Electronic Supplementary Information (ESI) for:

Ruthenium Olefin Metathesis Catalysts Featuring Unsymmetrical N-Heterocyclic Carbenes

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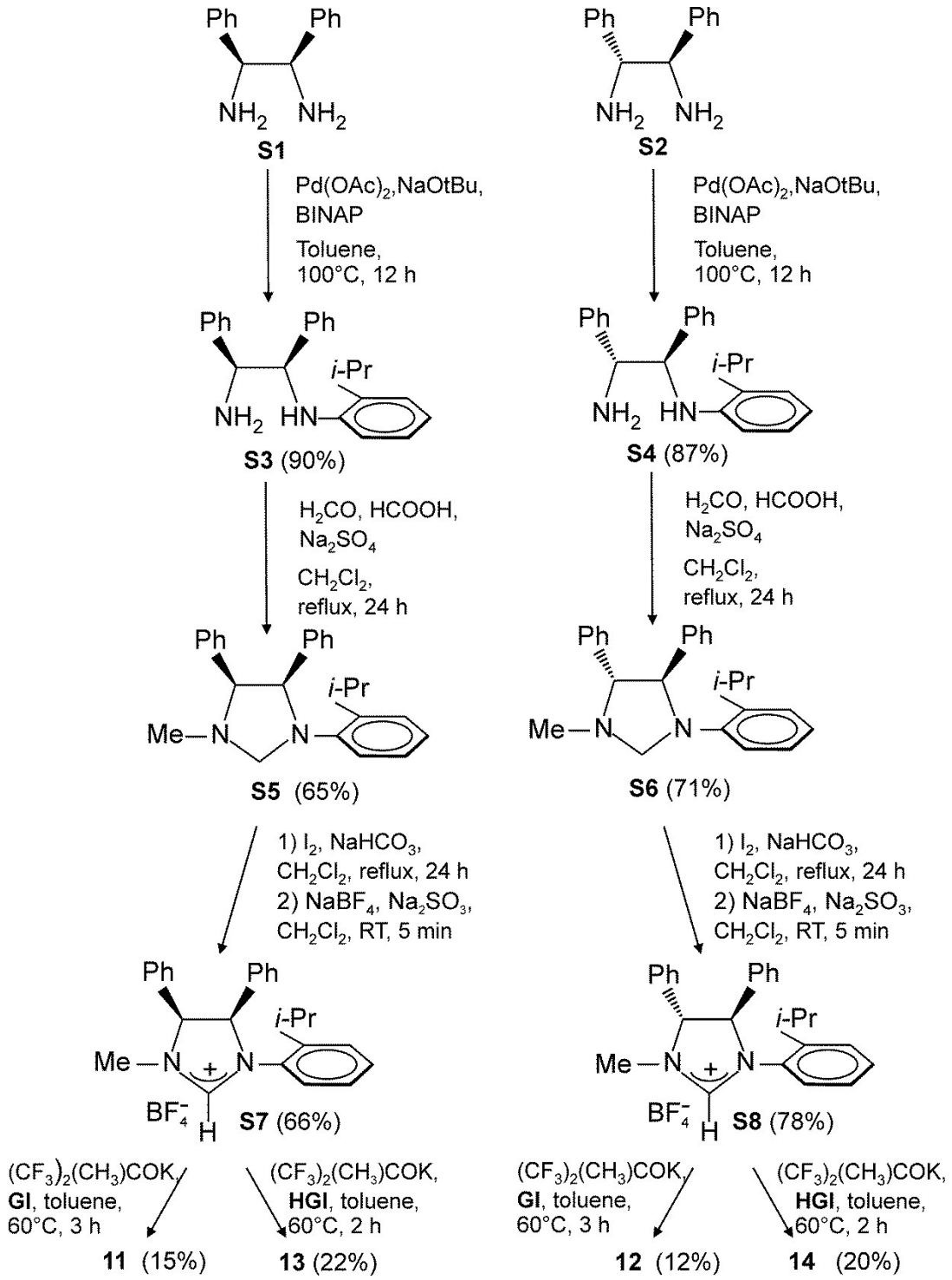
Experimental Procedure

1. General Information

All reactions involving organometallic compounds were performed under nitrogen using standard Schlenk and glove-box techniques. Solvents were dried and distilled before use. Deuterated solvents were degassed under a N_2 flow and stored over activated 4 Å molecular sieves. Reagents were purchased from Sigma Aldrich Company and TCI chemicals and used without further purifications. Substrates for metathesis reactions were prepared according to the literature. Flash column chromatography of organic molecules were performed using silica gel 60 (230-400 mesh) from Sigma Aldrich Company and flash column chromatography of complexes were performed, under nitrogen flow, using silica gel 60 (230-400 mesh) from TSI Cambrige. Analythical thin-layer chromatography (TLC) was performed using silica gel 60 F254 precoated plates with a fluorescent indicator. The visualization was performed using UV-light and $KMnO_4$ or I_2 stains. NMR spectra were recorded on Bruker Avance 250 spectrometer (250 MHz for ^1H; 62.5 MHz for ^{13}C), Bruker AM 300 spectrometer (300 MHz for ^1H; 75 MHz for ^{13}C), Bruker AVANCE 400 spectrometer (400 MHz for ^1H; 100 MHz for ^{13}C; 161.97 MHz for ^{31}P) and Bruker ASCEND 600 spectrometer (600 MHz for ^1H; 150 MHz for ^{13}C). NMR sample were prepared dissolving about 10 mg of compounds in 0.5 mL of deuterated solvent. ^1H and ^{13}C chemical shifts are listed in parts per million (ppm) downfield from TMS and are referenced from the solvent peaks or TMS. ^{31}P chemical shifts are referenced using H_3PO_4 as external standard. Spectra are reported as follows: chemical shift (δ ppm), multiplicity and integration. Multiplicity are abbreviated as follows: singlet (s), doublet (d), triplet (t), multiplet (m), broad (br), overlapped (o). Elemental analysis for C, H, N were recorded on a ThermoFinnigan Flash EA 1112 and were performed according to standard microanalytical procedures. ESI-MS were performed on a Waters Quattro Micro triple quadrupole mass spectrometer equipped with an electrospray ion source. Infrared spectra were recorded with a Bruker Vertex70 spectrometer. Enantiomeric excesses were determined by chiral GC (Supelco β-DEX 120, 30 m x 0.25 mm) or by chiral HPLC (JASCO MD-4015 Photo diode array detector, PU-4180 RMPLC Pump) and were compared to racemic samples. Optical activity was determined using a JASCO P2000 polarimeter.

2. Synthetic scheme for ruthenium complexes 11-14



Scheme S1

3. General procedure for the monoarilation of primary diamines

Under nitrogen atmosphere, in a round bottom flask, 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP) (0.2 eq.), palladium acetate (0.1 eq.), sodium *t*butoxide (2 eq.) and toluene (C = 0.05 M) were introduced. The orange solution was stirred for a few minutes. Then the diamine (1.5 eq.) and *o*-*i*propylphenylbromide (1 eq.) were added and the reaction mixture was heated to 100 °C overnight. After this time the purple mixture was cooled at room temperature, diluted with hexane, then filtered through a plug of silica gel and eluting with methanol. The crude yellow oil was purified by flash column chromatography on silica gel (hexane:ethyl acetate 9:1 to 6:4) to give the desired product.

Synthesis of *meso*-N^1-(2-*i*propylphenyl)-1,2-diphenylethylendiamine (**S3**)

Following the general procedure using *meso*-1,2-diphenylethylendiamine (**S1**) the desired product was obtained as a yellow oil (MW=330.5 g/mol, Yield=90%). ^{1}H NMR signals and ^{13}C NMR signals were congruent with those reported in the literature.[1]

Synthesis of (*R,R)*-N^1-(2-*i*propylphenyl)-1,2-diphenylethylendiamine (**S4**)

Following the general procedure using (*1R,2R)*-(+)-1,2-diphenylethylendiamine (**S2**) the desired product was obtained as a yellow oil (MW=330.5 g/mol, Yield=87%).

^{1}H NMR (CD_2Cl_2, 400 MHz): δ 7.33-7.23 (m, 10H), 7.08 (d, ^3J=7.5Hz, 1H), 6.80 (t, ^3J=7.9Hz, 1H), 6.55 (t, ^3J=7.3Hz, 1H), 6.14 (d, ^3J=8.2Hz, 1H), 5.45 (br s, 1H), 4.52 (br s, 1H), 4.39 (d, ^3J=4.2 Hz, 1H), 3.06 (m, 1H), 1.36 (d, ^3J=6.8Hz, 3H), 1.23 (d, ^3J=6.8Hz, 3H).

^{13}C NMR (CD_2Cl_2, 75 MHz): δ 144.2, 143.8, 142.4, 132.6, 128.9, 128.7, 127.7, 127.5, 127.3, 127.1, 126.6, 125.1, 116.9, 111.5, 63.5, 61.6, 27.8, 22.8, 22.4.

ESI+MS: *m/z* =331 (MH+). $[\alpha]_D^{20}$ = +36.2 (*c*=0.5, CH_2Cl_2).

4. General procedure for the alkylation of the monoarilated diamines

In a flask containing the amine (1 eq.), formaldehyde (5eq.), Na_2SO_4 (14.5 eq.), two drops of formic acid and CH_2Cl_2 (C=0.1M) were added. The reaction mixture was heated to reflux for 24 hours and then was filtered, concentrated and purified by flash column chromatography on silica gel (hexane:ethyl acetate 9:1).

[1] V. Paradiso, V. Bertolasi, F. Grisi, Organometallics, 2014, **33**, 5932.

Synthesis of 1-(2-^{i}propylphenyl)-3-methyl-4,5-diphenylimidazolidine (**S5**)

Following the general procedure using **S3** the desired product was obtained as a transparent oil (MW=356.5 g/mol, Yield=65%).

^{1}H NMR (CD_2Cl_2, 400 MHz): δ 7.22-6.93 (m, 14H), 5.02 (d, 1H, ^{2}J=8.5Hz), 4.65 (d, 1H, ^{3}J=4.1Hz), 4.06 (d, 1H, ^{2}J=8.5Hz), 3.82 (m, 1H), 3.55 (d, 1H, ^{3}J=4.1Hz), 2.32 (s, 3H), 1.29 (d, 3H, ^{3}J=7.0Hz), 1.04 (d, 3H, ^{3}J=7.0Hz).

^{13}C NMR (CD_2Cl_2, 75 MHz): δ 146.8, 145.2, 140.7, 139.3, 129.3, 129.1, 127.8, 127.5, 127.0, 126.9, 126.7, 125.1, 122.8, 80.3, 75.4, 70.9 , 38.7, 27.3, 24.9, 24.3.

ESI+MS: *m/z* =357 (MH+).

Synthesis of (*4R,5R*)-1-(2-^{i}propylphenyl)-3-methyl-4,5-diphenylimidazolidine (**S6)**

Following the general procedure using **S4** the desired product was obtained as a transparent oil (MW=356.5 g/mol, Yield=71%).

^{1}H NMR (CD_2Cl_2, 400 MHz): δ 7.19-6.95 (m, 14H), 4.61 (d, 1H, ^{2}J=8.5Hz), 4.35 (d, 1H, ^{3}J=4.5Hz), 4.29 (d, 1H, ^{3}J=4.5Hz), 3.59 (m, 1H), 3.41 (d, 1H, ^{2}J=8.5Hz), 2.24 (s, 3H), 1.29 (d, 3H, ^{3}J=6.8Hz), 1.06 (d, 3H, ^{3}J=6.8Hz).

^{13}C NMR (CD_2Cl_2, 100 MHz): δ 147.3, 144.2, 140.4, 139.0, 128.7, 128.6, 128.4, 128.1, 128.0, 127.7, 126.8, 126.5, 123.7, 120.4, 80.5, 79.8, 75.1, 38.6, 27.9, 24.6, 24.1.

ESI+MS: *m/z* =357 (MH+). $[\alpha]_D^{20}$ = +76.0 (*c*=0.5, CH_2Cl_2).

5. General procedure for the synthesis of the tetrafluoroborate salts

In a flask containing the cyclic amine (1eq.) were added $NaHCO_3$ (1.3 eq.), I_2 (1 eq.) and CH_2Cl_2 (C=0.1M). The purple reaction mixture was heated to reflux for 24 hours and then a saturated acqueous solution of Na_2SO_3 and $NaBF_4$ were added. When the organic phase became yellow it was extracted, concentrated, dried with $MgSO_4$ and purified by column chromatography (methylene chloride:methanol 40:1) to afford the product.

Synthesis of N^1-methyl-N^3-(2-^{i}propylphenyl)-4,5-dihydro-3H-imidazol-3-ium-tetrafluoroborate (**S7**)

Following the general procedure using **S5** the desired product was obtained as a white solid (MW=442.3 g/mol, Yield=66%).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.69 (s, 1H), 7.45-6.86 (m, 14H), 6.27 (d, 1H, ^{3}J=12.4Hz), 5.83 (d, 1H, ^{3}J=12.4Hz), 3.34 (s, 3H), 3.26 (m, 1H), 1.27 (d, 3H, ^{3}J=7.0Hz), 1.21 (d, 3H, ^{3}J=7.0Hz).

^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.1, 144.9, 131.8, 130.7, 130.5, 129.9, 129.1, 129.1, 129.0, 128.9, 128.3, 128.1, 127.5, 127.3, 127.1, 73.1, 70.8, 34.6, 28.3, 24.6, 24.2.

ESI+MS: *m/z* =356[(M+)-BF_4^-].

Synthesis of (*4R,5R*)-N^1-methyl-N^3-(2-*i*propylphenyl)-4,5-dihydro-3H-imidazol-3-ium-tetrafluoroborate (**S8**)

Following the general procedure using **S6** the desired product was obtained as a white solid (MW=442.3 g/mol, Yield=78%).

^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.53 (s, 1H), 7.51-6.68 (m, 14H), 5.25 (d, 1H, ^3J=9.6Hz), 5.08 (d, 1H, ^3J=9.6Hz), 3.24 (s, 3H), 2.92 (m, 1H), 1.10 (d, 3H, ^3J=6.9Hz), 0.98 (d, 3H, ^3J=6.9Hz).

^{13}C NMR (CD_2Cl_2, 100 MHz): δ 158.5, 146.3, 134.6, 134.2, 131.6, 130.9, 130.7, 130.4, 129.9, 128.9, 128.3, 127.8, 127.6, 127.4, 78.2, 75.1, 34.3, 28.6, 24.4, 24.1.

ESI+MS: *m/z* =356 [(M+)-BF_4^-]. $[\alpha]_D^{20}$ = +233.8 (*c*=0.5, CH_2Cl_2).

6. General procedure for the synthesis of catalysts 11 and 12

In glove box potassium hexafluoro*t*butoxide (1 eq.) and dry toluene (C = 0.1 M) were introduced in a vial followed by the tetrafluoroborate salt (1 eq.). After five minutes the Grubbs first generation catalyst (0.5 eq.) was added. The reaction mixture was stirred for three hours and purified by flash column chromatography on silica gel (hexane:diethyl ether 9:1).

Synthesis of [1-(2-*i*propylphenyl)-3-methyl-4,5-diphenyl-2-imidazolidinylidene] (dichloro)(benzilydene) (tricyclohexylphosphine)ruthenium (**11**)

The product is a mixture of two isomers (major:minor 1:0.4) and was obtained as a brown solid (MW=897.0 g/mol, Yield= 15%).

