# Supporting Information for

# Olefin Metathesis Catalyst: Stabilization Effect of Backbone Substitutions of *N*-Hetrocyclic Carbene

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**CONTENTS**

## *Materials and Methods*

All reactions involving metal complexes were conducted in oven-dried glassware under a nitrogen atmosphere with anhydrous solvents, using standard Schlenk and glovebox techniques. Anhydrous solvents were obtained via elution through a solvent column drying system.[1] $RuCl_2(PCy_3)_2(=CHC_6H_5)$ was obtained from Materia, Inc. Silica gel used for the purification of organometallic complexes was obtained from TSI Scientific, Cambridge, MA (60 Å, pH 6.5–7.0). NMR chemical shifts are reported in ppm downfield from $Me_4Si$, by using the residual solvent peak as internal standard for $^1$H and $^{13}$C, and $H_3PO_4$ (δ 0.0) for $^{31}$P. Data for NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. IR spectra were recorded on a Perkin-Elmer Paragon 1000 Spectrophotometer. Gas chromatography data was obtained using an Agilent 6850 FID gas chromatograph equipped with a DB-Wax Polyethylene Glycol capillary column (J&W Scientific). X-ray crystallographic structures were obtained by the Beckman Institute X-ray Crystallography Laboratory of the California Institute of Technology. Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K., and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition numbers 651006 (**13**) and 678270 (**19**). The screening of the catalysts, in ring-closing metathesis (RCM), cross metathesis (CM), and ring-opening metathesis polymerization reactions (ROMP), was conducted according to literature procedures.[2] The initiation kinetics studies were conducted according to literature procedures.[3]

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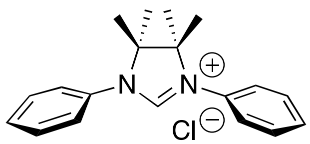
[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518–1520.
[2] Ritter, T.; Hejl, A.; Wenzel, A. G.; Funk, T. W.; Grubbs, R. H. *Organometallics* **2006**, *25*, 5740-5745.
[3] Sanford, M. S.; Love, J. A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2001**, *123*, 6543-6554.

## *Experimental*

**4,4,5,5-Tetramethyl-1,3-diphenyl-4,5-dihydro-1*H*-imidazol-3-ium chloride (10)**

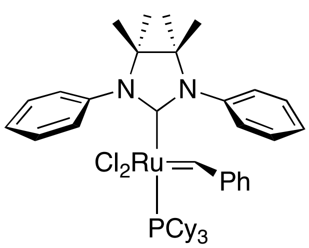



**10**

Diamine **9**[4] (2.07 g, 7.72 mmol) was dissolved in diethyl ether (20 ml) and treated with a solution of hydrogen chloride (4 M in dioxane, 7.7 ml) to precipitate the diamine hydrochloride salt. The white solid was collected by filtration and washed with copious amount of diethyl ether. The solid was placed in a flask and added triethyl orthoformate (25 ml). The resulting mixture was stirred at 130 °C for 10 min then cooled. After cooling to room temperature, the white solid was collected by filtration washing with large amount of diethyl ether and then with acetone to give the desired imidazolidinium chloride salt **10** (1.91 g, 6.07 mmol, Y = 79%).

$^1$H NMR (300 MHz, $CD_2Cl_2$): δ 9.37 (s, 1H), 7.69-7.66 (m, 4H), 7.54-7.52 (m, 6H), 1.46 (s, 12H). $^{13}$C NMR (75 MHz, $CD_2Cl_2$): δ 156.8, 133.3, 130.4, 130.0, 128.6, 74.0, 21.5. IR: 3015 (m), 2981 (m), 1616 (s), 1585 (s), 1491 (s), 1455 (s), 1390 (m), 1292 (m), 1269 (s), 1154 (s), 1078 (w), 782 (m), 768 (m), 701 (s). HRMS Calc'd for $C_{19}H_{23}N_2$: 279.1861. Meas: 279.1852.

**$RuCl_2$(4,4,5,5-Tetramethyl-1,3-diphenylimidazolin-2-ylidene)(=CH–Ph)($PCy_3$) (12)**




**12**

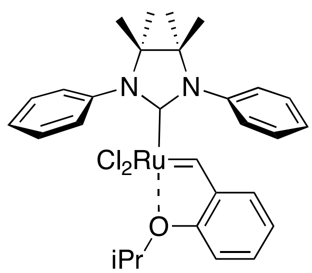
A mixture of **10** (288 mg, 0.915 mmol) and dry benzene (20 ml) was added KHMDS (182 mg, 0.915 mmol) under nitrogen atmosphere, and the resulting mixture was stirred at room temperature for 15 minutes, after which time, $RuCl_2(PCy_3)_2(=CHC_6H_5)$ (500 mg, 0.608 mmol) was added in one portion. After stirred at room temperature for overnight, the reaction mixture was concentrated under vacuum. The dark brown residue was added dry hexane (10 ml), and the mixture was stirred at room temperature for 20 minutes. The brown precipitation was collected by filtration and washed with hexane and then with methanol to give the desired ruthenium complex **12** (275 mg, 0.335 mmol, Y = 55%). Full characterization of **12** was difficult due to its instability.

$^1$H NMR (500 MHz, $C_6D_6$): δ 19.61 (d, $J$ = 3.8 Hz, 1H), 8.11 (d, $J$ = 6.7 Hz, 2H), 7.36-6.67 (m, 13H), 2.25-2.18 (m, 3H), 1.68-1.54 (m, 15H), 1.34-1.25 (m, 6H), 1.17-1.06 (m, 9H), 0.87 (s, 6H), 0.85 (s, 6H). $^{13}$C NMR (125 MHz, $C_6D_6$): δ 300.8, 217.2, 216.6, 151.8, 139.3, 137.9, 133.9,

[4] Garry, M. *Ann Chim France* **1942**, *17*, 5-99.

131.1, 129.5, 129.4, 129.2, 129.1, 128.9, 128.7, 128.5, 128.3, 128.0, 127.8, 127.7, 70.8, 70.7, 70.5, 33.4, 33.3, 29.6, 28.5, 28.4, 27.1, 22.5, 22.0. $^{31}$P NMR (121 MHz, $C_6D_6$): δ 22.35.

**$RuCl_2$(4,4,5,5-Tetramethyl-1,3-diphenylimidazolin-2-ylidene)(=CH–*o*-$^{i}$PrPh) (13)**

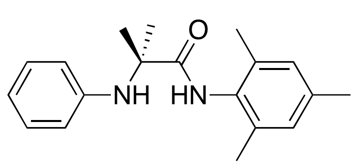


**13**

A mixture of **12** (200 mg, 0.240 mmol), *o*-isopropoxy-β-methylstyrene (**14**) (64 mg, 0.365 mmol), and *p*-toluenesulfonic acid (51 mg, 0.268 mmol) in benzene was stirred at 40 °C for 1 hour. After cooled to room temperature, the mixture was evaporated under vacuum and the residue was washed with methanol. The green solid thus obtained was recrystallized from benzene/*n*-pentane to give **13** as a dark green, crystalline solid (65 mg, 0.109 mmol, Y = 45%). X-ray quality crystal was obtained by a slow diffusion of pentane into a benzene solution.

$^{1}$H NMR (500 MHz, $C_6D_6$): δ 16.62 (s, 1H), 8.27 (d, *J* = 7.5 Hz, 2H), 7.56 (d, *J* = 7.1 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 7.3 Hz, 1H), 7.17-7.03 (m, 4H), 6.96 (dd, *J* = 7.5, 1.6 Hz, 1H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.38 (d, *J* = 8.3 Hz, 1H), 4.49 (sept, *J* = 6.2 Hz, 1H), 1.38 (d, *J* = 6.2 Hz, 6H), 0.97 (s, 6H), 0.91 (s, 6H). $^{13}$C NMR (125 MHz, $CD_2Cl_2$): δ 296.1 (d, $J_{C–H}$ = 22 Hz), 208.0, 152.8, 144.0, 140.5, 138.7, 132.5, 131.4, 130.4, 129.7, 129.2, 129.2, 128.9, 128.5, 128.5(4), 128.5(3), 128.4(8), 122.6, 121.8, 113.2, 75.0, 71.5, 70.3, 22.3, 22.2, 21.8, 21.7. IR: 3062 (w), 2979 (m), 2935 (w), 1589 (m), 1494 (s), 1453 (m), 1396 (s), 1370 (s), 1289 (m), 1267 (s), 1152 (s), 1114 (m), 954 (m), 938 (m), 844 (w), 808 (w), 770 (m), 748 (m), 714 (s) $cm^{-1}$. HRMS Calc'd for $C_{29}H_{34}Cl_2N_2ORu$: 598.1092. Meas: 598.1070.

***N*-Mesityl-2-methyl-2-(phenylamino)propanamide (15)**

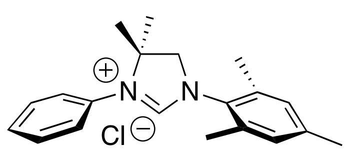


**15**

2-bromo-2-methylpropanoyl bromide (4.50 g, 19.57 mmol) was added to a mixture of 2,4,6-trimethylaniline (2.41g, 17.78 mmol), triethylamine (3.60 g, 35.56 mmol), and $CH_2Cl_2$ (20 ml) at 0 °C under Ar atmosphere. The cooling bath was removed after the addition was completed, and the reaction mixture was stirred at room temperature for 1.5 hour, after which time the mixture was diluted with $CH_2Cl_2$ (20 ml) and added aqueous solution of $NH_4Cl$. After the aqueous phase was separated, the organic layer was washed with brine and dried over anhydrous $MgSO_4$. Filtration and concentration of the filtrate gave 2-bromo-*N*-mesityl-2-methylpropanamide as a pale yellow solid (5.05g, 17.78 mmol, 100%). A solution of this amide (284 mg, 1.00 mmol) in dry THF (5 ml) was added to a mixture of sodium hydride (60% in mineral oil, 80 mg, 2.00 mmol), aniline (112 mg, 1.20 mmol) and THF (5 ml), and the resulting mixture was stirred for overnight at room temperature. The mixture was then added an aqueous solution of $NH_4Cl$ (15 ml), extracted with ethyl acetate (20 ml × 2), and the combined organic layer was washed with brine then dried over anhydrous $Na_2SO_4$. After filtration, the filtrate was concentrated under vacuum, and the residue was purified by column chromatography on silica (eluent: Hexane/Ethyl acetate = 5/1 ~ 4/1) to give **15** as a white solid (255 mg, 0.86 mmol, Y = 86%).

$^1$H NMR (300 MHz, $CDCl_3$): δ 8.35 (s, 1H), 7.25-7.17 (m, 2H), 6.84-6.71 (m, 5H), 3.98 (s, 1H), 2.23 (s, 3H), 2.11 (s, 6H), 1.63 (s, 6H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 173.8, 144.5, 136.4, 134.8, 131.0, 129.0, 119.2, 116.2, 58.4, 26.2, 20.8, 18.6. IR: 3341 (m), 3310 (s), 2987 (w), 1666 (s), 1607 (m), 1488 (s), 1376 (m), 1318 (m), 1264 (m), 1210 (m), 1162 (m), 850 (m), 749 (s), 696 (m) $cm^{-1}$. HRMS Calc'd for $C_{19}H_{24}N_2O$: 297.1967. Meas: 297.1956.

**1-Mesityl-4,4-dimethyl-3-phenyl-4,5-dihydro-1H-imidazol-3-ium chloride (16)**



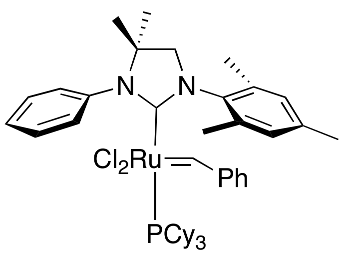

**16**

A solution of **15** (100 mg, 0.337 mmol) in dry dimethoxyethane (2 ml) was added lithium aluminum hydride (80 mg, 2.1 mmol), and the mixture was refluxed for 1 day. After cooling to room temperature, the reaction was quenched by adding $H_2O$ (0.08 ml), 15% aqueous NaOH (0.08 ml), and $H_2O$ (0.24 ml) successively. The white precipitation was filtered off and the filtrate was purified by column chromatography on silica (eluent: Hexane/Ethyl acetate = 10/1) to give $N^1$-mesityl-2-methyl-$N^2$-phenylpropane-1,2-diamine as a pale yellow solid (54 mg, 0.192 mmol, Y = 57%). The diamine (1.45 g, 5.14 mmol) was converted to the corresponding dihydrochloride salt (1.83 g, 5.14 mmol, 100%) by treating with HCl solution (4 M in dioxane). A mixture of this salt (500 mg, 1.4 mmol) and triethyl orthoformate (4.7 ml) was stirred at 130 °C for 5 min then cooled. After cooling to room temperature, the white precipitation was collected by filtration washing with large amount of diethyl ether and then with acetone to give the desired imidazolidinium chloride salt **16** (367 mg, 1.12 mmol, Y = 80%).

