507689
C	4.286581	-2.555010	4.159427
C	4.548488	-2.886037	2.806071
H	5.153707	-3.774592	2.571792
C	4.047974	-2.085709	1.772007
H	4.254722	-2.328345	0.720566
O	1.711660	-1.905613	-0.174331
C	0.902639	-2.751306	-0.901415
C	0.141096	-2.331563	-2.011112
H	0.117148	-1.271155	-2.319505
C	-0.621749	-3.276988	-2.710089
H	-1.230042	-2.955460	-3.568408
C	-0.622257	-4.639374	-2.322009
C	0.158035	-5.043629	-1.207784
H	0.162152	-6.099763	-0.899489
C	0.910806	-4.104201	-0.499667
H	1.513345	-4.396477	0.372386
C	7.644644	-1.496256	-2.949720
C	4.797480	-3.379825	5.218916
C	-1.415068	-5.601997	-3.033750
N	5.211569	-4.055992	6.086564
N	8.711536	-1.853267	-3.289441
N	-2.072491	-6.393800	-3.602327

	F 2.825891 5.043848 -2.835450 F 1.963927 6.325516 -1.088034 F 2.029355 7.137601 -3.215805 F 0.864847 5.360505 -4.040615 F 0.006284 6.647809 -2.303766	

12.3 Computational details for the Hardness and Electrophilicity

The chemical potential and molecular hardness for the N-electron system with total energy *E* and external potential $v(\vec{r})$ are defined as the following first and second derivatives of the energy with respect to N:[20]

$$\mu = \left(\frac{\partial E}{\partial N}\right)_{v(\vec{r})} = -\chi \quad (1)$$

and,

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{v(\vec{r})} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right)_{v(\vec{r})} \quad (2)$$

In numerical applications, μ and η are calculated using the finite difference approximation,

$$\mu \approx -\frac{1}{2}(\mathrm{IP} + \mathrm{EA}) \quad (3)$$

and

$$\eta \approx \frac{1}{2}(\mathrm{IP} - \mathrm{EA}) \quad (4)$$

where the vertical ionization potential (IP) and the electron affinity (EA) are obtained from the energy of the neutral, anionic and the cationic clusters at the geometry of the corresponding N-electron neutral copper cluster,

$$\mathrm{IP} = \left[E(N-1) - E(N)\right] \quad (5)$$

$$\mathrm{EA} = \left[E(N) - E(N+1)\right] \quad (6)$$

The electrophilicity index is in turn defined as [21]

$$\omega = \frac{\mu^2}{2\eta} \quad (7)$$

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