^{1}H NMR (C_6D_6, 400 MHz): δ 20.64 (minor isomer, d, $^3J_{HP}$=9.4Hz, 0.4H), 19.63 (major isomer, s, 1H, Ru=CHPh), 8.63-6.17 (overlapped signals of both isomers, 28H), (only signals of major isomer are shown below) 5.31 (d, ^3J=10.6Hz, 1H), 5.18 (d, ^3J=10.6Hz, 1H), 3.97 (s, 3H), 3.81-3.66 (o m, 2.6H), 2.68 (br m, 3H), 2.45 (br m, 1H), 2.34 (s, 1.2H), 2.08-0.88 (overlapped signals of both isomers, 50H).

^{13}C NMR (C_6D_6, 100 MHz): δ 294.8 (Ru=CHPh), 223.8 (*i*NCN, $^2J_{C\text{-}P}$=75.1Hz), 151.7, 146.5, 137.5, 134.6, 134.5, 134.1, 133.9, 132.9, 131.4, 126.0, 75.1, 72.9, 36.4, 33.2, 33.1, 32.0, 31.9, 30.5, 30.1, 29.7, 29.6, 28.2, 28.1, 27.2, 27.0, 26.8, 25.6. ^{31}P NMR (C_6D_6, 161.97 MHz): δ 34.8, 19.8.

Anal. Calcd for $C_{50}H_{65}Cl_2N_2PRu$ (897.0): C, 66.95, H, 7.30, N, 3.12. Found: C, 67.08, H, 7.49, H, 3.08.

Synthesis of (*4R,5R*)-[1-(2-*i*propylphenyl)-3-methyl-4,5-diphenyl-2-imidazolidinylidene] (dichloro)(benzilydene) (tricyclohexylphosphine)ruthenium (**12**)

The product is a mixture of two isomers (major:minor 1:0.5) and was obtained as a brown solid (MW=897.0 g/mol, Yield= 12%).

^{1}H NMR (C_6D_6, 400 MHz): δ 20.73 (minor isomer, d, $^3J_{HP}$=8.8Hz, 0.5H), 19.67 (major isomer, s, 1H, Ru=CHPh), 8.44-6.21 (overlapped signals of both isomers, 28H), (only signals of major isomer are shown below) 4.85 (d, ^3J=3.7Hz, 1H), 4.80 (d, ^3J=3.7Hz, 1H), 3.90 (s, 3H), 3.51 (m, 1H), 2.72 (m, 3H), 2.08-0.92 (overlapped signals of both isomers, 53H).

^{13}C NMR (C_6D_6, 100 MHz): δ 303.6 (Ru=CHPh), 295.4, 219.9 (*i*NCN, $^2J_{C\text{-}P}$=72.3Hz) 152.7, 151.5, 147.3, 146.7, 140.5, 140.2, 139.5, 138.3, 137.1, 79.1, 78.0, 77.7, 76.7, 36.8, 36.3, 33.3, 33.1, 32.0, 31.8, 30.5, 30.0, 29.8, 29.5, 29.7, 28.2, 28.1. ^{31}P NMR (C_6D_6, 161.97 MHz): δ 35.0, 20.8.

Anal. Calc. for $C_{50}H_{65}Cl_2N_2PRu$ (897.0): C, 66.95, H, 7.30, N, 3.12. Found: C, 66.98, H, 7.42, N, 3.18.

7. General procedure for the synthesis of complexes 13 and 14

In glove box potassium hexafluoro*t*butoxide (1 eq.) and dry toluene (C = 0.1 M) were introduced in a vial followed by the tetrafluoroborate salt (1 eq.). After five minutes the Hoveyda-Grubbs first generation catalyst (0.66 eq.) was added. The reaction mixture was stirred for two hours and purified by flash column chromatography on silica gel (hexane:diethyl ether 5:1).

Synthesis of [1-(2-*i*propylphenyl)-3-methyl-4,5-diphenyl-2-imidazolidinylidene] (dichloro)(2-ipropoxyphenylmethylene)ruthenium (**13**)

The product was obtained as a green solid (MW=674.7 g/mol, Yield= 22%).

^{1}H NMR (C_6D_6, 400 MHz): δ 16.22 (s, 1H, Ru=CH-*o*-O*i*PrC_6H_4), 7.51 (d, ^3J=7.9Hz, 1H), 7.13-6.97 (om, 5H), 6.89-6.86 (m, 3H), 6.74-6.64 (om, 7H), 6.50-6.47 (om, 2H), 5.49 (d, ^3J=10.33Hz, 1H), 4.80 (d, ^3J=10.33Hz, 1H), 4.72 (m, 2H), 4.06 (s, 3H), 3.52 (m, 1H), 1.77 (m, 6H), 1.24 (m, 6H).

^{13}C NMR (C_6D_6, 100 MHz): δ 289.4 (Ru=CH-*o*-O*i*PrC_6H_4), 214.9, 153.6, 149.0, 144.5, 139.8, 134.5, 134.2, 133.6, 122.8, 113.5, 75.6, 72.7, 37.5, 30.6, 28.6, 24.8, 24.7, 22.6, 22.5. Anal. Calc. for $C_{35}H_{38}Cl_2N_2ORu$ (675.7): C, 62.31, H, 5.68, N, 4.15. Found: C, 62.49, H, 5.96, N, 4.07.

Synthesis of (*4R,5R*)-[1-(2-*i*propylphenyl)-3-methyl-4,5-diphenyl-2-imidazolidinylidene] (dichloro)(2-ipropoxyphenylmethylene)ruthenium (**14**)

The product was obtained as a green solid (MW=674.7 g/mol, Yield= 20%).

^{1}H NMR (C_6D_6, 400 MHz): δ 16.16 (s, 1H, Ru=CH-*o*-O^{i}PrC_6H_4), 7.52-6.92 (om, 15H), 6.68 (m, 1H), 6.58 (br s, 1H), 6.47 (d, ^3J=8.0Hz, 1H), 4.79-4.70 (om, 4H), 3.99 (s, 3H), 3.48 (br m, 1H), 1.75 (m, 6H), 1.25 (br d, 3H) 1.01 (d, ^3J=6.8Hz, 3H).^{13}C NMR (C_6D_6, 100 MHz): δ 288.5 (Ru=CH-*o*-O^{i}PrC_6H_4), 212.2, 153.8, 149.0, 144.6, 144.4, 140.8, 140.4, 139.8, 133.4, 130.1, 129.9, 129.6, 129.5, 127.7, 127.6, 127.5, 127.0, 123.0, 122.7, 113.7, 82.7, 80.5, 76.8, 76.2, 75.8, 37.8, 37.6, 32.9, 31.4, 30.8, 30.4, 28.4, 28.1, 26.8, 25.2.

Anal. Calc. for $C_{35}H_{38}Cl_2N_2ORu$ (674.7): C, 62.31, H, 5.68, N, 4.15. Found: C, 62,45, H, 5,86, N, 4,10.

8. General procedure for the synthesis of rhodium complexes 39 e 40

In glove box the tetrafluoroborate salt (1 eq.), potassium bis(trimethylsilyl)amide (KHMDS, 1 eq.) and dry toluene (0.02M) were introduced in a vial. After few minutes, a solution of $[RhCl(COD)]_2$ (2 eq.) in dry toluene was added. After two hours at room temperature the mixture was concentrated and purified by column chromatography on silica gel (methylene chloride:ethanol 95:5).

Synthesis of 1-(2-*i*propylphenyl)-3-cyclohexyl-4,5-diphenyl-2-imidazolidinylidene] chloro(η^4-1,5-cyclooctadiene)rhodium (**39**)

The product was obtained as a yellow solid (MW=669.1 g/mol, Yield= 84%) as a mixture of two isomers (major:minor 1:0.2)

^{1}H NMR (CD_2Cl_2, 600 MHz): δ 8.71 (major isomer, d, 1H,^3J=7.6Hz), 8.31 (minor isomer, d, 0.2H ^3J=7.6Hz), (only major isomer signals are shown below) 7.33-7.29 (o m, 3H), 7.23 (d, ^3J=7.4Hz, 2H), 7.07 (o m, 5H), 6.98 (br s, 4H), 5.66 (m, 1H), 5.65 (d, ^3J=11.0Hz, 1H), 5.35 (d, ^3J=11.0Hz, 1H), 4.93 (br s, 2H), 3.50 (br s, 1H), 3.08 (m, 1H), 2.82 (br s, 1H), 2.40-2.38 (o m, 2H), 2.25 (br s, 1H), 2.08 (br d, 1H), 1.93-1.82 (o m, 4H), 1.70-1.64 (o m, 4H), 1.56-1.54 (o m, 2H), 1.45-1.32 (o m, 2H), 1.29 (d, ^3J=6.6Hz, 3H), 1.09 (d, ^3J=6.6Hz, 3H), 0.94 (o m, 1H), 0.84 (o m, 1H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 216.9 (J_{Rh-C}=48.1Hz), 144.2, 138.3, 135.9, 134.4, 133.2, 128.1, 128.0, 127.9, 127.7, 126.3, 126.0, 98.0 (J_{Rh-C}=6.6Hz), 97.8 (J_{Ru-C}=6.3Hz), 74.3, 68.8 (J_{Rh-C}=14.2Hz), 68.1, 66.5 (J_{Ru-C}=13.3Hz), 62.9, 33.6, 33.4, 33.3, 33.2, 31.9, 28.9, 28.8, 28.6, 27.0, 26.9, 25.9, 24.7, 24.6.

Anal. Calc. for $C_{38}H_{46}ClN_2Rh$ (669.1): C, 68.21, H, 6.93, N, 4.19. Found: 67.87, H, 7.05, N, 4.16.

Synthesis of (*4R*,*5R*)1-(2-*i*propylphenyl)-3-cyclohexyl-4,5-diphenyl-2-imidazolidinylidene] chloro(η^4-1,5-cyclooctadiene)rhodium (**40**)

The product was obtained as a yellow solid (MW=669.1 g/mol, Yield= 79%). ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 8.48 (d, 1H,^{3} J=7.8Hz), 7.48-7.18 (o m, 14H), 5.61 (br t, 1H), 4.96 (br s, 1H), 4.86 (br m, 1H), 4.76 (dd, ^{3} J=15.4Hz, 2H), 4.29 (br s, 1H), 3.82 (br m, 1H), 2.99 (m, 1H), 2.96 (br s, 1H), 2.54 (o m, 1H), 2.45 (m, 1H), 2.28 (m, 1H), 2.01 (m, 1H), 1.88-1.56 (o m, 7H), 1.48-1.36 (o m, 3H), 1.27 (d, ^3J=7.0Hz, 3H), 1.03 (d, ^3J=6.7Hz, 3H), 0.98 (o m, 1H), 0.80 (o m, 1H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 214.9 (J_{Rh-C}=47.2Hz), 145.1, 142.5, 139.6, 137.5, 133.7, 129.5, 129.4, 129.3, 129.0, 128.9, 128.6, 128.3, 127.3, 126.3, 126.0, 125.9, 125.6, 98.9 (J_{Rh-C}=6.0Hz), 97.9 (J_{Rh-C}=6.0Hz), 79.0, 78.9, 78.7, 70.4, 68.2 (J_{Rh-C}=14.7Hz), 67.3 (J_{Rh-C}=14.1Hz), 61.0, 34.7, 34.3, 31.6, 29.2, 28.3, 27.7, 26.9.

Anal. Calc. for $C_{38}H_{46}ClN_2Rh$ (669.1): C, 68.21, H, 6.93, N, 4.19. Found: 68.32, H, 7.11, N, 4.10.

8. General procedure for the synthesis of complexes 41 and 42

Carbon monoxide was bubbled into a solution of **39** or **40** in dry methylene chloride (C=0.013M) for 1 hour at room temperature. The light yellow solution was concentrated and the solid was washed three times with the minimum amount of cold pentane.

Synthesis of 1-(2-*i*propylphenyl)-3-cyclohexyl-4,5-diphenyl-2-imidazolidinylidene] dicarbonylchloro rhodium (**41**)

The product was obtained as a yellow solid (MW=617.0 g/mol, Yield= 73%) and as a mixture of three isomers (major:minor1:minor2 1:0.5:0.3).

^{1}H NMR (CD_2Cl_2, 600 MHz):), (only major isomer signals are shown below) δ 7.87 (d, 1H, ^3J=7.9Hz), 7.23-6.71 (o m, 14H), 5.78 (d, ^3J=10.8, 1H), 5.40 (d, ^3J=10.8, 1H), 4.56 (brt, 1H), 3.07 (m, 1H), 2.11-1.02 (o m, 17H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 206.3 (J_{Rh-C}=38.9Hz), 186.8 (J_{Rh-C}=53.4Hz), 183.5 (J_{Rh-C}=75.5Hz), 148.2, 145.5, 137.2, 135.7, 134.1, 133.1, 129.9, 129.4, 128.9, 128.4, 128.2, 128.1, 127.9, 126.8, 126.2, 74.7, 68.3, 61.9, 34.3, 33.0, 28.9, 27.7, 26.4, 26.2, 25.7, 25.6, 24.9.

IR (KBr): νCO 2080 (trans) and 1999 cm^{-1} (cis).

Anal. Calc. for $C_{32}H_{34}ClN_2O_2Rh$ (617.0): C, 62.29, H, 5.55, N, 4.54. Found: C, 62.35, H, 5.87, N, 4.36.

Synthesis of (*4R,5R*)-1-(2-*i*propylphenyl)-3-cyclohexyl-4,5-diphenyl-2-imidazolidinylidene] dicarbonylchloro rhodium (**42**)

The product was obtained as a yellow solid (MW=617.0 g/mol, Yield= 64%) and as a mixture of two isomers (major:minor 1:0.3).

^{1}H NMR (CD_2Cl_2, 600 MHz): (only major isomer signals are shown below) 7.45-7.03 (o m, 14H), 5.01 (br d, 1H), 4.93 (br t, 1H), 4.76 (br d, 1H), 3.15 (m, 1H), 2.97 (m, 1H), 2.36 (o m, 1H), (2.32 br s, 2H), 1.85-1.03 (o m, 11H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 203.2 (J_{Rh-C}=40.4Hz), 186.7 (J_{Rh-C}=54.3Hz), 183.7 (J_{Rh-C}=73.9Hz), 146.1, 141.4, 138.9, 136.5, 133.9, 129.7, 129.6, 129.4, 129.3, 129.2, 129.0, 127.5, 126.7, 126.4, 126.1, 79.0, 71.8, 61.1, 32.0, 31.7, 30.1, 27.8, 26.3.

IR (KBr): νCO 2075 (trans) and 1992 cm^{-1} (cis).

Anal. Calc. for $C_{32}H_{34}ClN_2O_2Rh$ (617.0): C, 62.29, H, 5.55, N, 4.54. Found: C, 62.44, H, 5.39, N, 4.46.

Catalysis

1. RCM of Diethyldiallyl malonate (**15**) (**Figure 1**)

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (1%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR probe. After that, 19.3 μL (0.080 mmol) of **15** were injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **17** by integrating the methylene protons in the starting material, δ 2.61 (dt) in CD_2Cl_2 or 2.84 (dt) in C_6D_6, and those in the product, δ 2.98 (s) in CD_2Cl_2 or 3.14 (s) in C_6D_6.

2. RCM of Diethyldiallylmethallylmalonate (**19**) (**Figure 2**)

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (1%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR probe. After that, 20.5 μL (0.080 mmol) of **19** were injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **21** by integrating the methylene protons in the starting material, δ 2.67 (s), 2.64 (dt) in CD_2Cl_2 or 2.96 (d), 2.93 (s) in C_6D_6, and those in the product, δ 2.93 (s), 2.88 (m) in CD_2Cl_2 or 3.18 (m), 3.07 (s) in C_6D_6.