$^1$H NMR (300 MHz, $CDCl_3$): δ 9.76 (s, 1H), 7.65-7.62 (m, 2H), 7.49-7.47 (m, 3H), 6.92 (s, 2H), 4.13 (s, 2H), 2.39 (s, 6H), 2.27 (s, 3H), 1.69 (s, 6H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 158.4, 140.2, 134.9, 132.3, 130.2, 130.0, 129.9, 129.8, 127.4, 68.6, 63.7, 26.7, 20.9, 18.1. IR: 3401 (m), 2975 (w), 1624 (s), 1592 (m), 1301 (w), 1263 (m), 1219 (m), 856 (w), 776 (w) $cm^{-1}$. HRMS Calc'd for $C_{20}H_{25}N_2$: 293.2018. Meas: 293.2021.

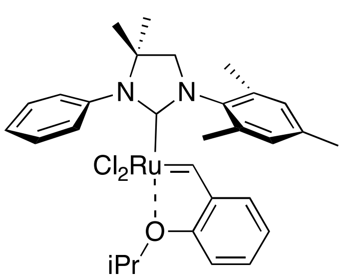
**$RuCl_2$(1-Mesityl-4,4-dimethyl-3-phenylimidazolin-2-ylidene)(=CH–Ph)($PCy_3$) (18) and $RuCl_2$(1-Mesityl-4,4-dimethyl-3-phenylimidazolin-2-ylidene)(=CH–*o*-$^{i}$PrPh) (19)**

The phosphine complex **18** and the phosphine-free complex **19** was prepared from **16** according to the procedure described for the synthesis of **13**. X-ray quality crystal of **19** was obtained by a slow diffusion of pentane into a $CH_2Cl_2$ solution.




**18**

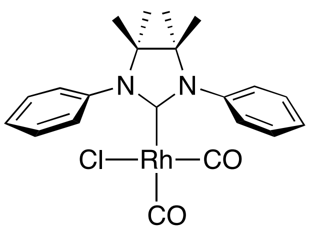
$^{1}H$ NMR (500 MHz, $CD_2Cl_2$): δ 19.14 (s, 1H), 8.77 (br s, 1H), 7.89-7.87 (m, 2H), 7.51 (t, $J$ = 7.6 Hz, 2H), 7.44 (tt, $J$ = 7.4, 1.2 Hz, 1H), 7.39 (t, $J$ = 7.4 Hz, 1H), 7.10 (t, $J$ = 7.6 Hz, 2H), 6.71 (br s, 2H), 5.84 (br s, 1H), 3.66 (br s, 2H), 2.65-1.99 (m, 5H), 1.91 (s, 3H), 1.94-1.87 (m, 3H), 1.53-1.47 (m, 9H), 1.36 (s, 6H), 1.39-1.23 (m, 6H), 0.98-0.89 (m, 16H). $^{13}C$ NMR (125 MHz, $CD_2Cl_2$): δ 296.8, 218.1, 217.5, 151.8, 138.3, 137.7, 136.9, 136.1, 135.0, 129.7, 129.4, 129.1, 128.9, 128.6, 128.2, 65.9, 65.2, 32.7, 32.5, 29.2, 28.3, 28.2, 27.7, 26.7, 21.2, 18.8. IR ($CD_2Cl_2$): 2931 (s), 2852 (m), 1987 (w), 1487 (m), 1447 (m), 1400 (m), 1301 (m), 1175 (m), 778 (w) $cm^{-1}$. HRMS Calc'd for $C_{45}H_{63}Cl_2N_2PRu$: 834.3150. Meas: 834.3165.




**19**

$^{1}H$ NMR (500 MHz, $C_6D_6$): δ 16.49 (s, 0.5H), 16.48 (s, 0.5H), 7.99-7.96 (m, 2H), 7.57-7.49 (m, 4H), 7.10 (d, $J$ = 0.6 Hz, 2H), 6.91 (d, $J$ = 4.4 Hz, 2H), 6.86 (d, $J$ = 8.1 Hz, 1H), 4.90 (sept, $J$ = 6.2 Hz, 1H), 3.91 (s, 2H), 2.46 (s, 3H), 2.33 (s, 6H), 1.47 (s, 6H), 1.22 (d, $J$ = 6.2 Hz, 6H). $^{13}C$ NMR (125 MHz, $CD_2Cl_2$): δ 297.6 (d, $J_{C–H}$ = 18 Hz), 209.9, 152.6, 145.1, 139.4, 138.8, 138.1, 136.5, 135.6, 130.1, 1230.0, 129.4, 128.9(0), 128.8(6), 122.9, 122.5, 113.4, 75.4, 66.0, 65.5, 27.8, 21.8, 21.5, 18.5. IR: 2967 (m), 1589 (m), 1572 (m), 1489 (m), 1472 (m), 1450 (m), 1380 (s), 1317 (m), 1286 (s), 1207 (m), 1179 (m), 1154 (m), 1113 (s), 1031 (w), 931 (m), 877 (w), 805 (w), 770 (w), 754 (m), 699 (m) $cm^{-1}$. HRMS Calc'd for $C_{34}H_{44}Cl_2N_2ORu$: 612.1249. Meas: 612. 1229.

**RhCl(CO)$_2$(4,4,5,5-Tetramethyl-1,3-diphenylimidazolin-2-ylidene) (32a)**

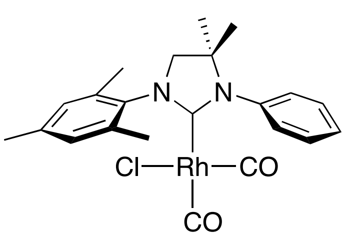


**32a**

The imidazolidinium salt **16** (33 mg, 0.10 mmol), KHMDS (20 mg, 0.10 mmol), and toluene (2 ml) was stirred at room temperature under $N_2$ for 15 min, and added to a suspension of [RhCl(COD)]$_2$ (20 mg, 0.04 mmol) in toluene (1 ml). The resulting mixture was stirred at room temperature for 1.5 hour, and then the solvent was removed under vacuum. The residue was purified by column chromatography on TSI silica (eluent: 2% EtOH in $CH_2Cl_2$) to give [(NHC)RhCl(COD)] **31a** as a yellow powder. A solution of **31a** in $CH_2Cl_2$ (3 ml) was bubbled with CO for 1 hour. The mixture was then concentrated under vacuum and the residue was washed with dry hexane (2 ml × 3). The resulting solid was dried under vacuum to give **32** (26 mg, 0.055 mmol, Y = 76% two steps).

$^1$H NMR (500 MHz, $CD_2Cl_2$): δ 7.49-7.36 (m, 10H), 1.28 (s, 6H), 1.27 (s, 6H). $^{13}$C NMR (125 MHz, $CD_2Cl_2$): δ 202.8 ($J_{C\text{–}Rh}$ = 40 Hz), 187.0 ($J_{C\text{–}Rh}$ = 54 Hz), 183.6 ($J_{C\text{–}Rh}$ = 76 Hz), 138.3, 131.7, 129.3, 129.1, 128.9, 72.1, 22.0, 21.9. IR ($CD_2Cl_2$): 2078, 1996 cm$^{-1}$. HRMS Calc'd for $C_{21}H_{22}ClN_2O_2Rh$: 472.0425. Meas: 472.0402.

**RhCl(CO)$_2$(1-Mesityl-4,4-dimethyl-3-phenylimidazolin-2-ylidene) (32b)**



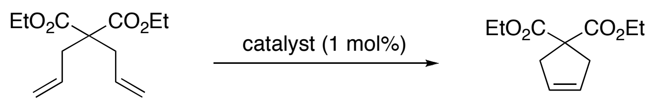
**32b**

The imidazolidinium **16** (33 mg, 0.10 mmol) was treated as described above to give **32b** (32 mg, 0.066 mmol, Y = 94% two steps).

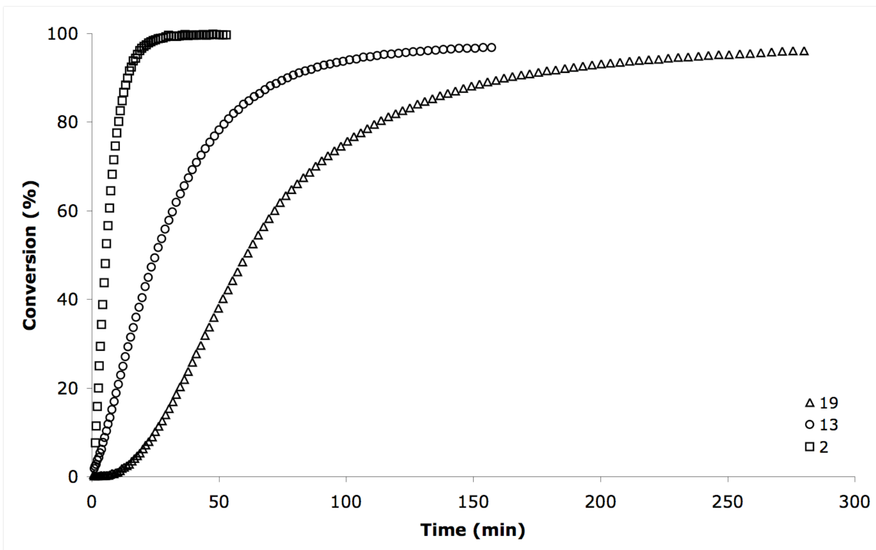
$^1$H NMR (500 MHz, $CD_2Cl_2$): δ 7.49-7.47 (m, 4H), 7.36 (s, 1H), 6.98 (br s, 2H), 3.77 (br s, 2H), 2.42 (br s, 6H), 2.33 (s, 3H), 1.46 (s, 6H). $^{13}$C NMR (125 MHz, $CD_2Cl_2$): δ 204.4 ($J_{C\text{–}Rh}$ = 40 Hz), 186.5 ($J_{C\text{–}Rh}$ = 54 Hz), 183.8 ($J_{C\text{–}Rh}$ = 75 Hz), 139.2, 137.8, 135.5, 131.7, 129.9, 129.2, 129.1, 128.9, 67.3, 65.4, 27.6, 21.4. IR ($CD_2Cl_2$): 2079, 1996 cm$^{-1}$. HRMS Calc'd for $C_{22}H_{24}N_2O_2Rh$: 451.0893. Meas: 451.0889.