3. RCM of Diethyldimethallylmalonate (**23**) (**Figure 3**)

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (5%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR Probe. After that, 21.6 μL (0.080 mmol) of **23** was injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **25** by integrating the methylene protons in the starting material, δ 2.71 (s) in CD_2Cl_2 or 2.98 (s) in C_6D_6, and those in the product, δ 2.89 (s) in CD_2Cl_2 or 3.15 (s) in C_6D_6.

4. RCM of N-Tosyl diallylamine (**16**) (**Figure 1**)

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (1%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR probe. After that, 17.2 μL (0.080 mmol) of **16** was injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **18** by integrating the methylene

protons in the starting material, δ 3.70 (dt) in CD_2Cl_2 or 3.71 (d) in C_6D_6, and those in the product, δ 4.00 (s) in CD_2Cl_2 or 3.90 (s) in C_6D_6.

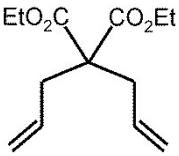
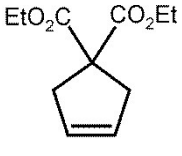
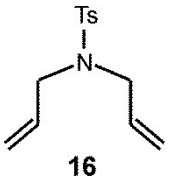
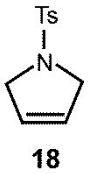
5. RCM of N-tosyl allylmethallylamine (**20**) (**Figure 2**).

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (1%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR Probe. After that, 19.4 μL (0.080 mmol) of **20** was injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **22** by integrating the methylene protons in the starting material, δ 3.63 (s), 2.64 (dt) in CD_2Cl_2 or 3.70 (d), 3.67 (s) in C_6D_6, and those in the product, δ 3.91 (s), 2.88 (m) in CD_2Cl_2 or 3.96 (m), 3.82 (s) in C_6D_6.

6. RCM of N-tosyl dimethallylamine (**24**) (**Figure 3**).

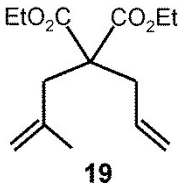
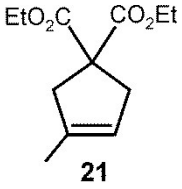
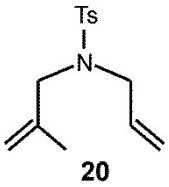
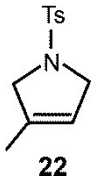
An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (5%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR Probe. After that, 20.2 μL (0.080 mmol) of **24** was injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **26** by integrating the methylene protons in the starting material, δ 3.61 (s) in CD_2Cl_2 or 3.69 (s) in C_6D_6, and those in the product, δ 3.87 (s) in CD_2Cl_2 or 3.90 (s) in C_6D_6.

Table S1. RCM of **15** and **16**

Entry[a]	Substrate	Product	Catalyst (mol%)	Time (min)	Yield[b] (%)
1	 **15**	 **17**	**7** (1)	60	52
2			**8** (1)	20	>97
3			**11** (1)	60	78
4			**12** (1)	22	>97
5			**GIItol** (1)	35	97
6			**9** (1)	20	>99
7			**10** (1)	4	>99
8			**13** (1)	5	>99
9			**14** (1)	3	>99
10			**HGIItol** (1)	4	>99
11	 **16**	 **18**	**7** (1)	32	60
12			**8** (1)	94	35
13			**11** (1)	65	60
14			**12** (1)	94	35
15			**GIItol** (1)	>99	27
16			**9** (1)	93	60
17			**10** (1)	>99	2
18			**13** (1)	>99	4
19			**14** (1)	>99	3
20			**HGIItol** (0.1)	>99	6

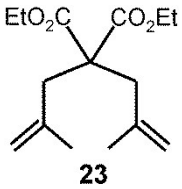
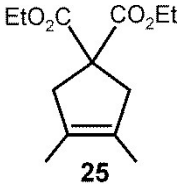
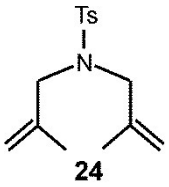
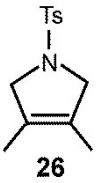
[a]Runs with catalysts **7**, **8**, **11**, **12** and **GIItol** were carried out in CD_2Cl_2 at 30°C; while runs with catalyst **9**, **10**, **13**, **14** and **HGIItol** were performed in C_6D_6 at 60°C. [b]Yields based on NMR analysis.

Table S2. RCM of **19** and **20**

Entry[a]	Substrate	Product	Catalyst (mol%)	Time (min)	Yield[b] (%)
1	 **19**	 **21**	**7** (1)	60	72
2			**8** (1)	60	91
3			**11** (1)	60	45
4			**12** (1)	60	84
5			**GIItol** (1)	60	79
6			**9** (1)	60	94
7			**10** (1)	8	>99
8			**13** (1)	11	99
9			**14** (1)	9	>99
10			**HGIItol** (1)	8	>99
11	 **20**	 **22**	**7** (1)	60	84
12			**8** (1)	24	98
13			**11** (1)	60	66
14			**12** (1)	30	96
15			**GIItol** (1)	45	99
16			**9** (1)	14	99
17			**10** (1)	4	>99
18			**13** (1)	7	>99
19			**14** (1)	5	>99
20			**HGIItol** (0.1)	11	>99

[a]Runs with catalysts **7**, **8**, **11**, **12** and **GIItol** were carried out in CD_2Cl_2 at 30°C; while runs with catalyst **9**, **10**, **13**, **14** and **HGIItol** were performed in C_6D_6 at 60°C. [b]Yields based on NMR analysis.

Table S3. RCM of **23** and **24**

Entry[a]	Substrate	Product	Catalyst (mol%)	Time (min)	Yield[b] (%)
1	 **23**	 **25**	**7** (5)	60	22
2			**8** (5)	60	57
3			**11** (5)	60	9
4			**12** (5)	60	30
5			**GIItol** (5)	60	70
6			**9** (5)	60	45
7			**10** (5)	60	>97
8			**13** (5)	60	37
9			**14** (5)	60	34
10			**HGIItol** (5)	60	97
11	 **24**	 **26**	**7** (5)	60	33
12			**8** (5)	60	64
13			**11** (5)	60	29
14			**12** (5)	60	31
15			**GIItol** (5)	60	92
16			**9** (5)	60	77
17			**10** (5)	60	97
18			**13** (5)	60	76
19			**14** (5)	60	77
20			**HGIItol** (1)	23	>99

[a]Runs with catalysts **7**, **8**, **11**, **12** and **GIItol** were carried out in CD_2Cl_2 at 30°C; while runs with catalyst **9**, **10**, **13**, **14** and **HGIItol** were performed in C_6D_6 at 60°C. [b]Yields based on NMR analysis.

7. ROMP of 1,5-cyclooctadiene (**27**) (**Figure 6**)

An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (0.1%mol) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR Probe. After that, 49.1 μL (0.40 mmol) of **35** was injected and the reaction was monitored as a function of time, determining the conversion by integrating the protons in the monomer at δ =2.36 (s) in CD_2Cl_2 or 2.22 (s) in C_6D_6, and those in the polymer, δ=2.09 (s) and 2.04 (s) in CD_2Cl_2 or 2.14 (s) and 2.11 (s) in C_6D_6. Those signals of the polymer are also used to determine the *E/Z* ratio. When the conversion is complete, the polymerization is quenched with a solution of ethylvinyl ether in methanol.

8. CM of Allylbenzene (**28**) and cis-(1,4)-Diacetoxy-2-butene (**29**) (**Scheme 1**)

In an oven-dried 4-ml vial (equipped with a magnetic stirrer) 66 μL (0.5 mmol) of **28** and 160 μL (1.0 mmol) of **29** were added simultaneously to a 2.5 mL solution of the catalyst (0.0013 mmol) in methylene chloride. The reaction mixture was refluxed under nitrogen overnight. The reaction mixture was purified on column chromatography eluting with hexane:ethyl acetate 9:1. The cross metathesis product **30** was obtained as a transparent oil and *E/Z* ratio was determined by NMR spectroscopy.

9. ARCM of **31** and **32** without additive (**Scheme 2**, **Table 3**)

In glove box, **31** or **32** (0.11 mmol, 1 eq.) was added to 2 mL of CD_2Cl_2 solution of the catalyst (0.00275 mmol, 0.025 eq.). The flask was stirred a 40°C for two hours for substrate **31** and for three hours for the alkene **32**. Yields were determined via NMR spectroscopy of the crude product. The reaction mixture was filtered on neutral alumina and injected into GC system without further purifications.

10. ARCM of **31** and **32** with NaI (**Scheme 2**, **Table 3**)

Under nitrogen atmosphere, to a 1 mL THF-d8 solution of the catalyst (0.0022 mmol, 0.04 eq.), NaI (0.055 mmol, 1 eq.) was added. The reaction mixture was stirred at room temperature for one hour. After that, **31** or **32** (0.055 mmol, 1 eq.) was added. Then, the flask was stirred a 40°C for for two hours for substrate **31** and for three hours for the alkene **32**. Yields were determined via NMR spectroscopy of the crude product. The reaction mixture was filtered on neutral alumina and injected into GC system without further purifications.

11. AROCM of **35** with styrene (**Scheme 3**, **Table 4**)

In glove box, **35** (0.43 mol, 1 eq.) and styrene (4.3 mmol, 10 eq.) was simultaneously added to 7.5 mL of CD_2Cl_2 solution of the catalyst (0.013 mmol, 0.03 eq.). The flask was stirred at room temperature for two hours for the for Grubbs second generation catalysts and three hours for Hoveyda-Grubbs second generation catalysts. The reaction mixture was then concentrated and purified via column chromatography (petroleum ether:diethyl ether 1:1) to afford the product as a transparent oil. About 1mg of the product was dissolved in 1 mL of 2-propanol (HPLC grade purity), filtered using a syringe filter and then injected into the HPLC system.

NMR spectra

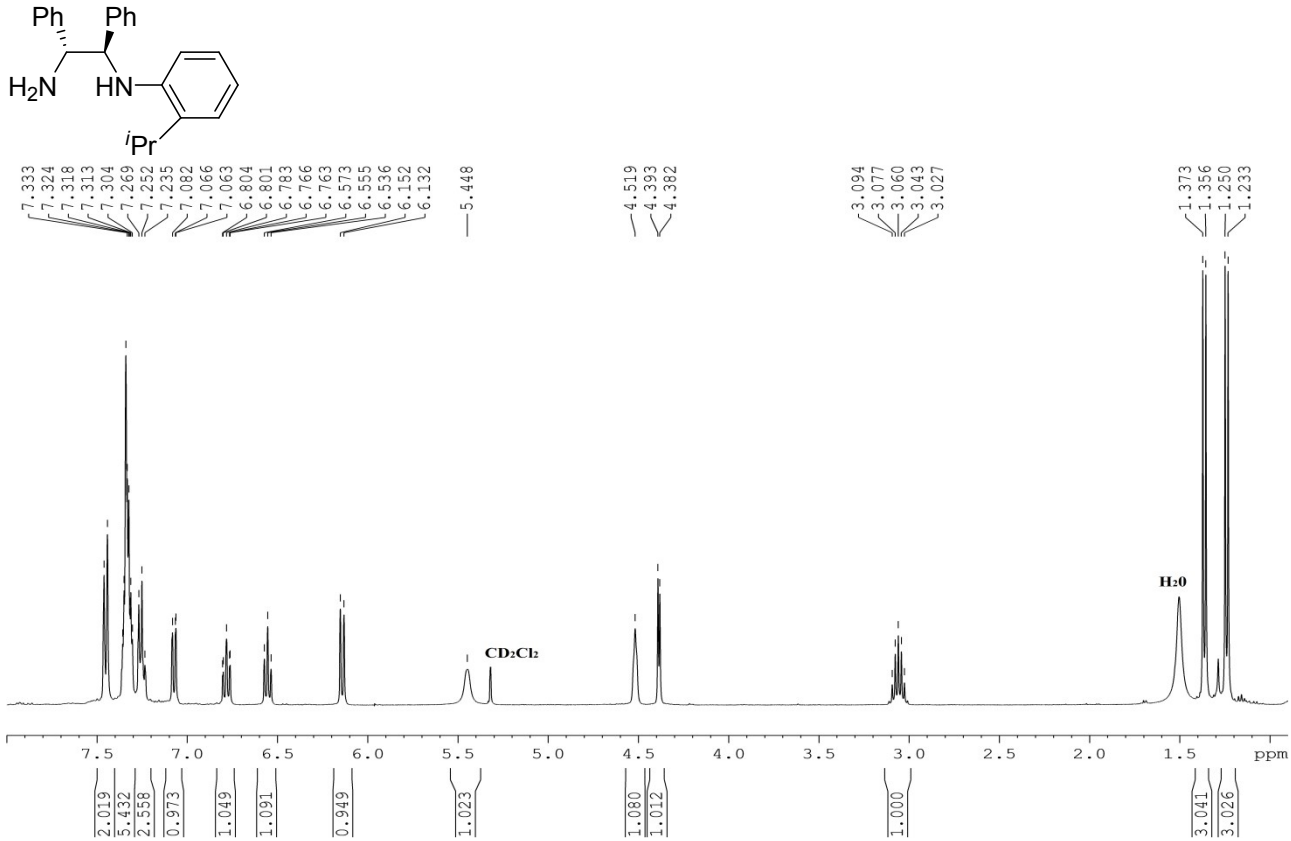


Figure S1: ^{1}H NMR spectrum of **S4** (CD_2Cl_2, 400MHz**)**

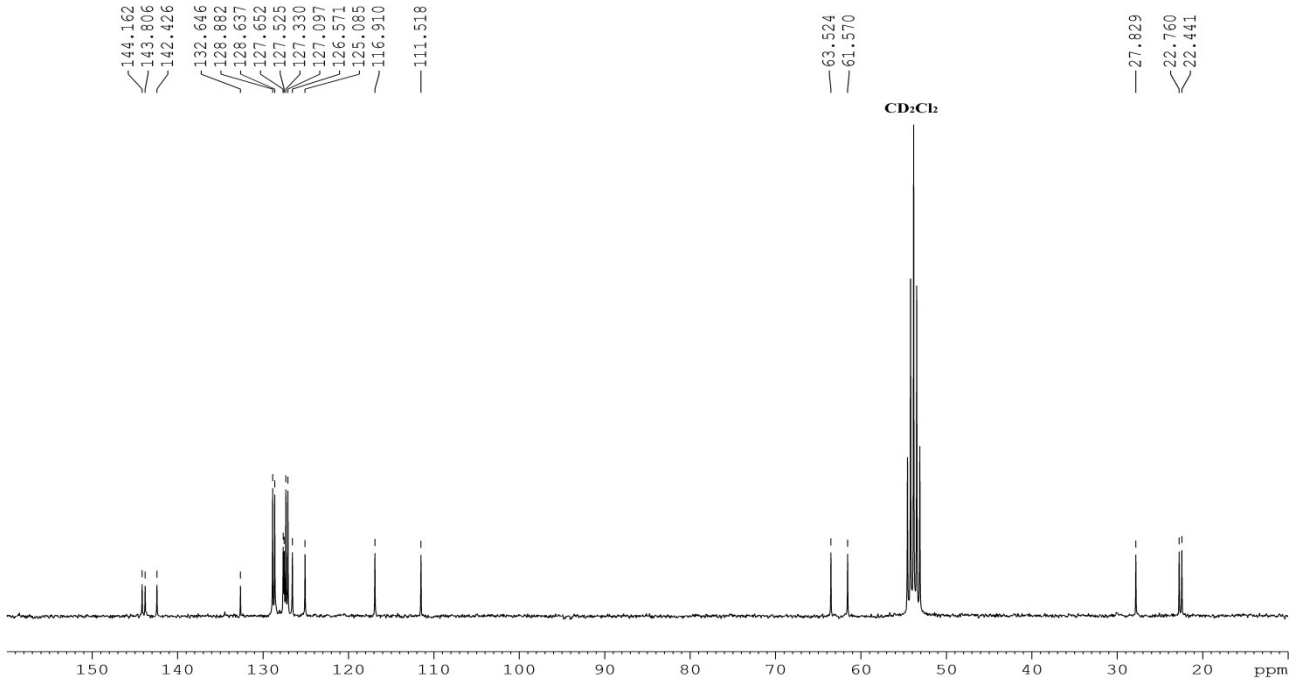


Figure S2: ^{13}C NMR {^{1}H} spectrum of **S4** (CD_2Cl_2, 75MHz)

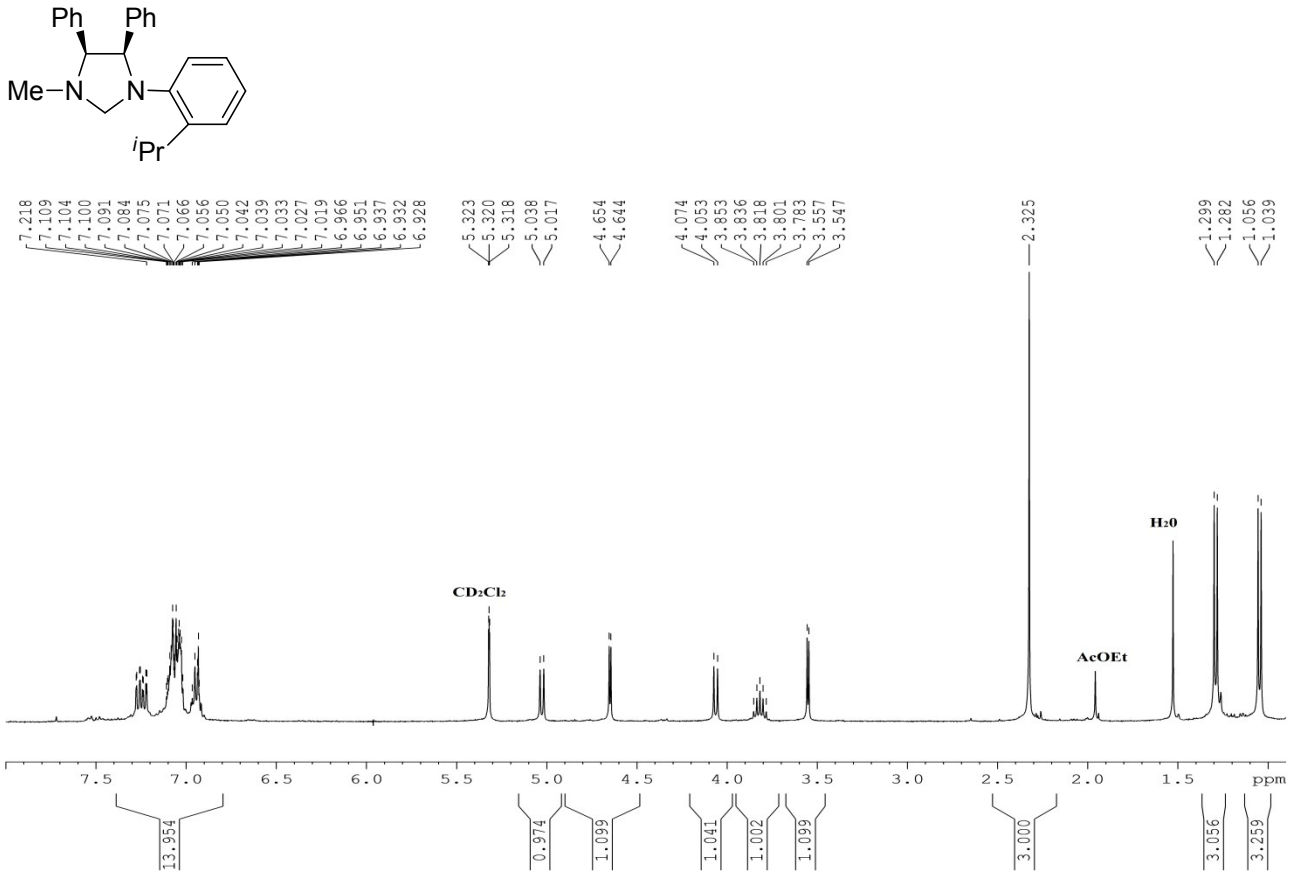


Figure S3: ^{1}H NMR spectrum of **S5** (CD_2Cl_2, 400MHz**)**

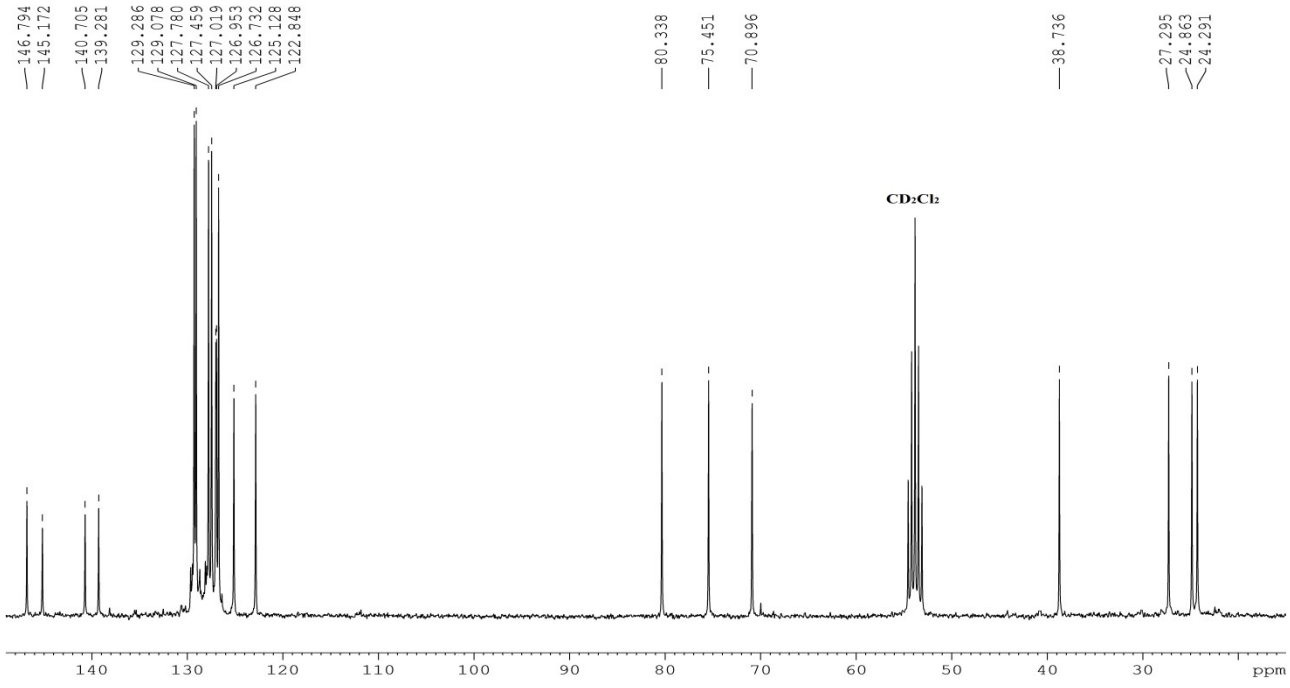


Figure S4: ^{13}CNMR {^{1}H}of **S5** (CD_2Cl_2, 75MHz)

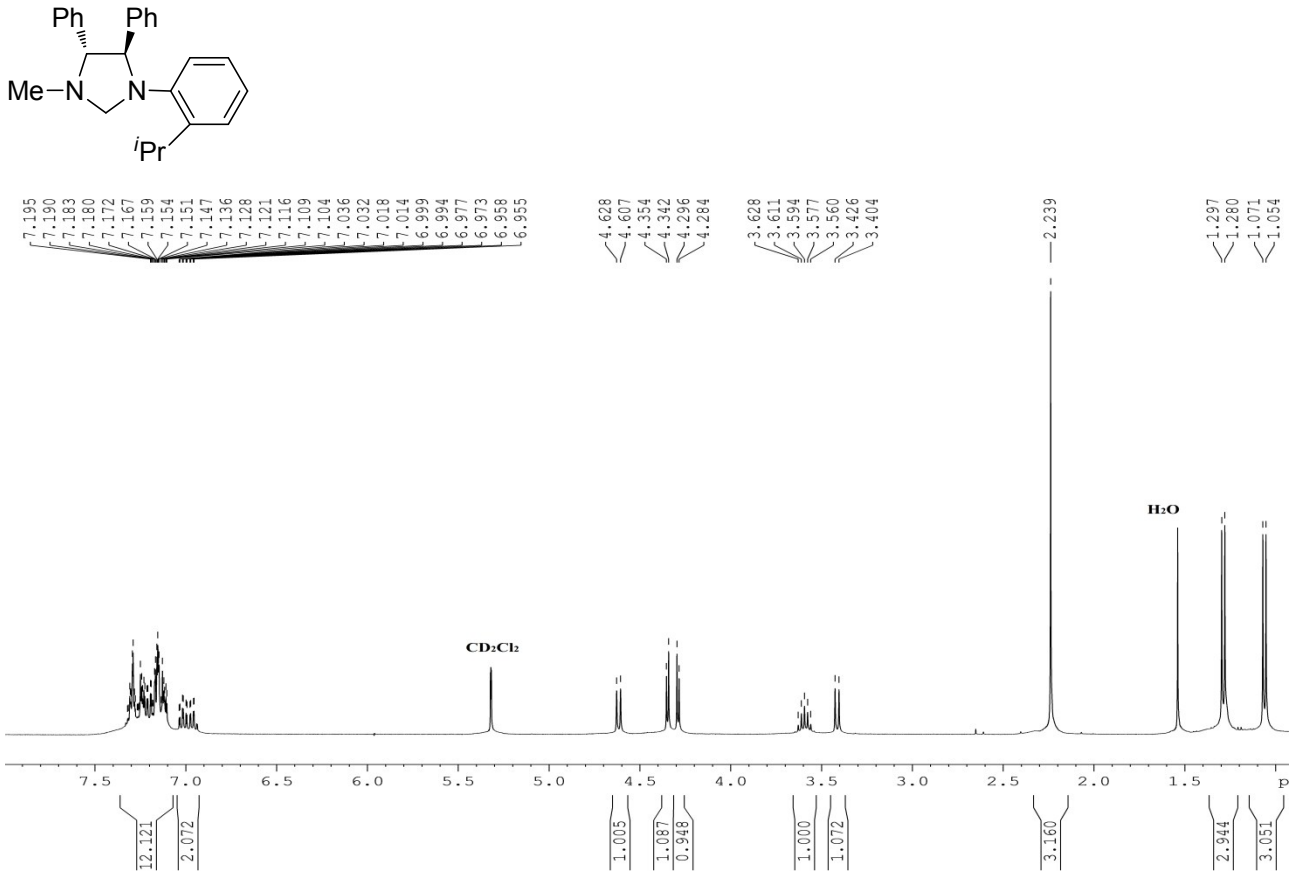


Figure S5: [1]HNMR spectrum of **S6** (CD_2Cl_2, 400MHz**)**

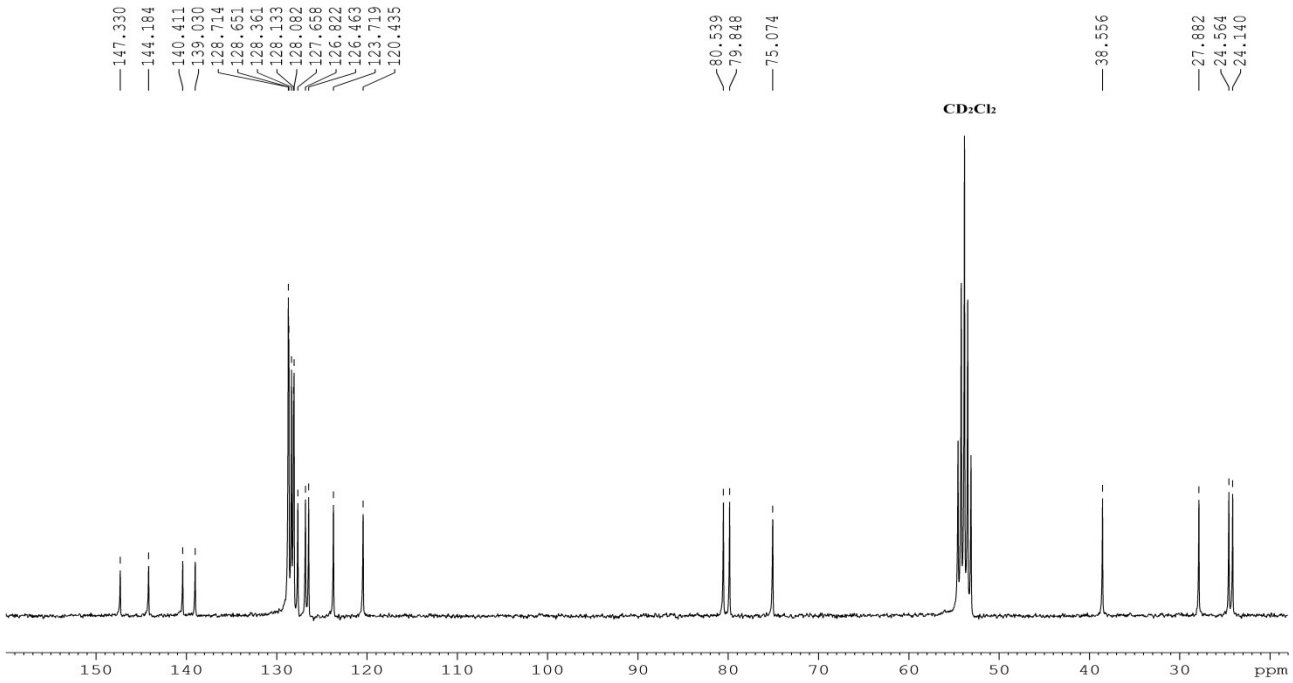


Figure S6: [13]CNMR {[1]H} of **S6** (CD_2Cl_2, 100MHz)