## Standard Activity Test: RCM Reactions

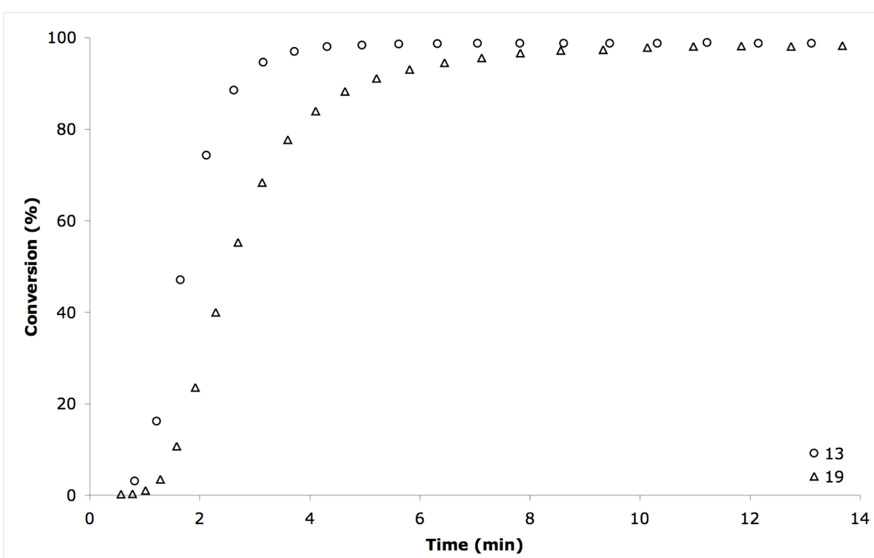
All tests were performed according to the experimental procedure described by Ritter et al.[1]

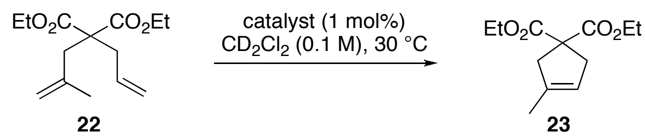



At 30 °C, $CD_2Cl_2$ (0.1 M)

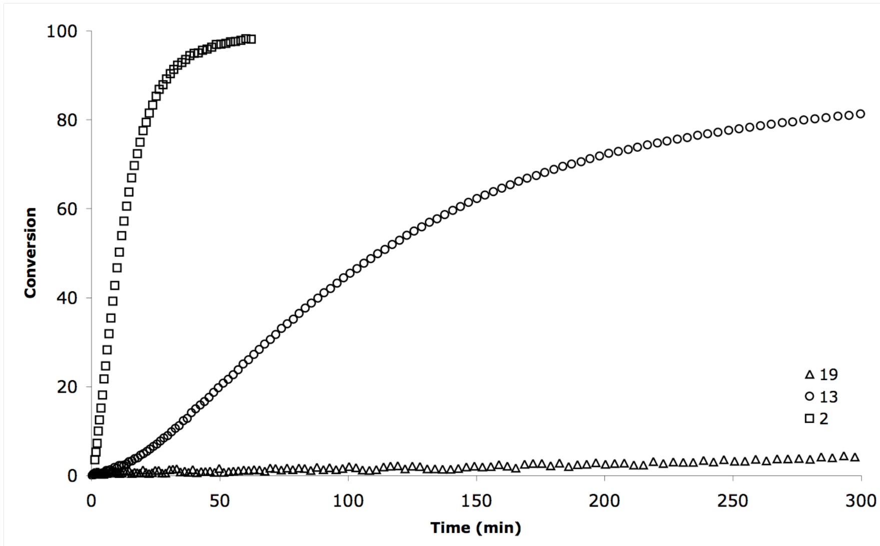



At 60 °C, $C_6D_6$ (0.1 M)

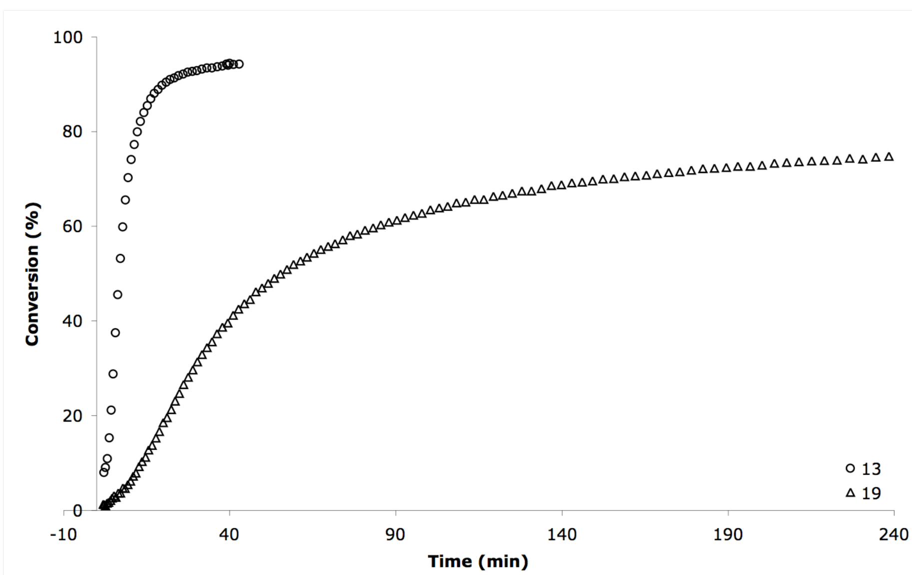


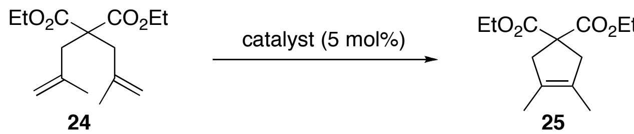



At 30 °C, $CD_2Cl_2$ (0.1 M)

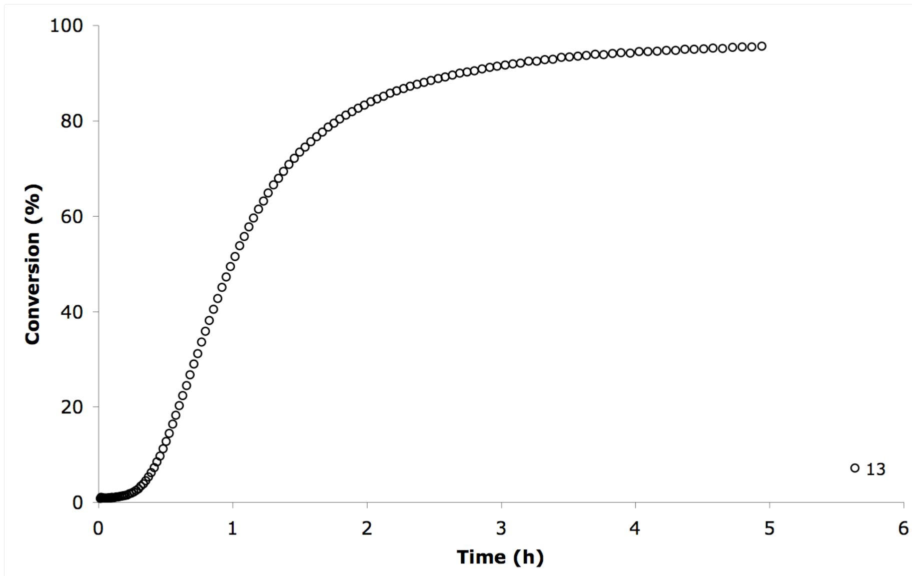



At 60 °C, $C_6D_6$ (0.1 M)

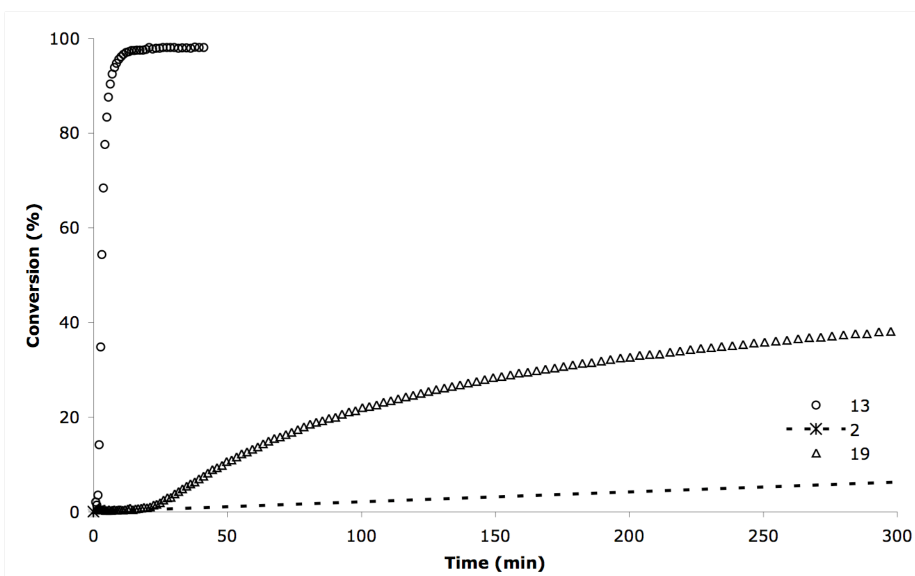




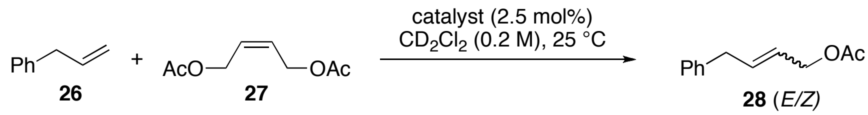

At 30 °C, $CD_2Cl_2$ (0.1 M)

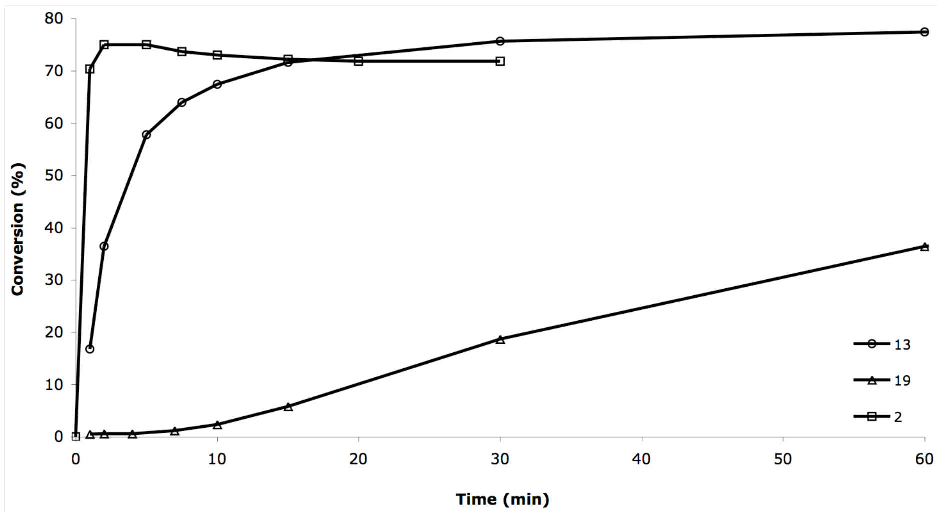



At 60 °C, $C_6D_6$ (0.1 M)