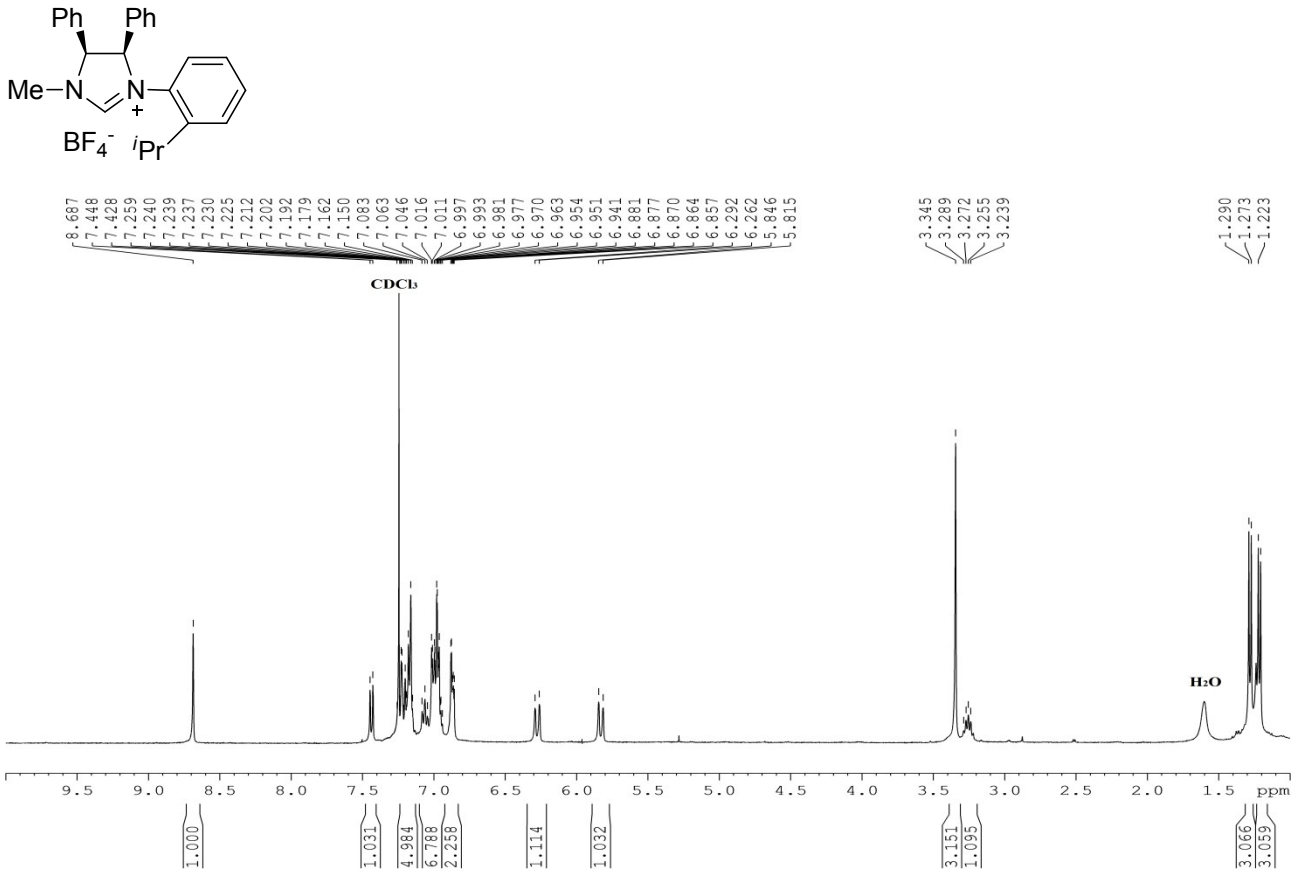


Figure S7: ^{1}H NMR spectrum of **S7** ($CDCl_3$, 400MHz**)**

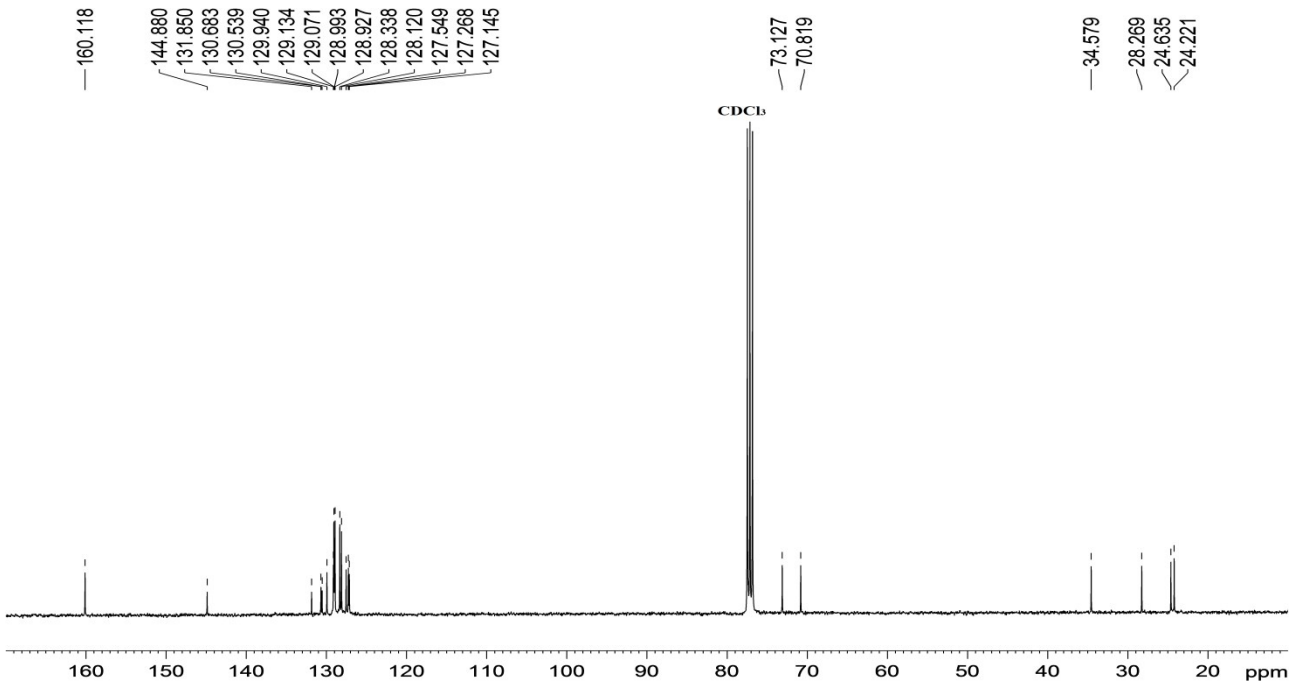


Figure S8: ^{13}C NMR $\{^{1}H\}$ spectrum of **S7** ($CDCl_3$, 100MHz)

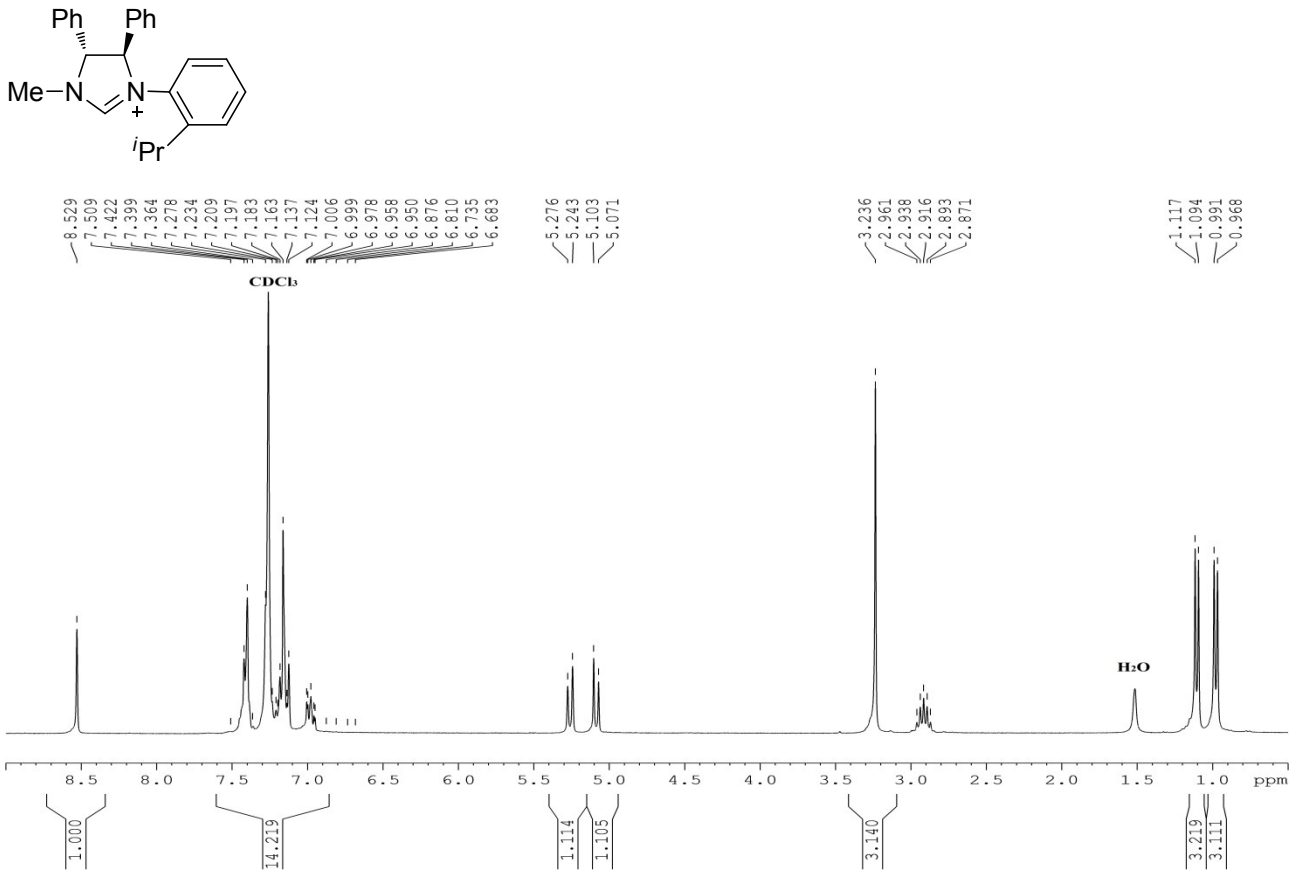


Figure S9: ^{1}H NMR spectrum of **S8** ($CDCl_3$, 400MHz**)**

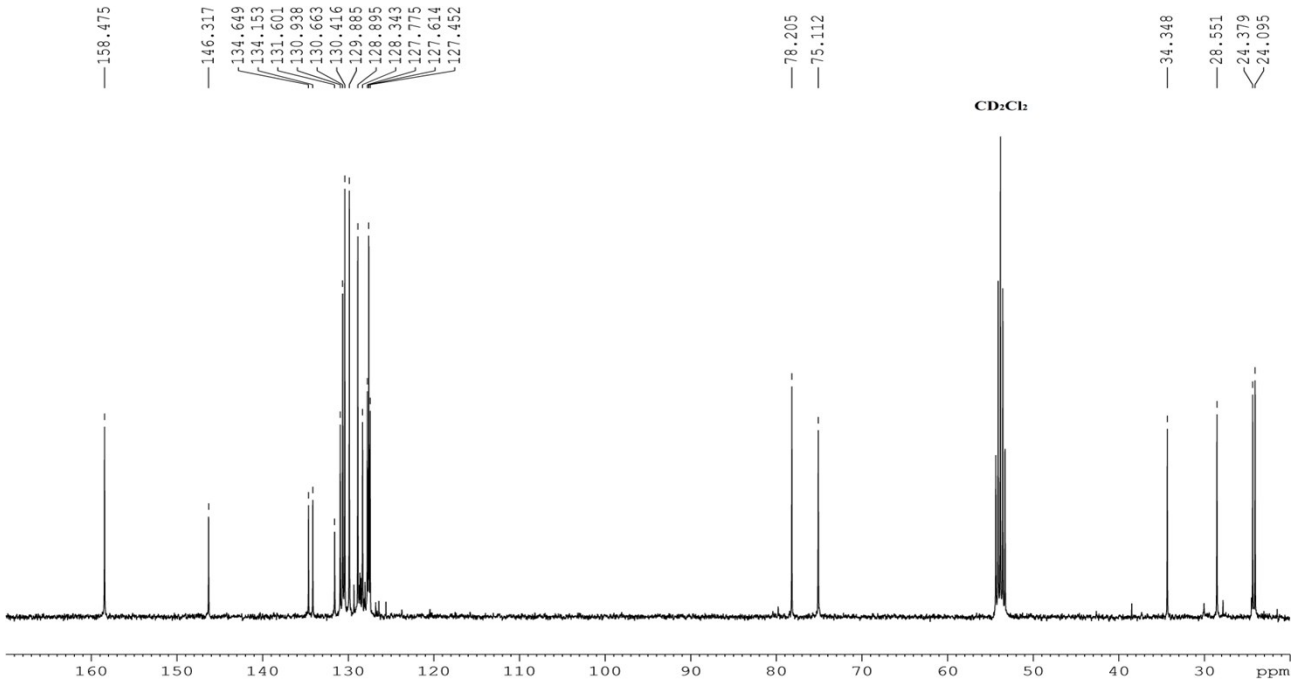


Figure S10: ^{13}C NMR $\{^{1}H\}$ spectrum of **S8** (CD_2Cl_2, 100MHz)

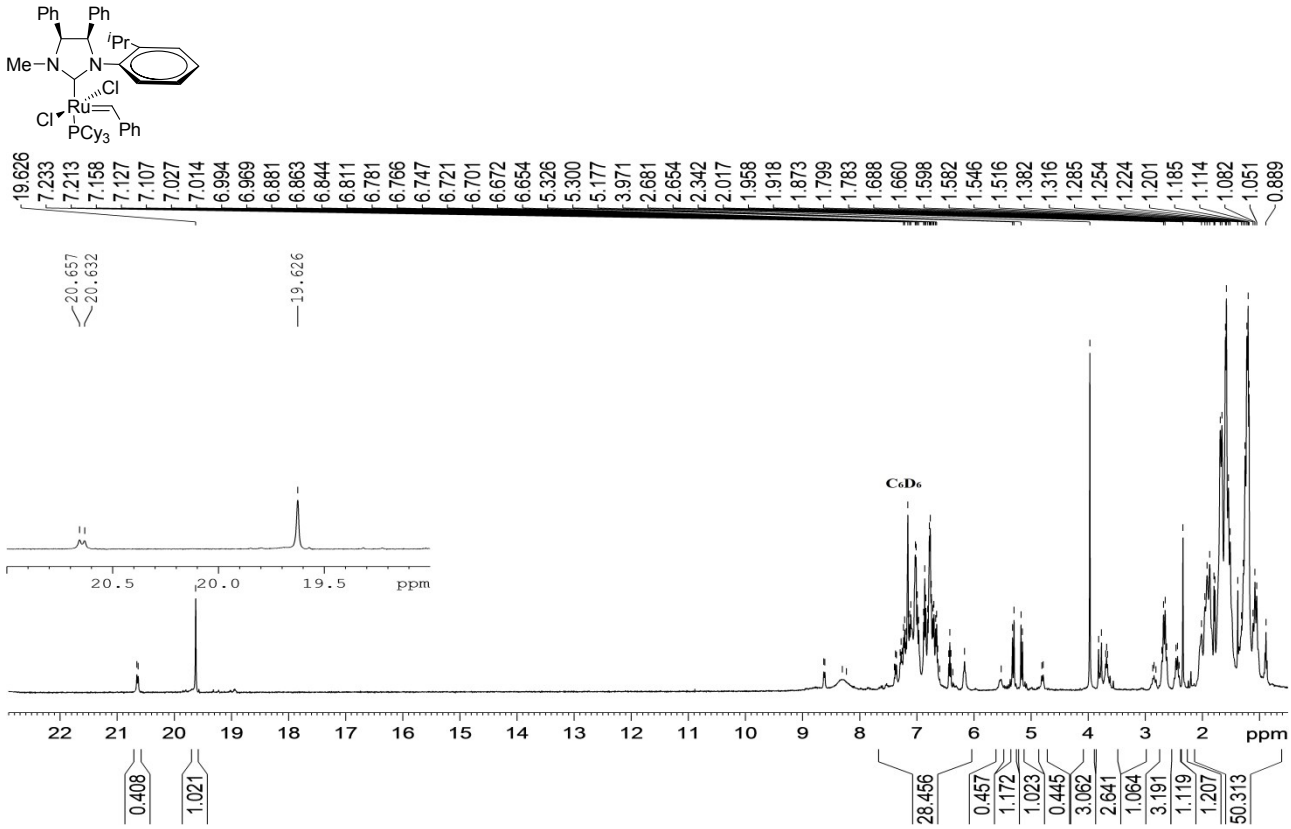


Figure S11: ^{1}H NMR spectrum of **11** (C_6D_6, 400MHz**)**

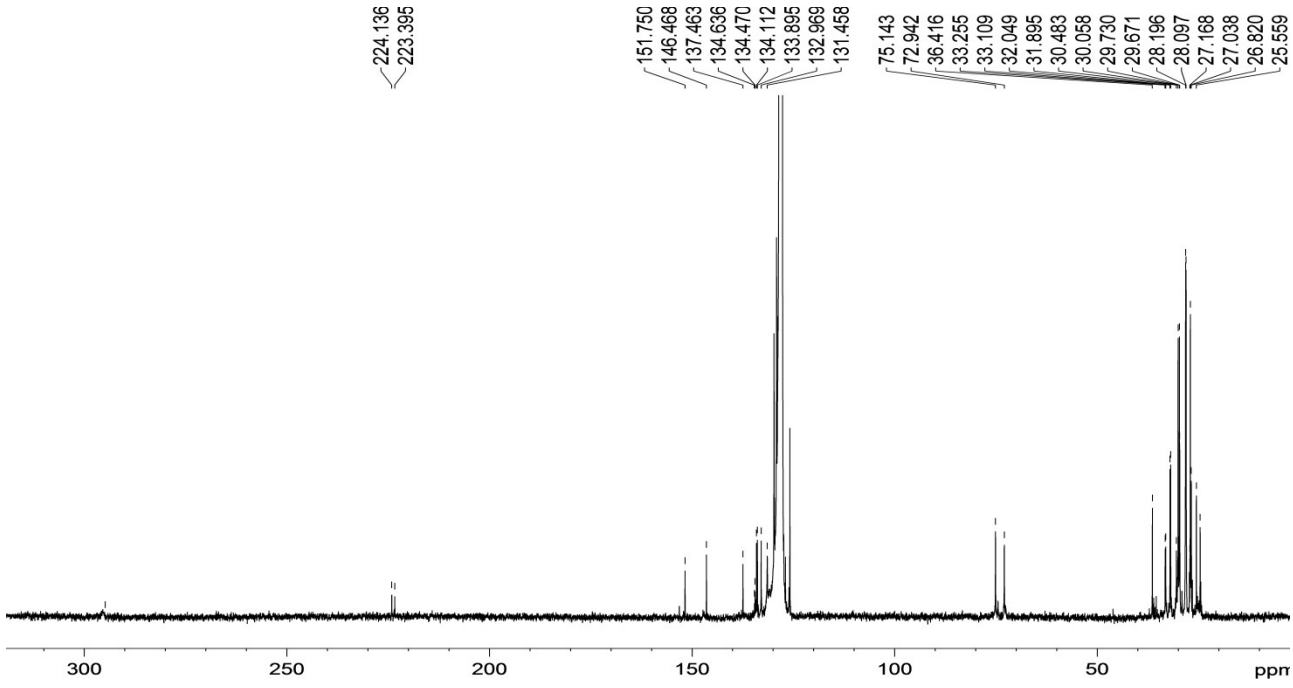


Figure S12: ^{13}C NMR {^{1}H}spectrum of **11** (C_6D_6, 100MHz)

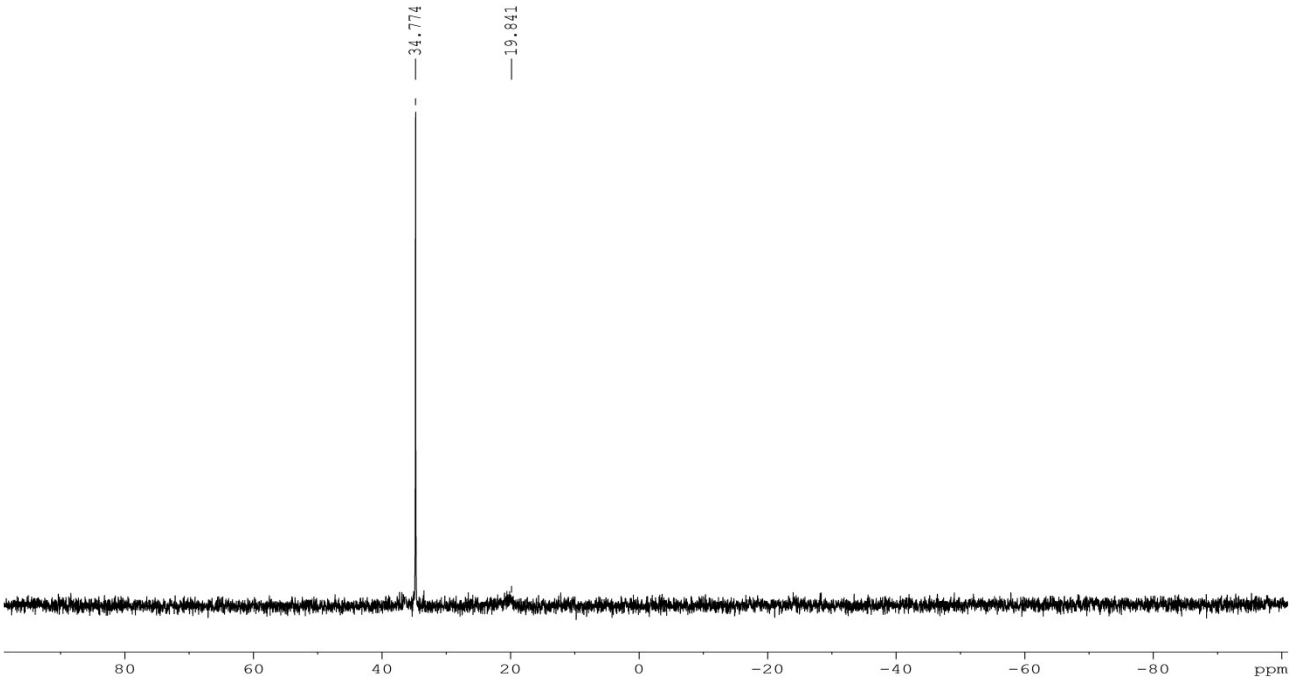


Figure S13: ^{31}P NMR $\{^{1}H\}$spectrum of **11** (C_6D_6, 161.97MHz)

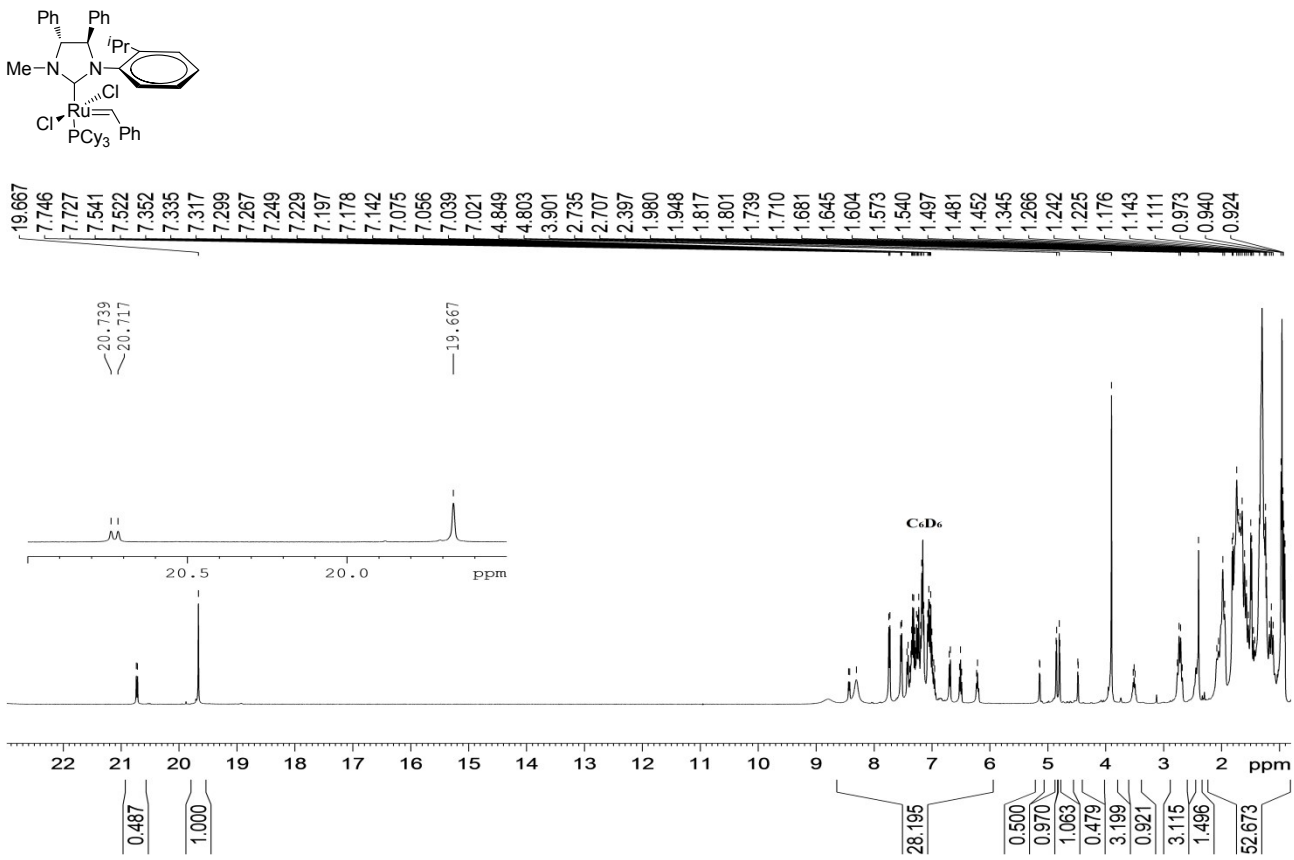


Figure S14: ^{1}H NMR spectrum of **12** (C_6D_6, 400MHz**)**

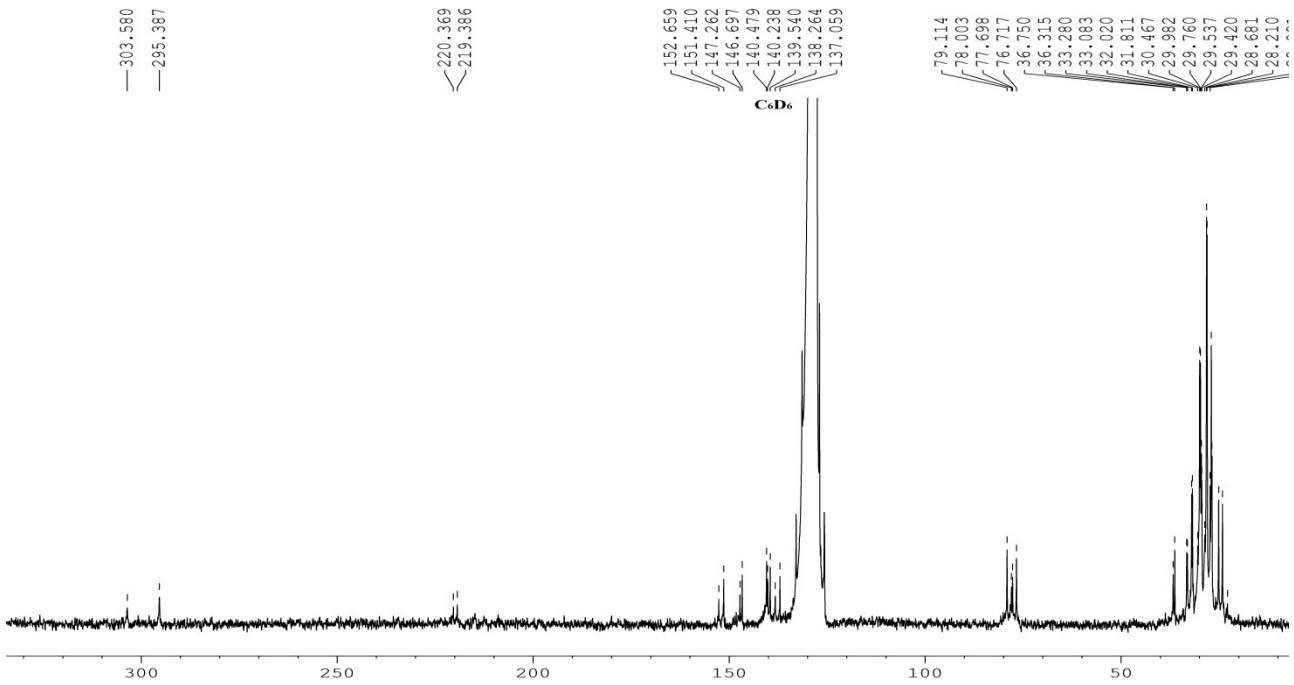


Figure S15: ^{13}C NMR {^{1}H}spectrum of **12** (C_6D_6, 75MHz)

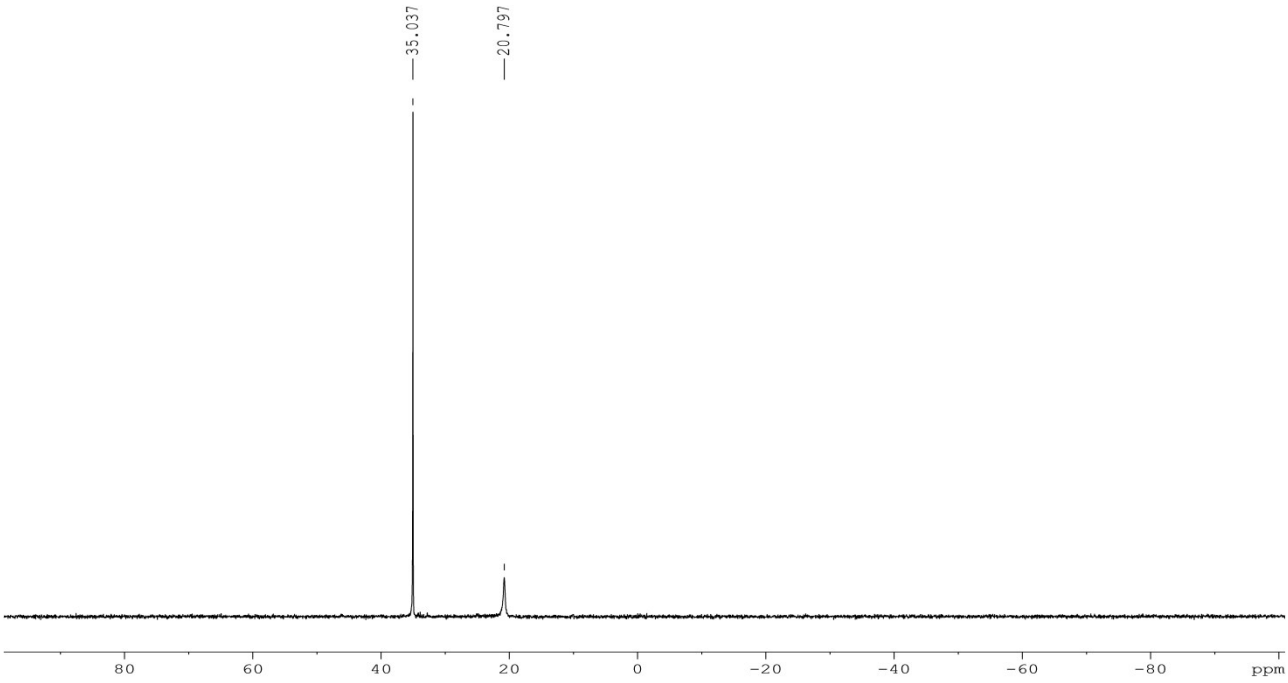


Figure S16: ^{31}P NMR $\{^{1}H\}$spectrum of **12** (C_6D_6, 161.97MHz)