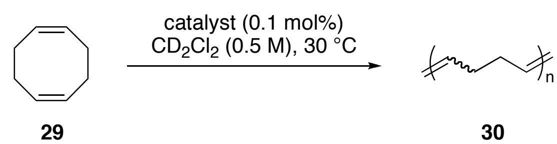


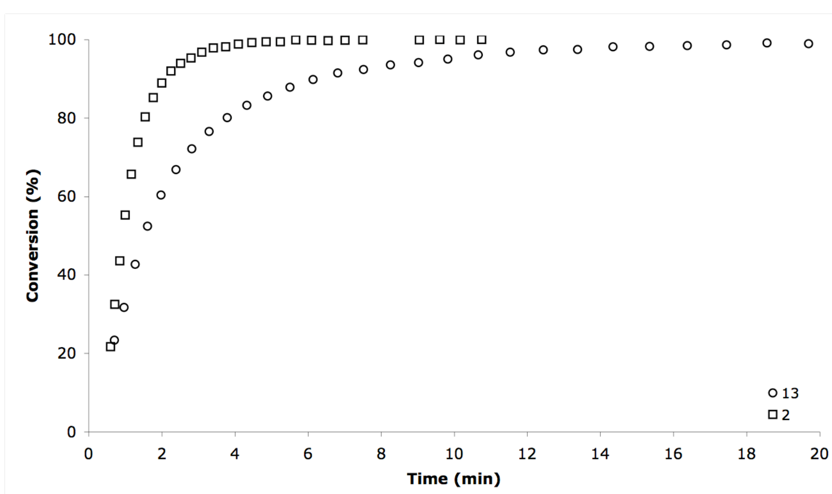
## CM Reactions



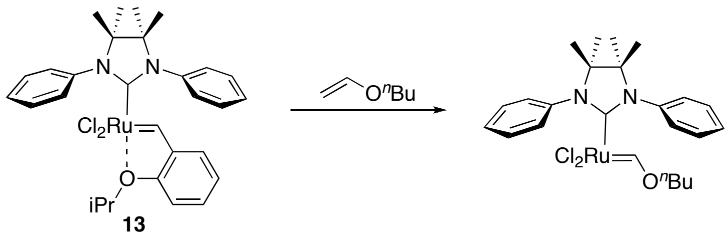

## ROMP of Cyclooctadiene

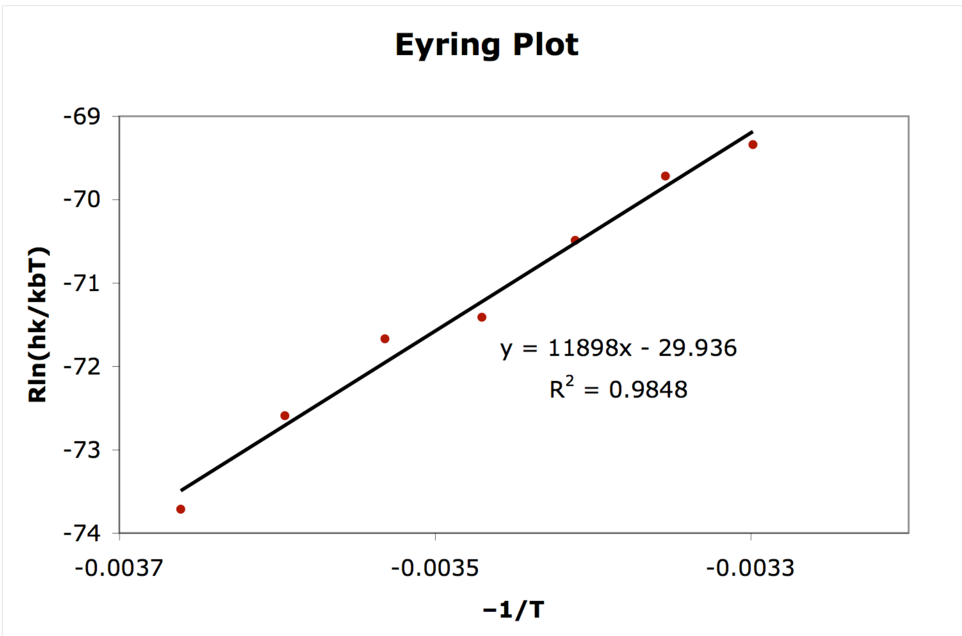


**Initiation Studies**

The initiation kinetics studies of compound **13** were conducted according to literature procedures.[2]

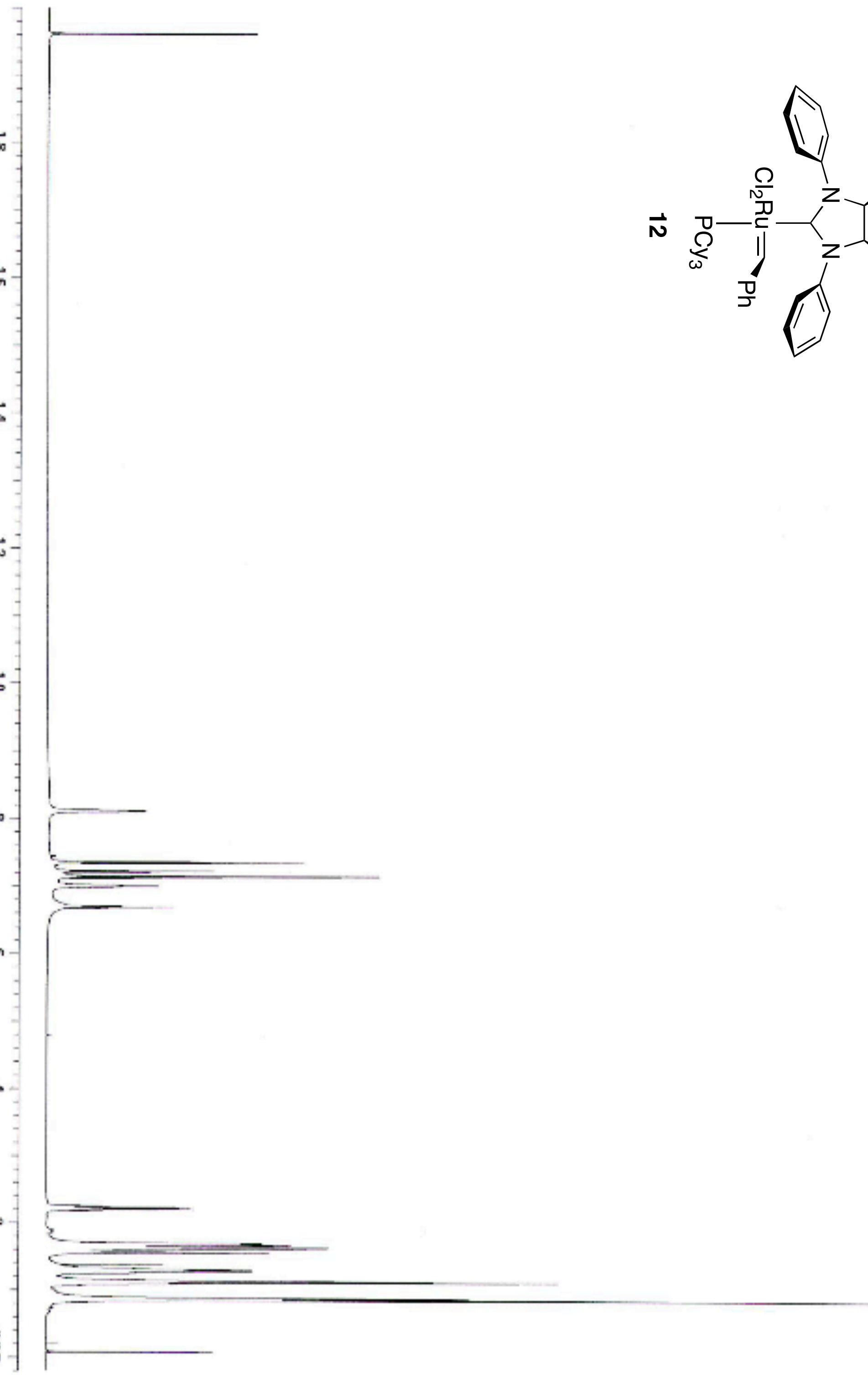


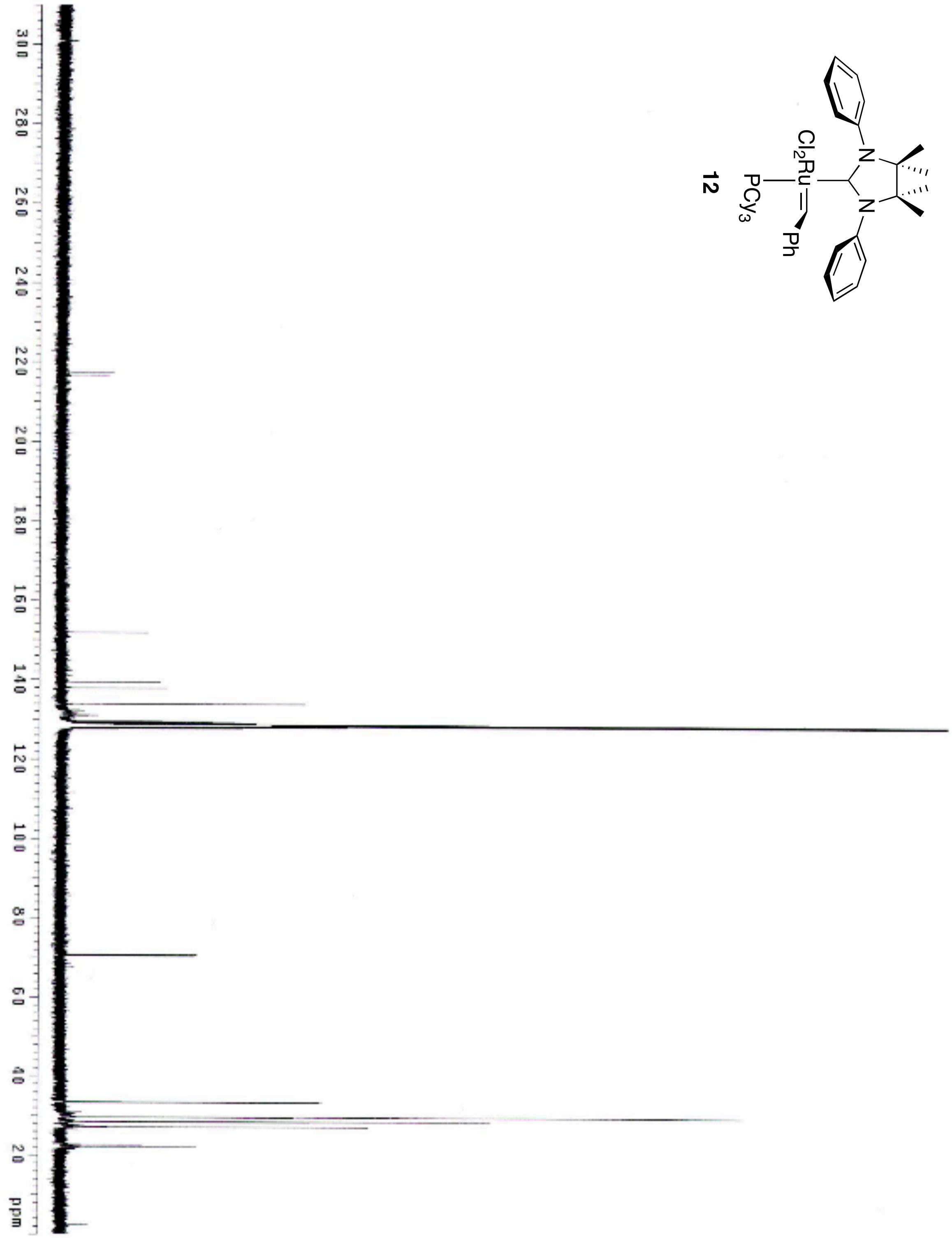

| (303 K) | **13** | **2** |
|---|---|---|
| $\Delta H^{\ddagger}$ (kcal/mol) | 11.9 (± 1.7) | 15.2 (± 0.8) |
| $\Delta S^{\ddagger}$ (e.u.) | −30 (± 6) | −19 (± 3) |
| $\Delta G^{\ddagger}$ (kcal/mol) | 21.0 (± 0.1) | 20.7 (± 0.01) |
| $k_{init}$ | $47 \times 10^{-4}$ | $67 \times 10^{-4}$ |