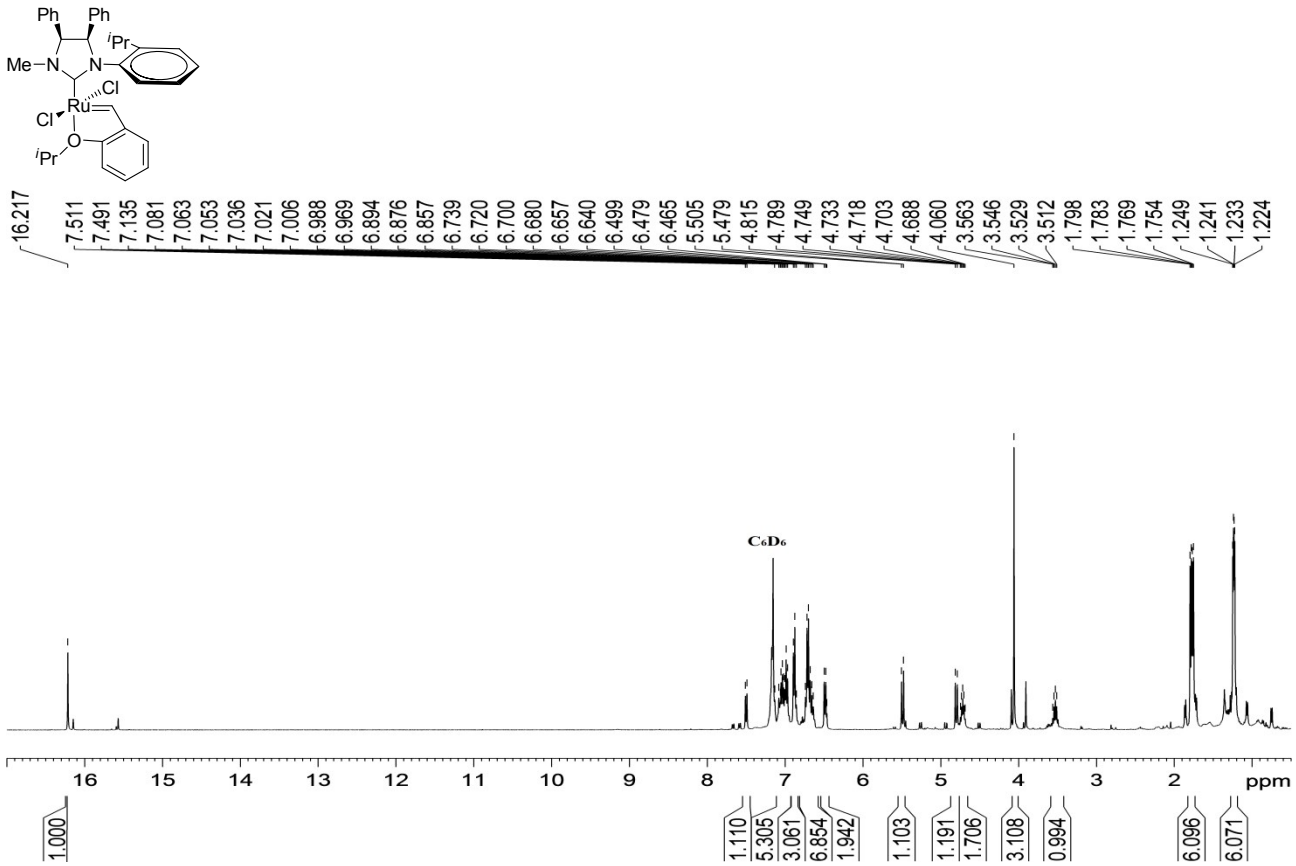


Figure S17: ^{1}H NMR spectrum of **13** (C_6D_6, 400MHz**)**

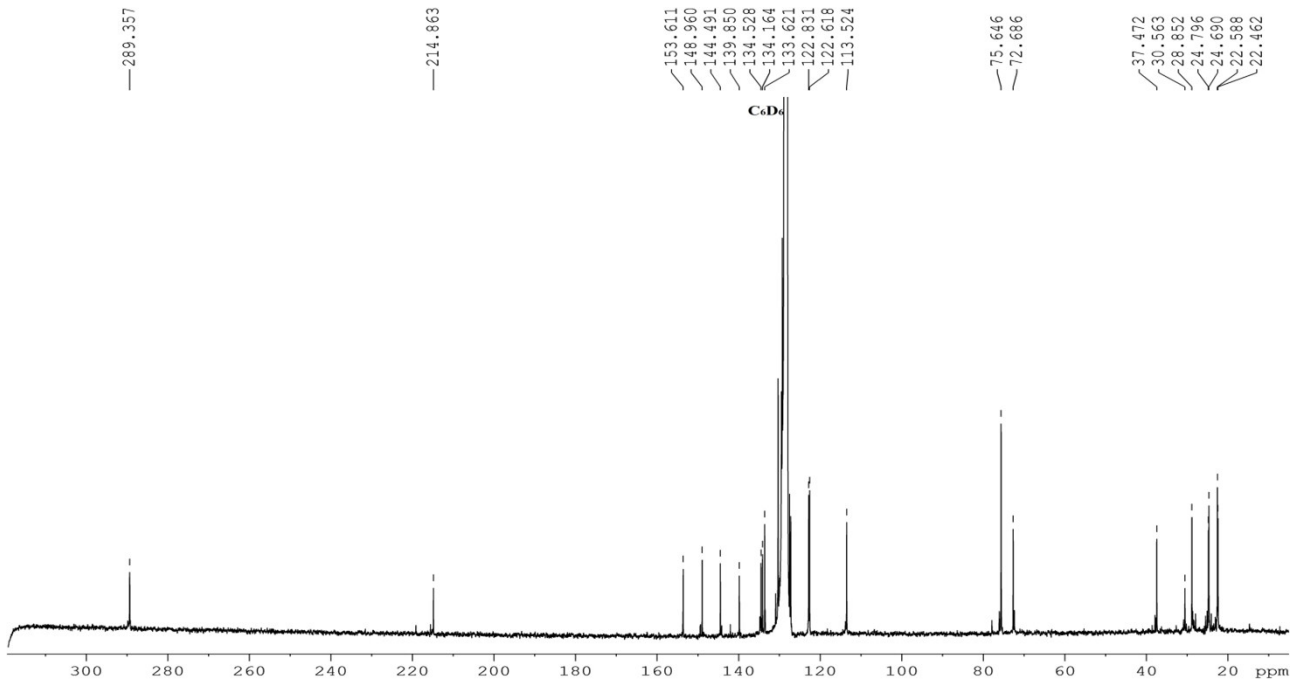


Figure S18: ^{13}C NMR {^{1}H}spectrum of **13** (C_6D_6, 75MHz)

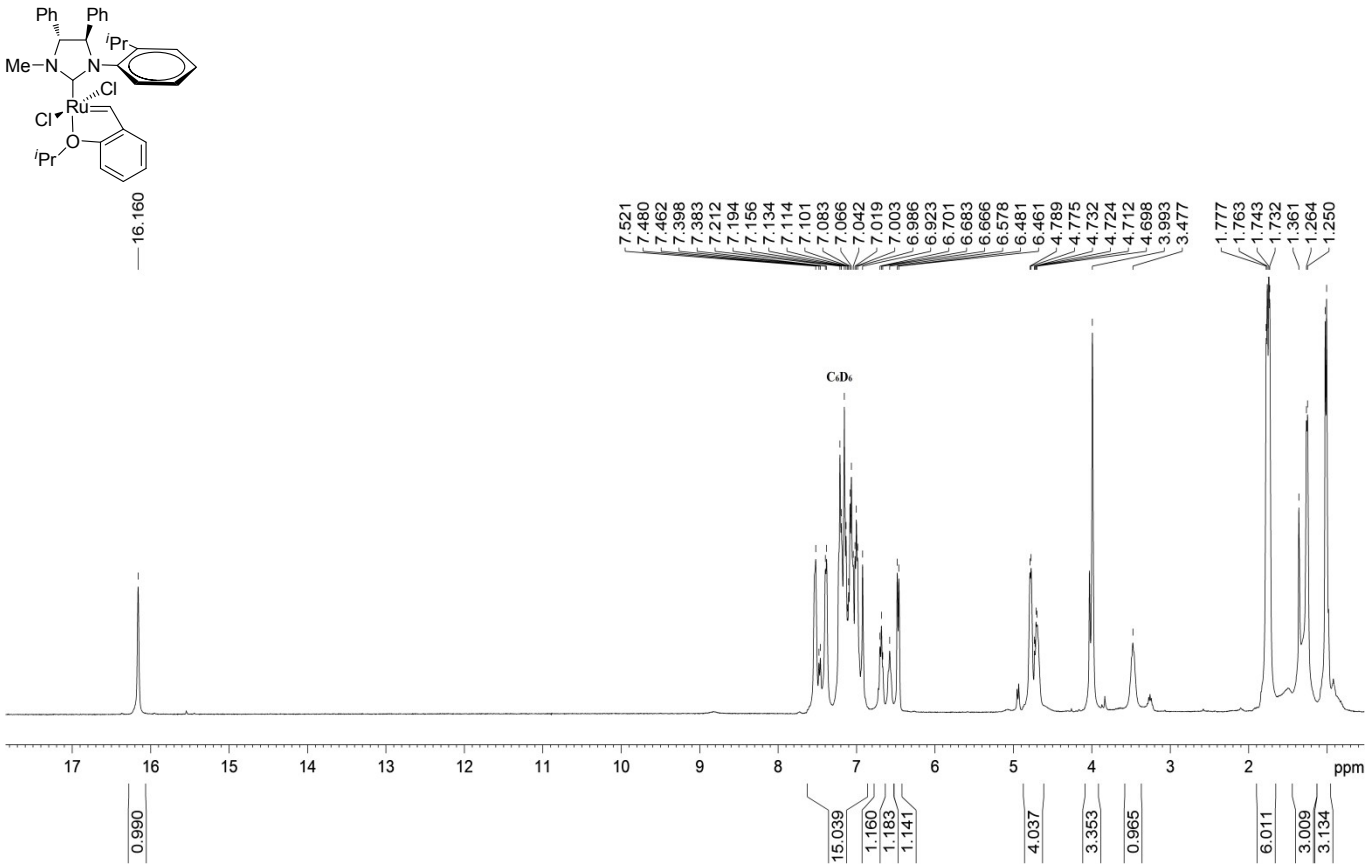


Figure S19: ^{1}H NMR spectrum of **14** (C_6D_6, 400MHz**)**

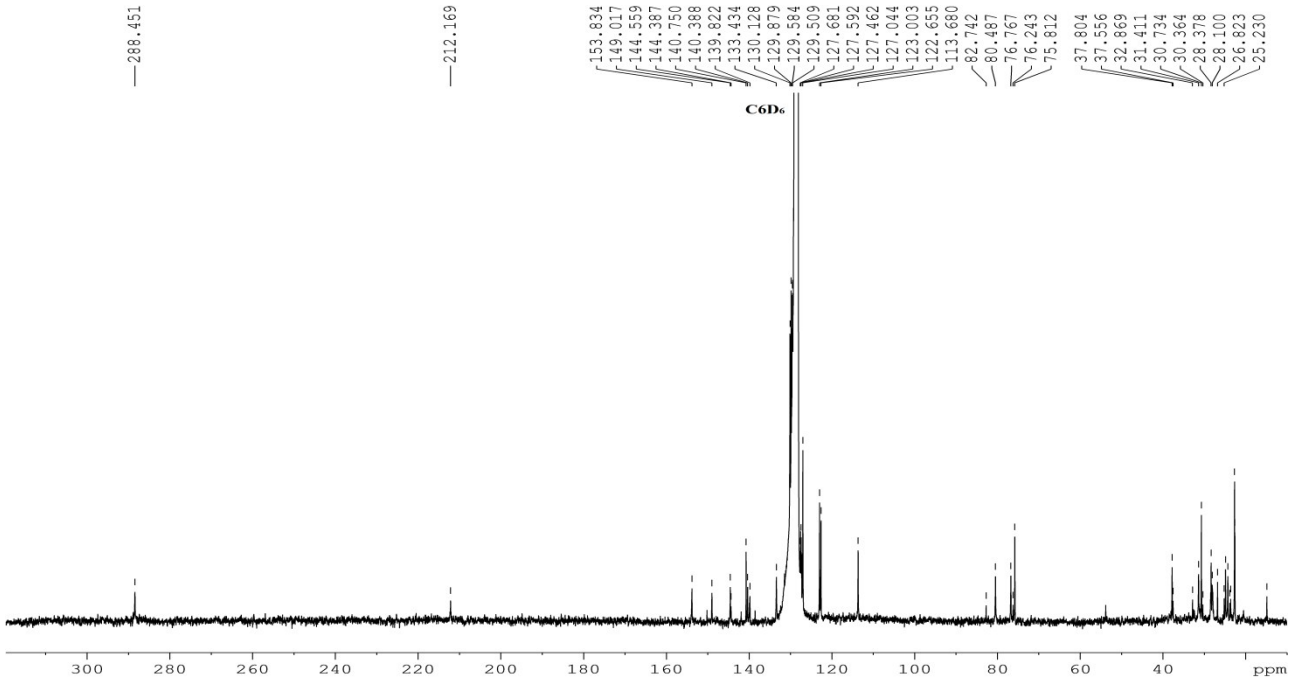


Figure S20: ^{13}C NMR {^{1}H}spectrum of **14** (C_6D_6, 75MHz)