**NMR Spectra**

$^1$H-NMR of **12**

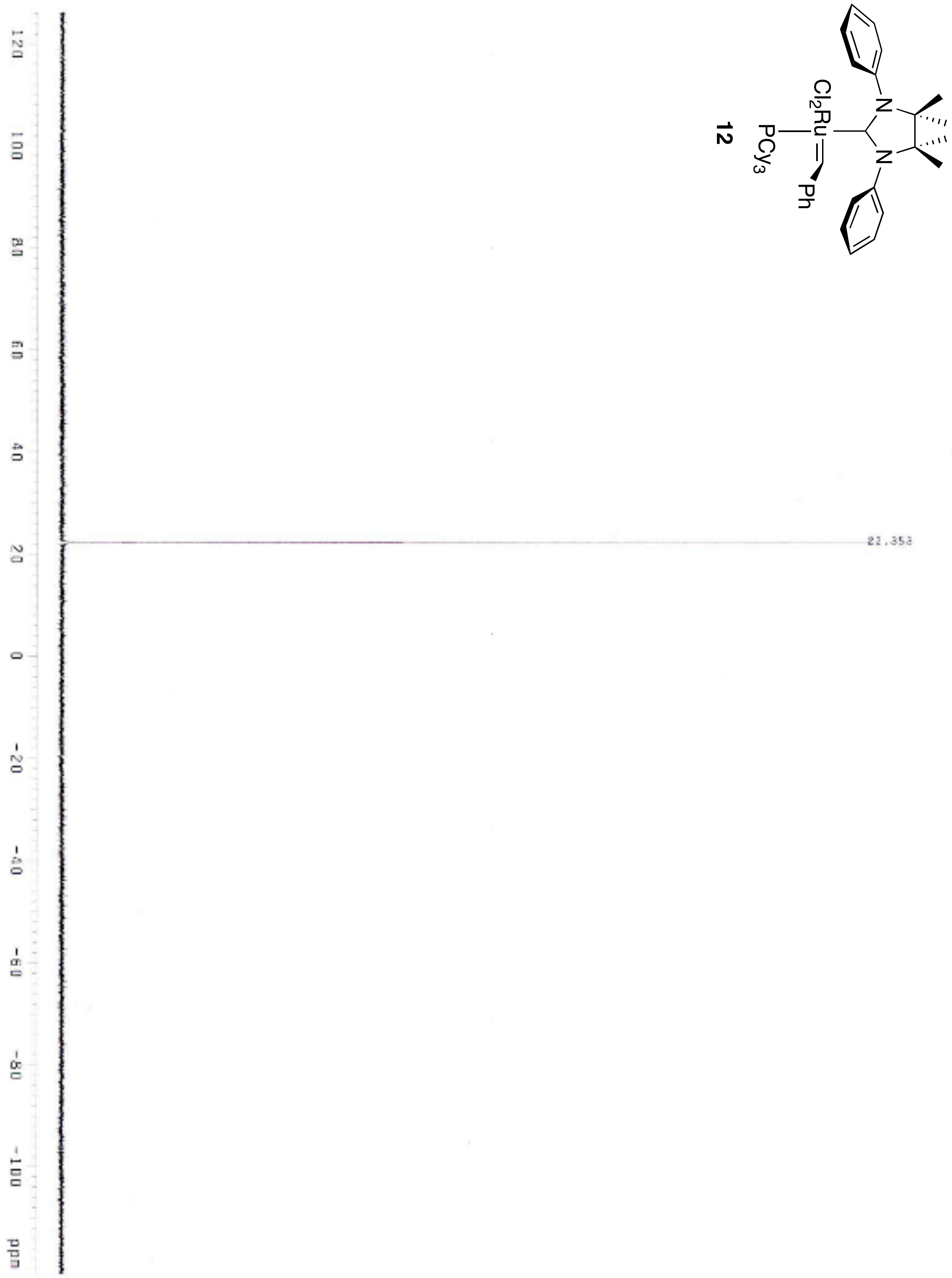


$^{13}$C-NMR of **12**

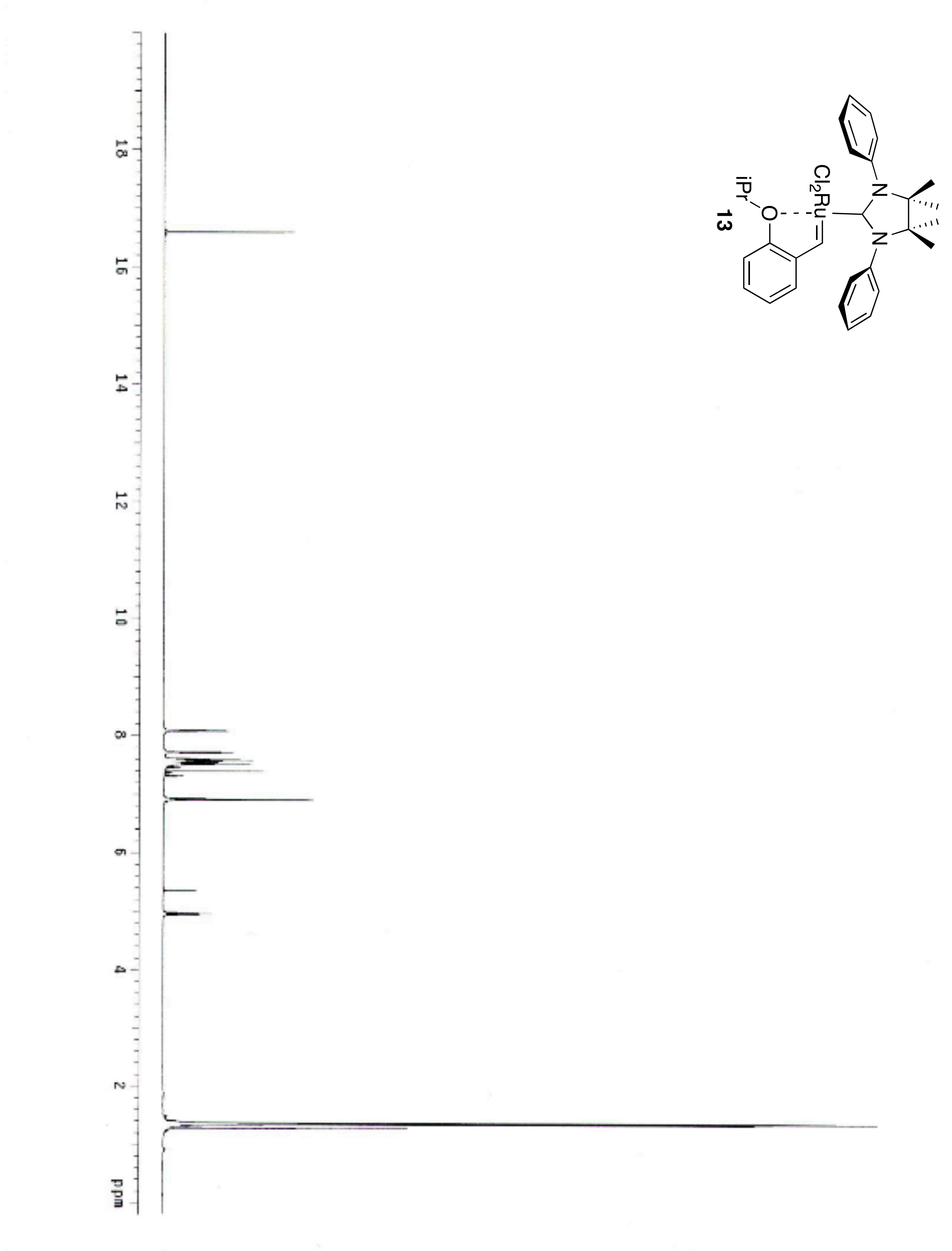



**12**

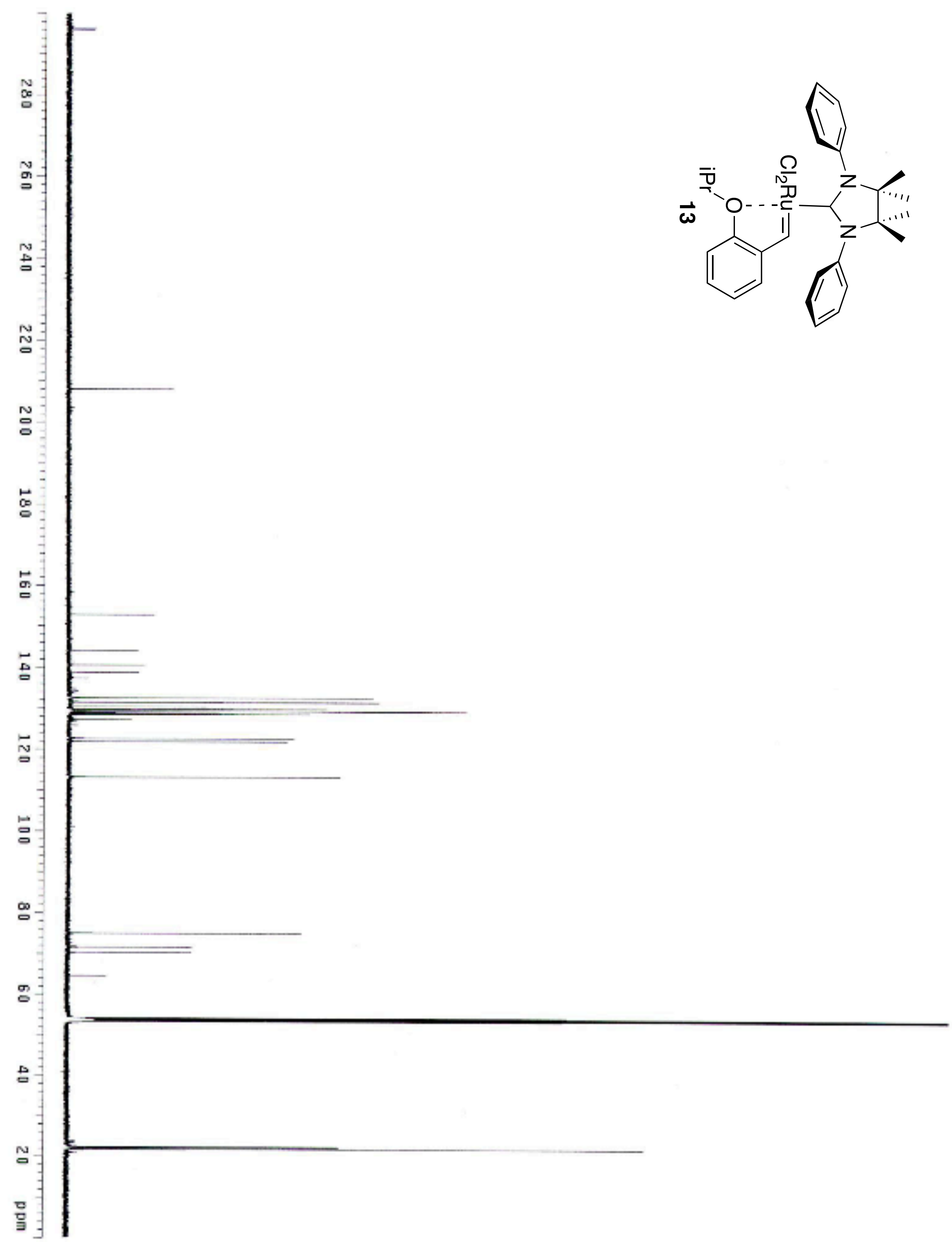
$^{31}$P-NMR of **12**



$^{1}$H-NMR of **13**

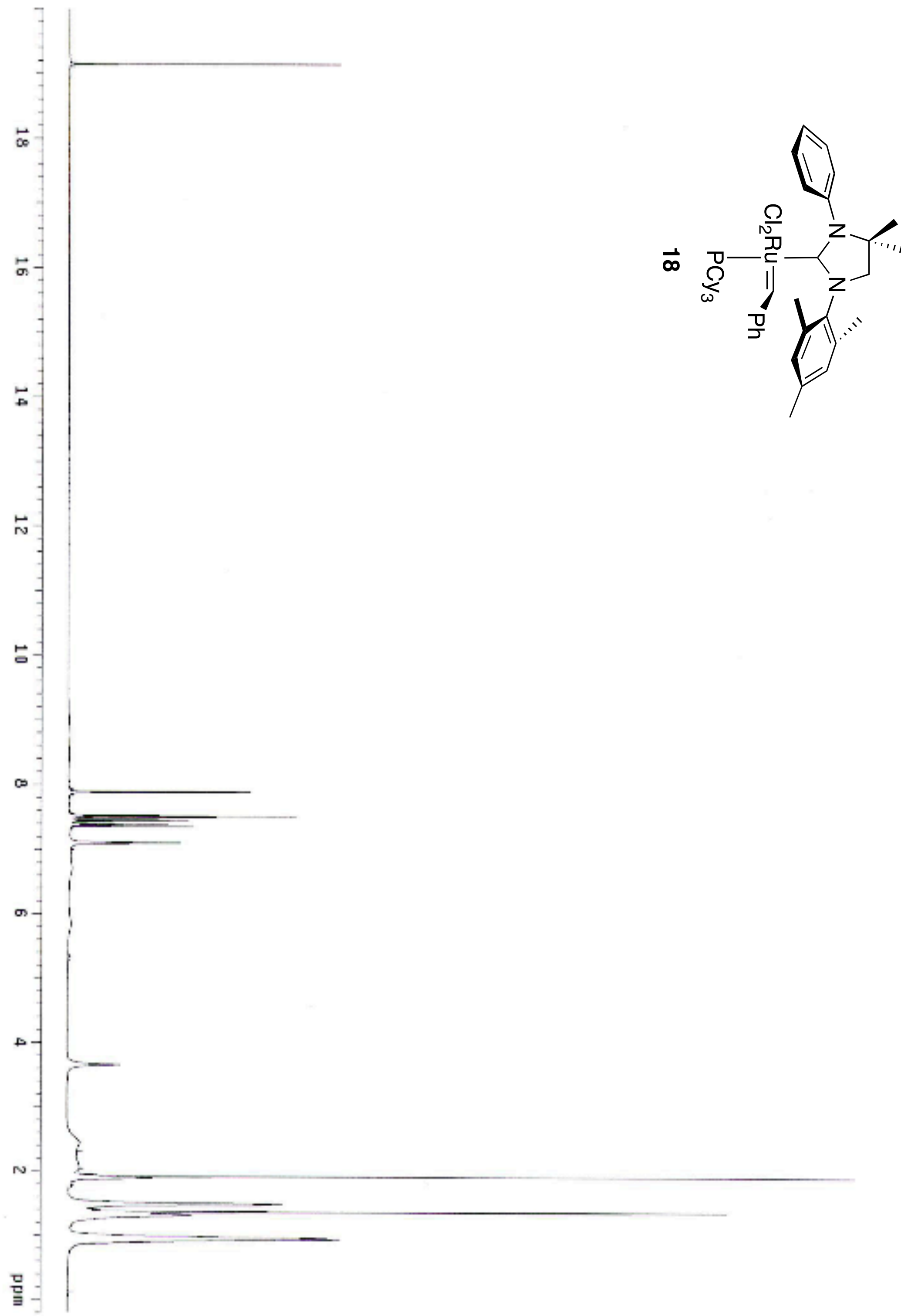


$^{13}$C-NMR of **13**

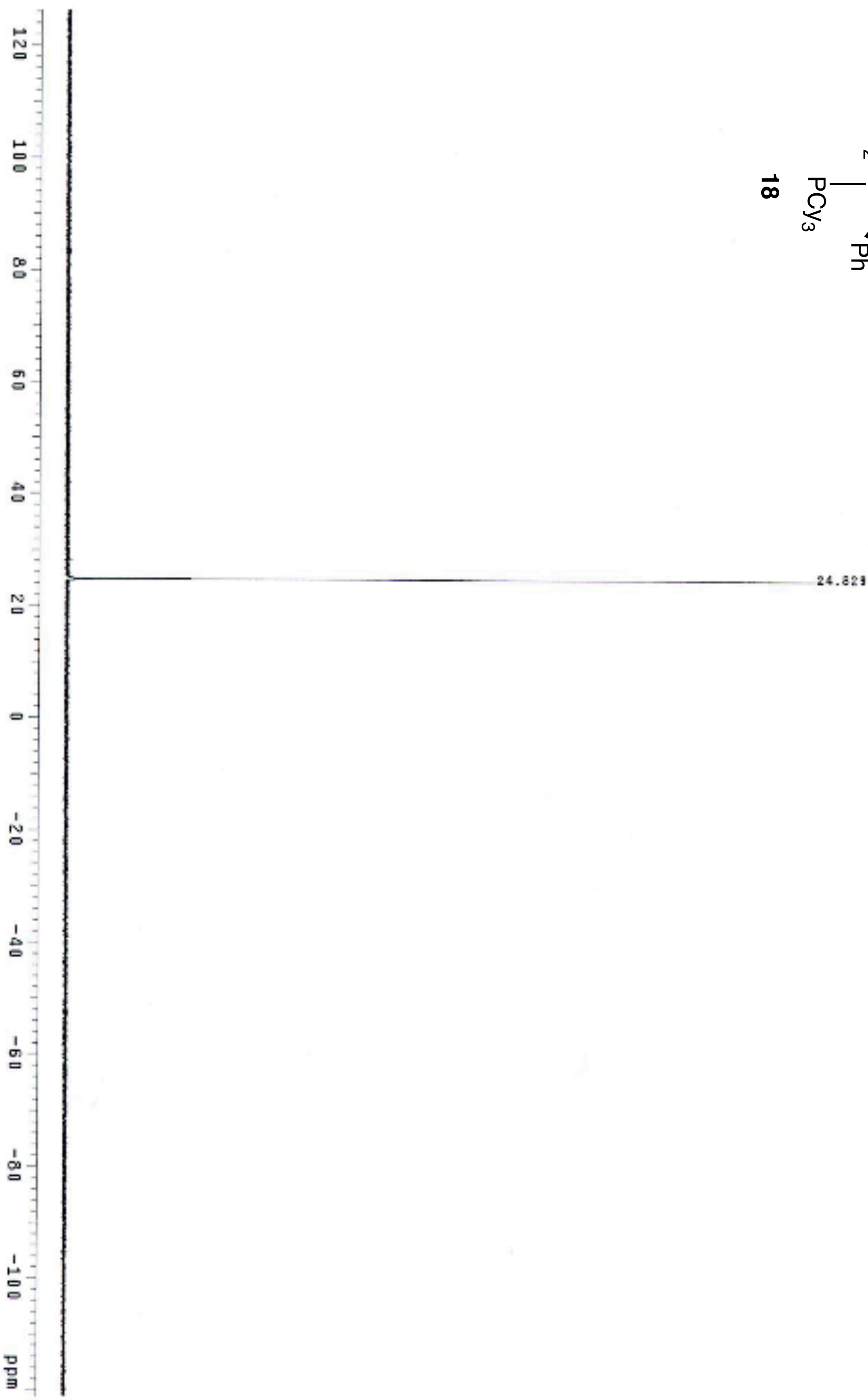


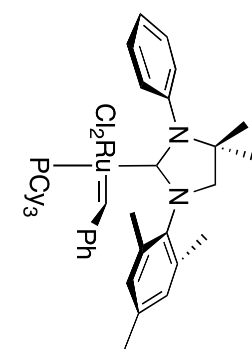
280
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm
Cl2Ru
iPr
O
N
N
13

[1]H-NMR of **18**



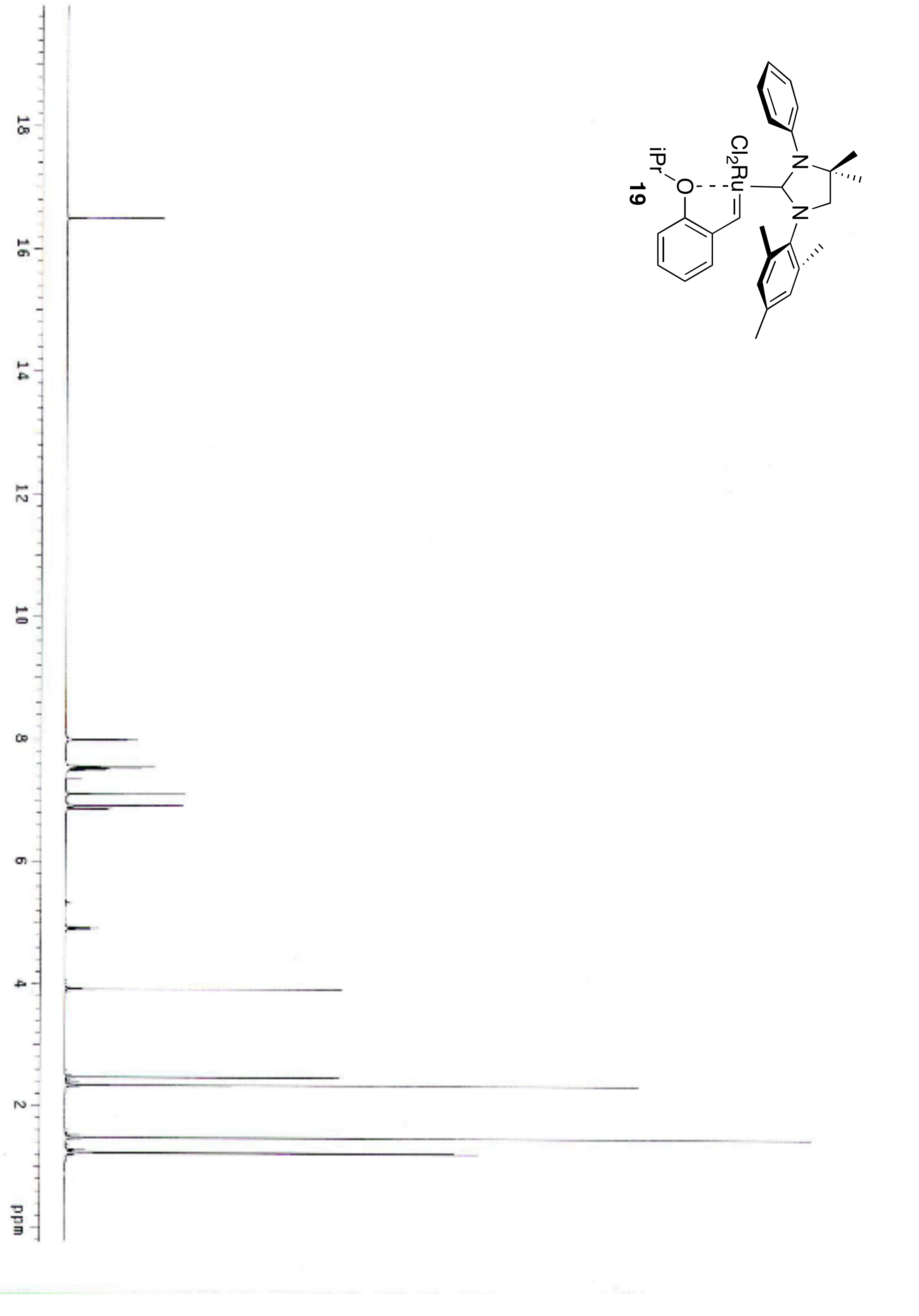
$^{31}$P-NMR of **18**



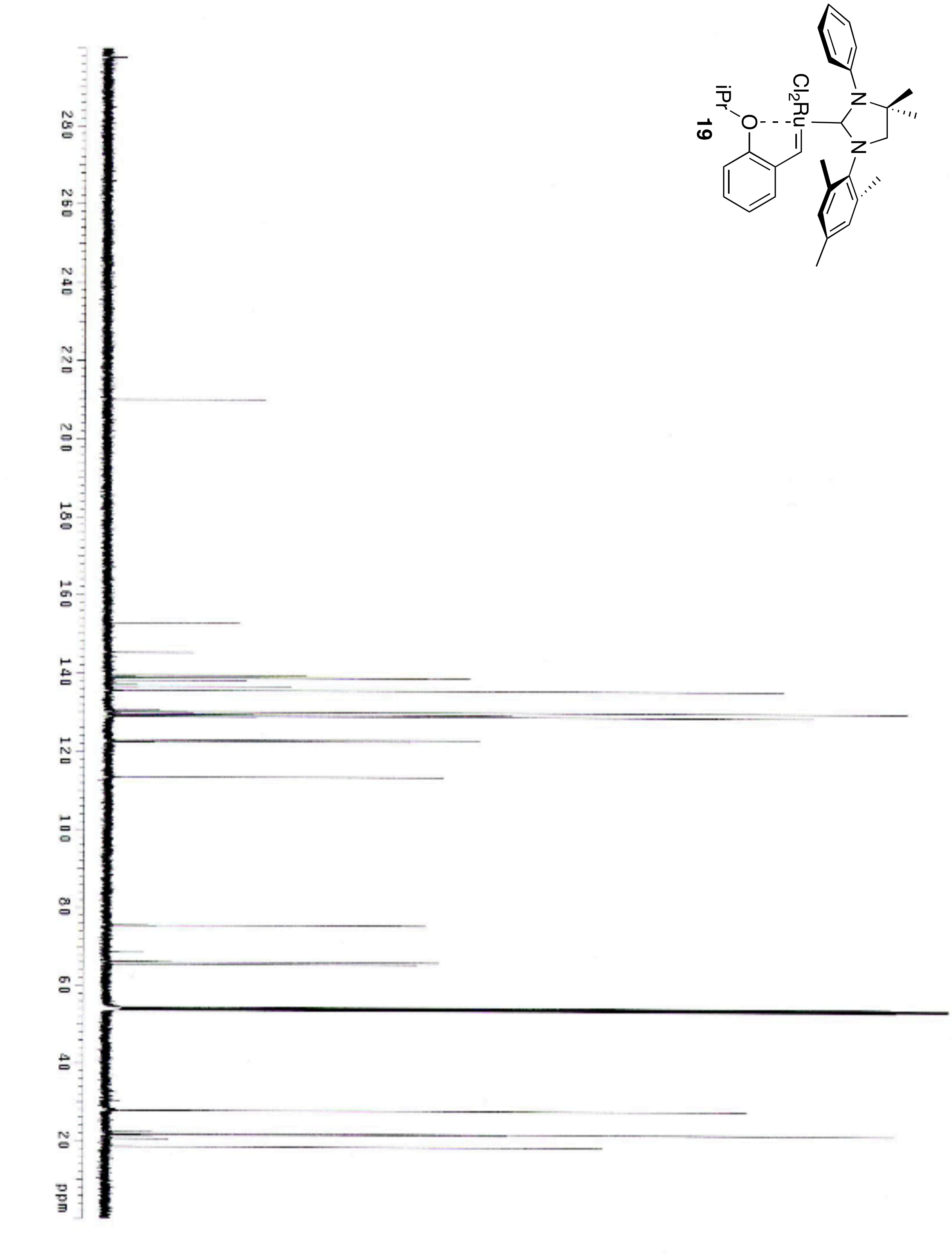




**18**

$^{1}$H-NMR of **19**

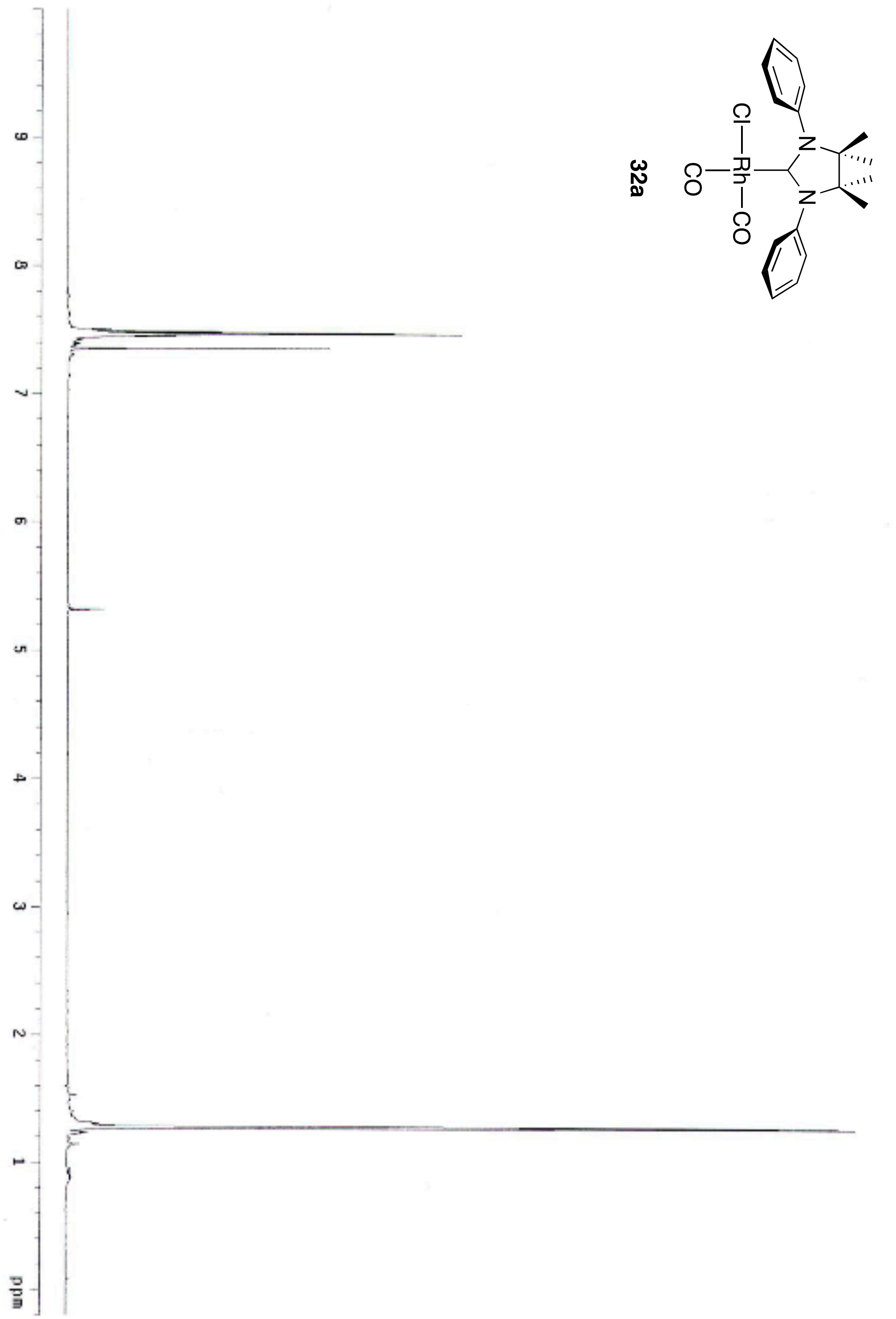


$^{13}$C-NMR of **19**

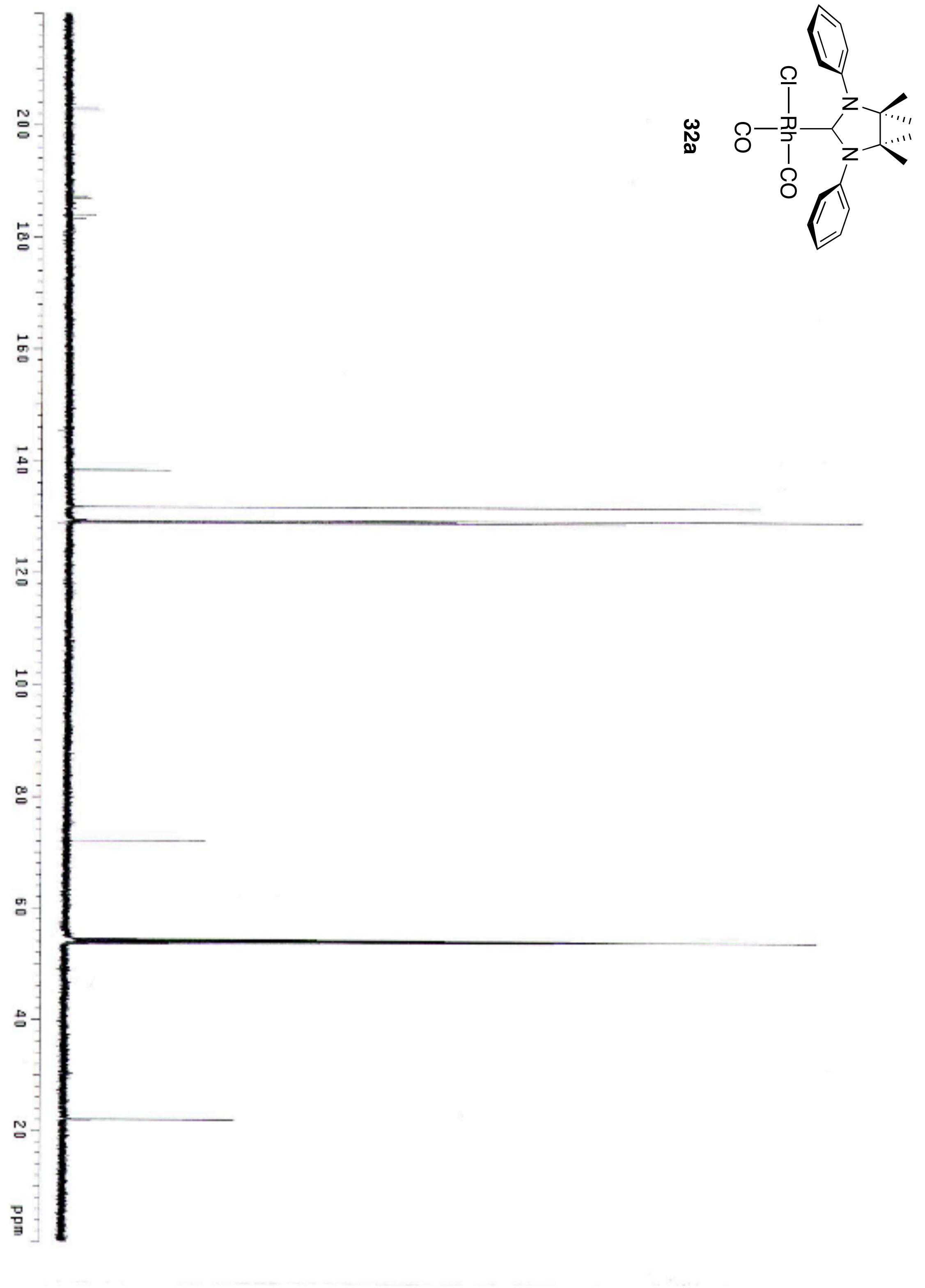


Cl2Ru
iPr
19
N
O
280
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm

[1]H-NMR of **32a**

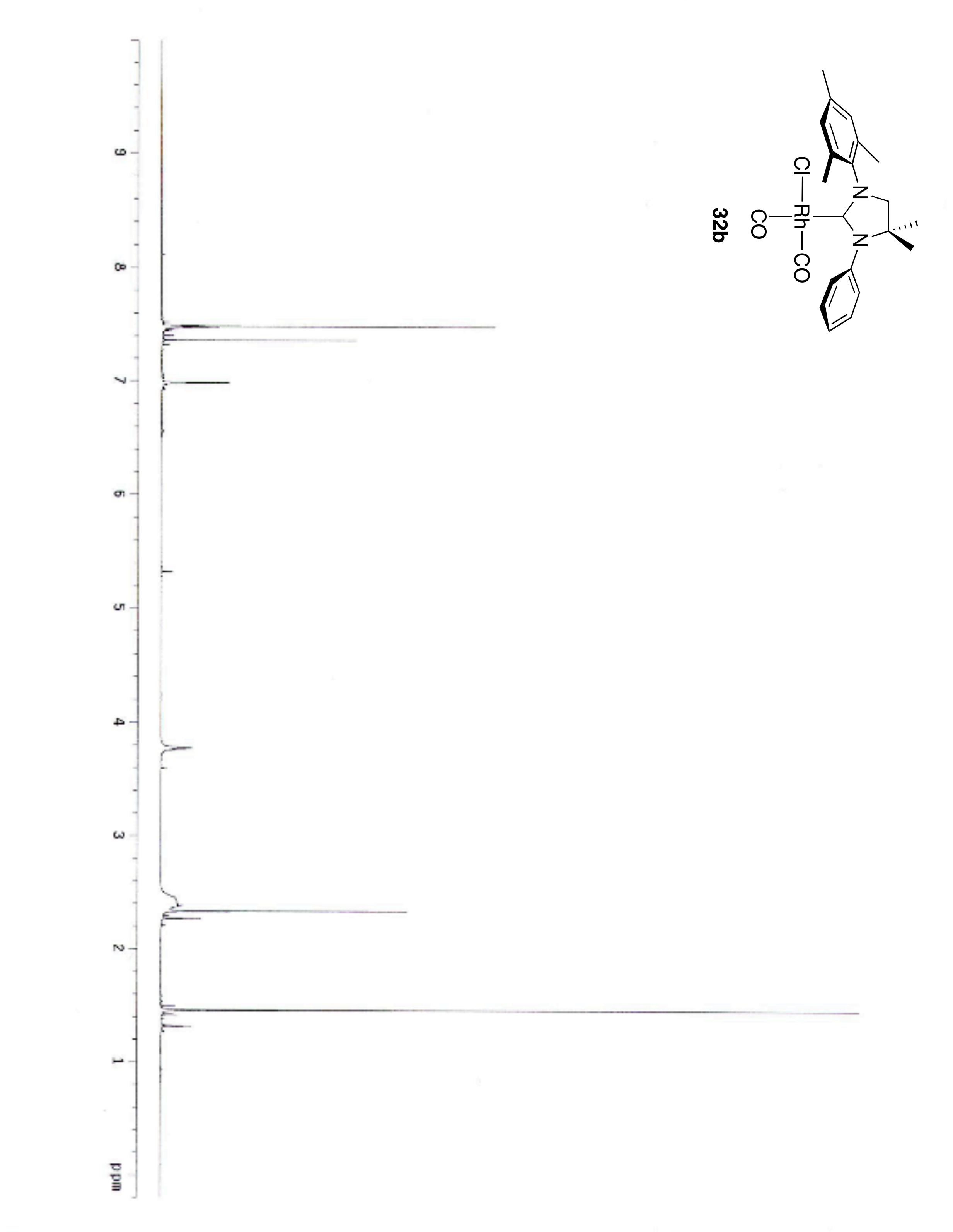


$^{13}$C-NMR of **32a**

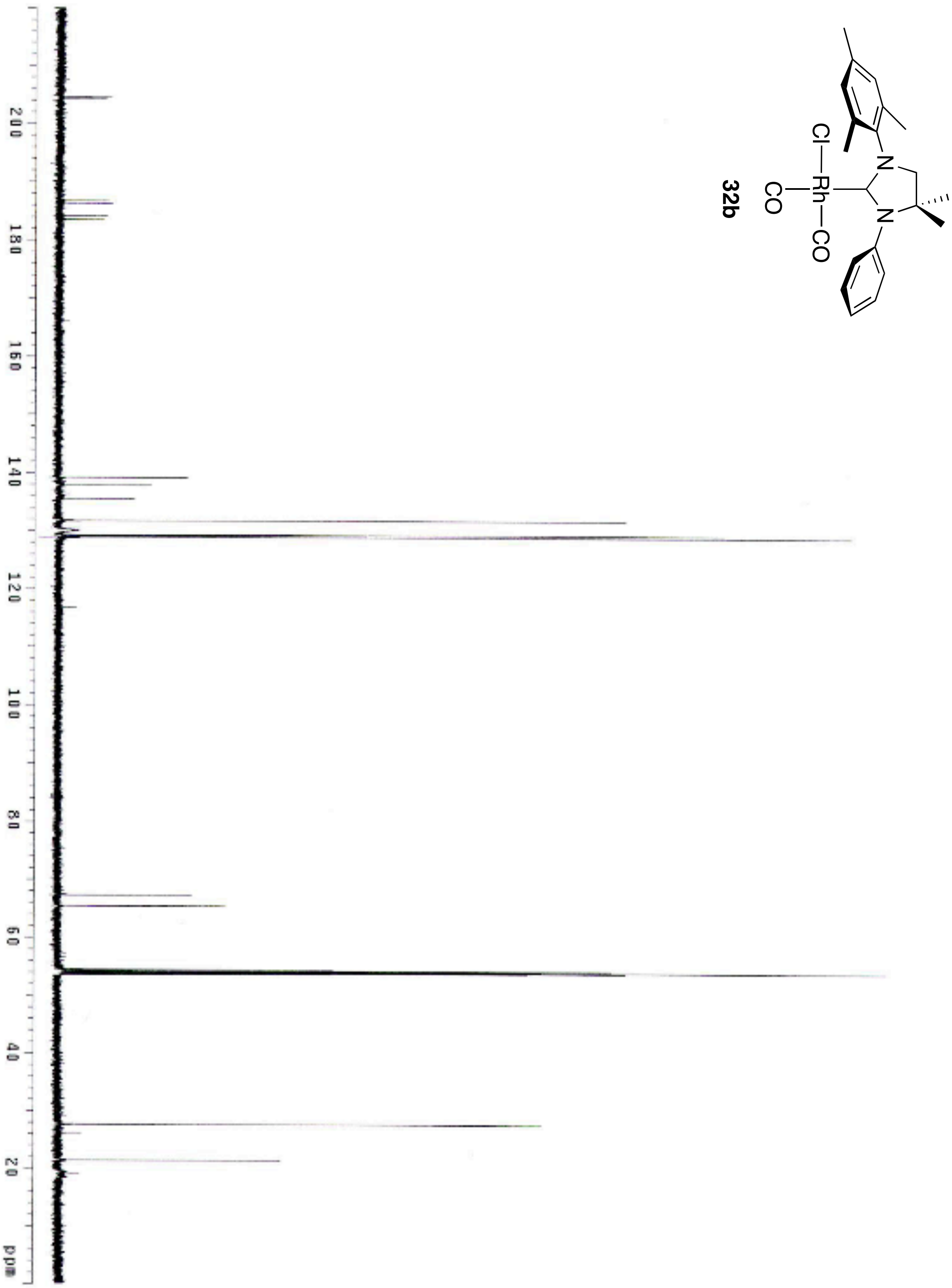



32a

[1]H-NMR of **32b**



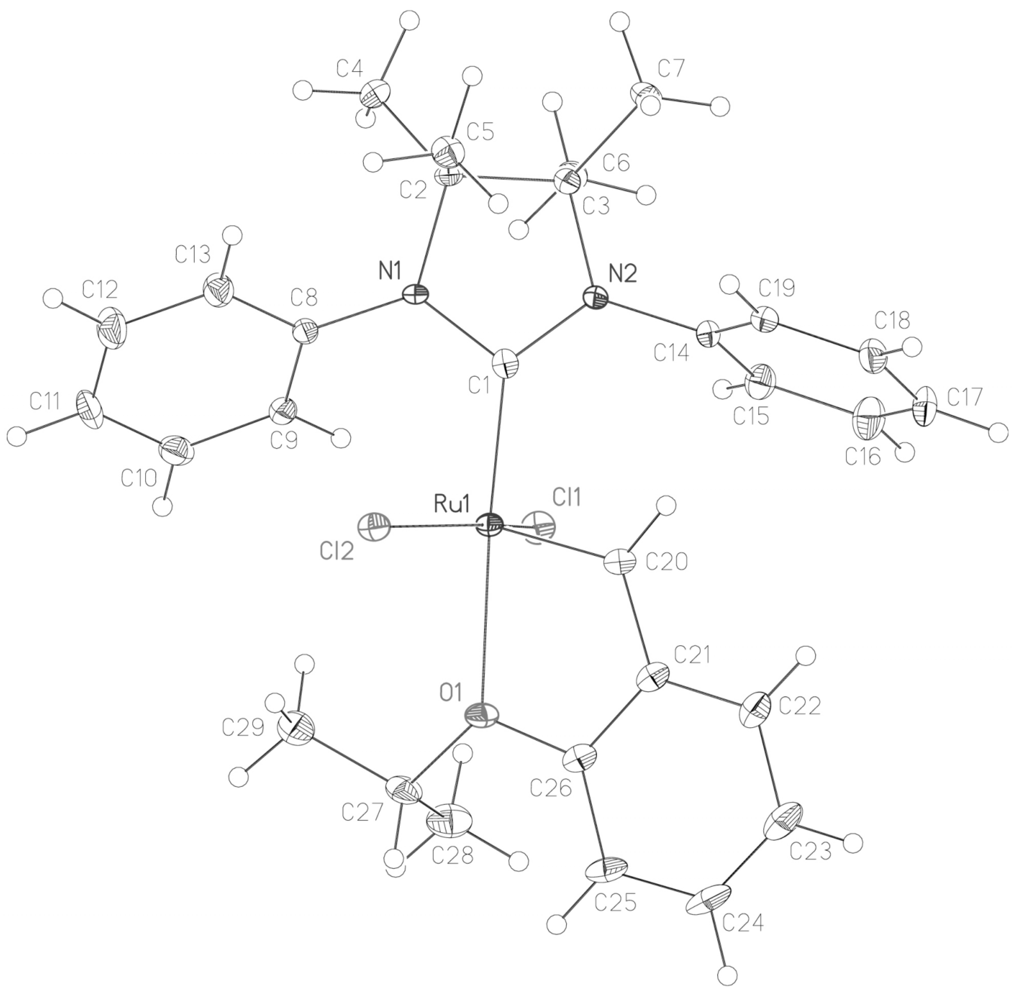
[13]C-NMR of **32b**




**32b**

**X-Ray Structural Analysis**

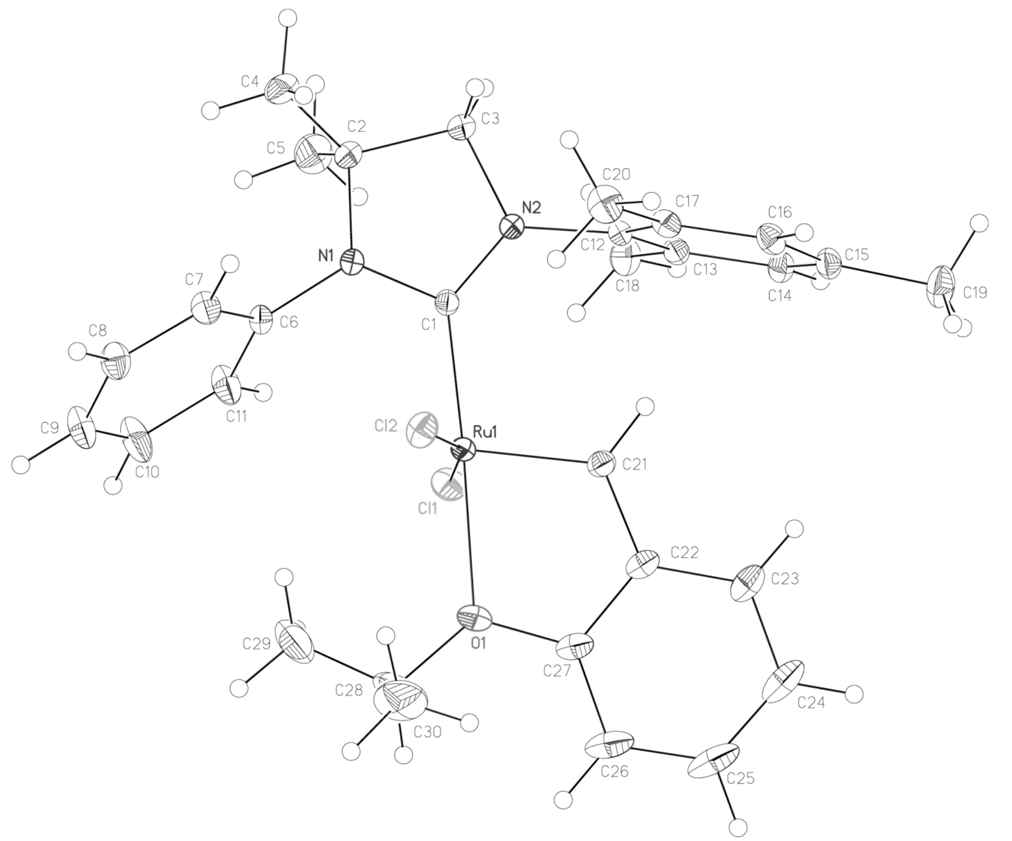
Minimum Overlap View of **13**




Selected Bond Lengths [Å] and Angles [°] for **13**

| | | | |
|---|---|---|---|
| Ru(1)-C(20) | 1.822(2) | C(20)-Ru(1)-C(1) | 98.53(8) |
| Ru(1)-C(1) | 1.959(2) | C(20)-Ru(1)-O(1) | 78.37(7) |
| Ru(1)-O(1) | 2.3068(14) | C(1)-Ru(1)-O(1) | 176.72(7) |
| Ru(1)-Cl(2) | 2.3354(5) | C(20)-Ru(1)-Cl(2) | 99.49(6) |
| Ru(1)-Cl(1) | 2.3549(5) | C(1)-Ru(1)-Cl(2) | 92.76(6) |
| | | O(1)-Ru(1)-Cl(2) | 88.85(4) |
| | | C(20)-Ru(1)-Cl(1) | 101.71(6) |
| | | C(1)-Ru(1)-Cl(1) | 90.98(6) |
| | | O(1)-Ru(1)-Cl(1) | 88.61(4) |
| | | Cl(2)-Ru(1)-Cl(1) | 157.668(19) |

Minimum Overlap View of **19**




Selected Bond Lengths [Å] and Angles [°] for **19**

| | | | |
|---|---|---|---|
| Ru(1)-C(21) | 1.8342(6) | C(21)-Ru(1)-C(1) | 102.96(2) |
| Ru(1)-C(1) | 1.9686(6) | C(21)-Ru(1)-O(1) | 79.51(2) |
| Ru(1)-O(1) | 2.2581(5) | C(1)-Ru(1)-O(1) | 177.51(2) |
| Ru(1)-Cl(2) | 2.33786(17) | C(21)-Ru(1)-Cl(2) | 98.94(2) |
| Ru(1)-Cl(1) | 2.35763(17) | C(1)-Ru(1)-Cl(2) | 90.426(18) |
| | | O(1)-Ru(1)-Cl(2) | 88.943(15) |
| | | C(21)-Ru(1)-Cl(1) | 98.37(2) |
| | | C(1)-Ru(1)-Cl(1) | 92.486(17) |
| | | O(1)-Ru(1)-Cl(1) | 87.354(14) |
| | | Cl(2)-Ru(1)-Cl(1) | 161.314(6) |