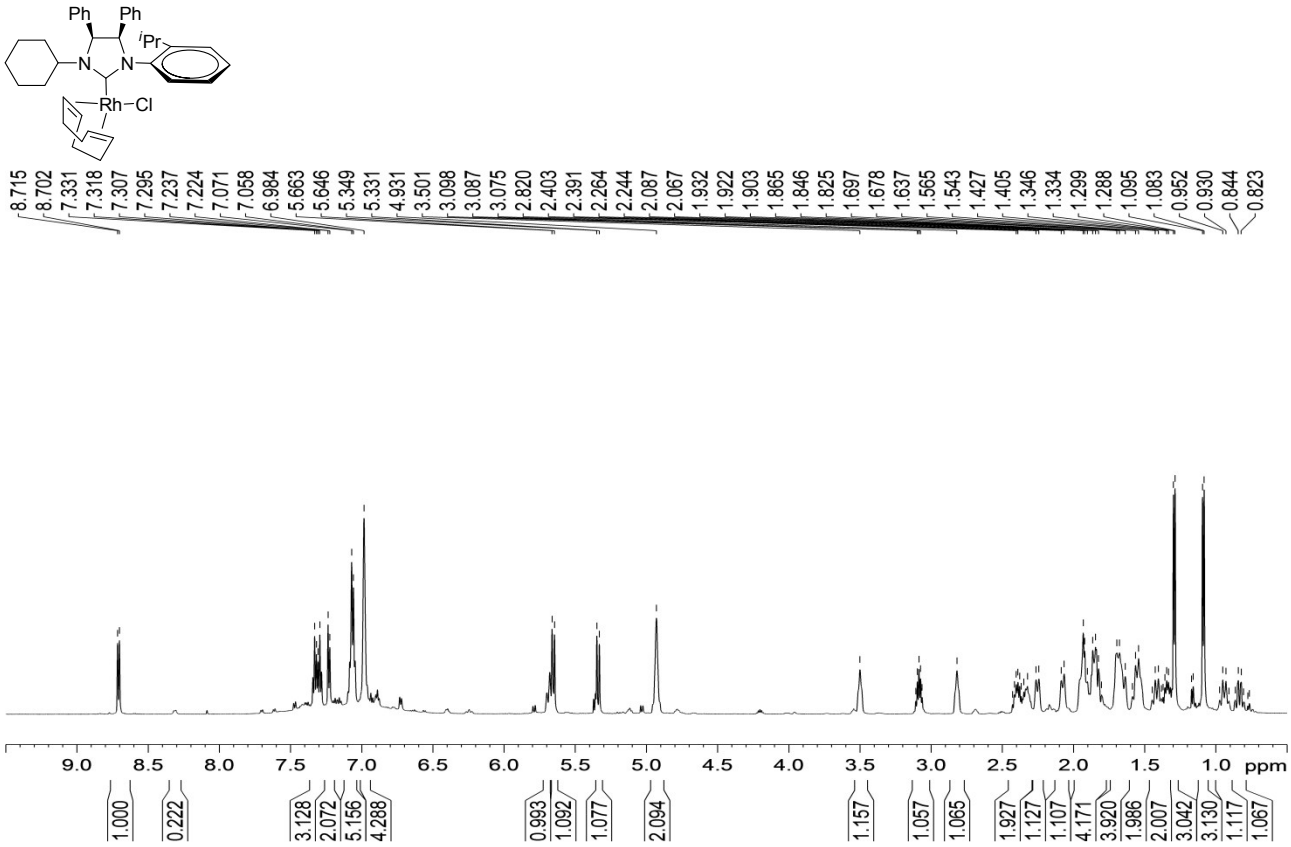


Figure S21: ^{1}H NMR spectrum of **39** (CD_2Cl_2, 600MHz**)**

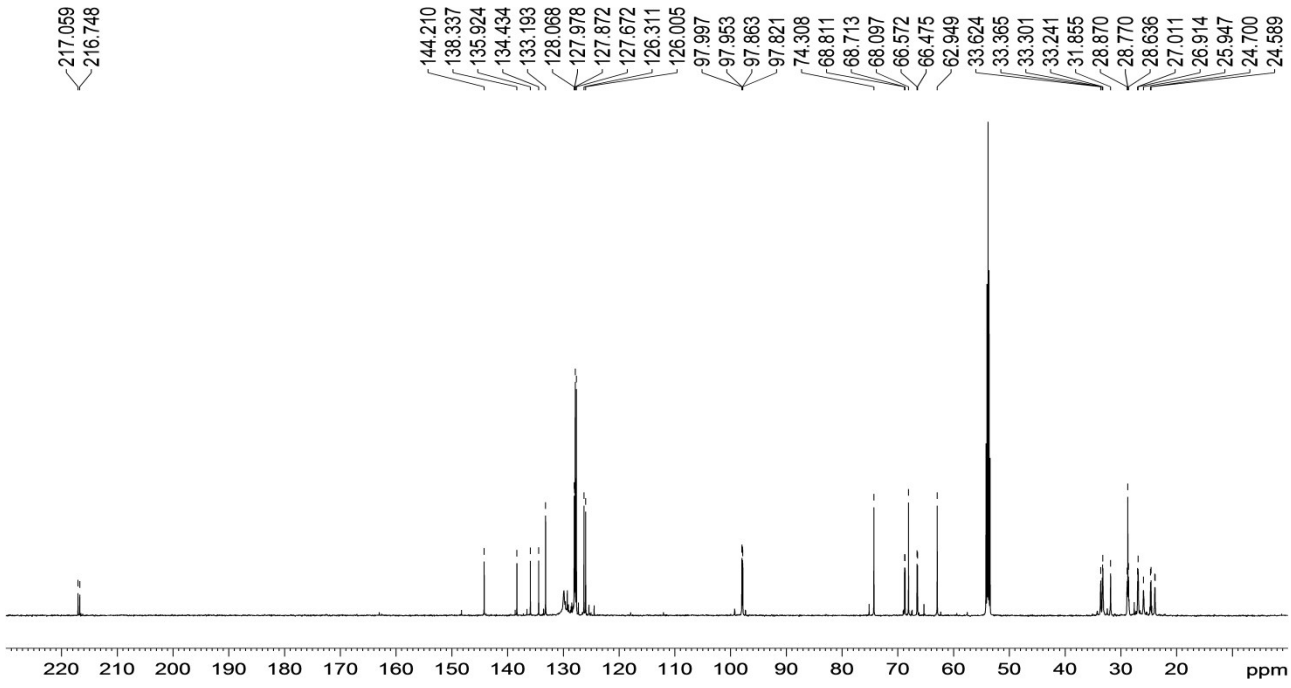


Figure S22: ^{13}C NMR {^{1}H}spectrum of **39** (CD_2Cl_2, 125MHz)

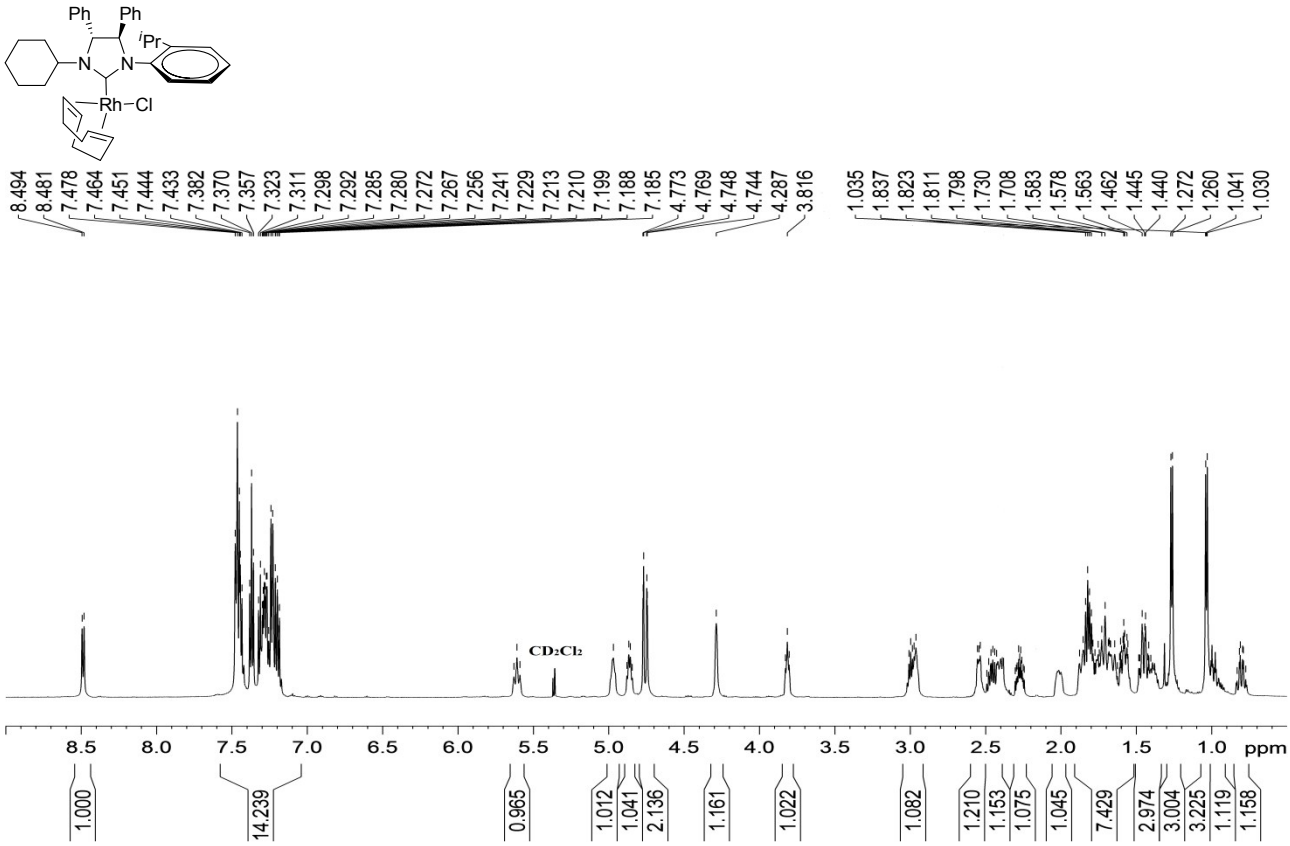


Figure S23: ^{1}H NMR spectrum of **40** (CD_2Cl_2, 600MHz**)**

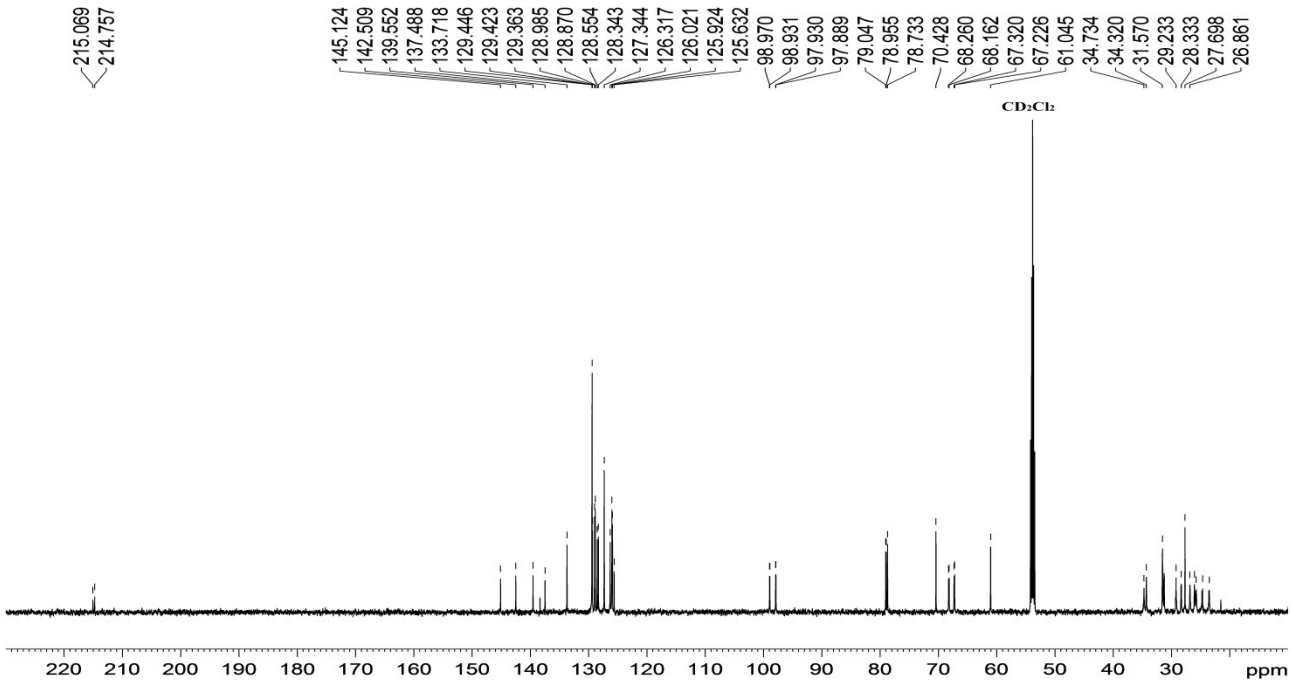


Figure S24: ^{13}C NMR {^{1}H}spectrum of **40** (CD_2Cl_2, 125MHz)

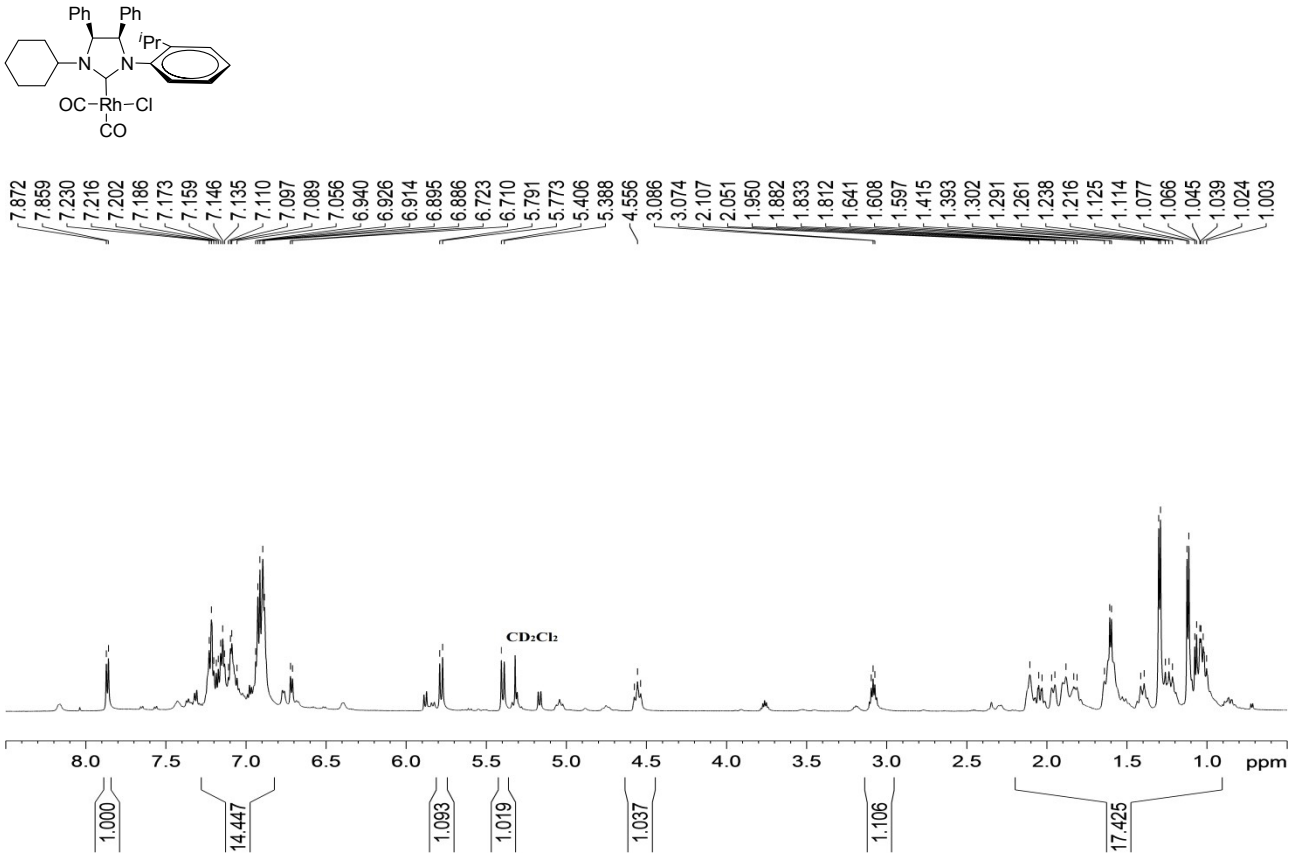


Figure S25: ^{1}H NMR spectrum of **41** (CD_2Cl_2, 600MHz**)**

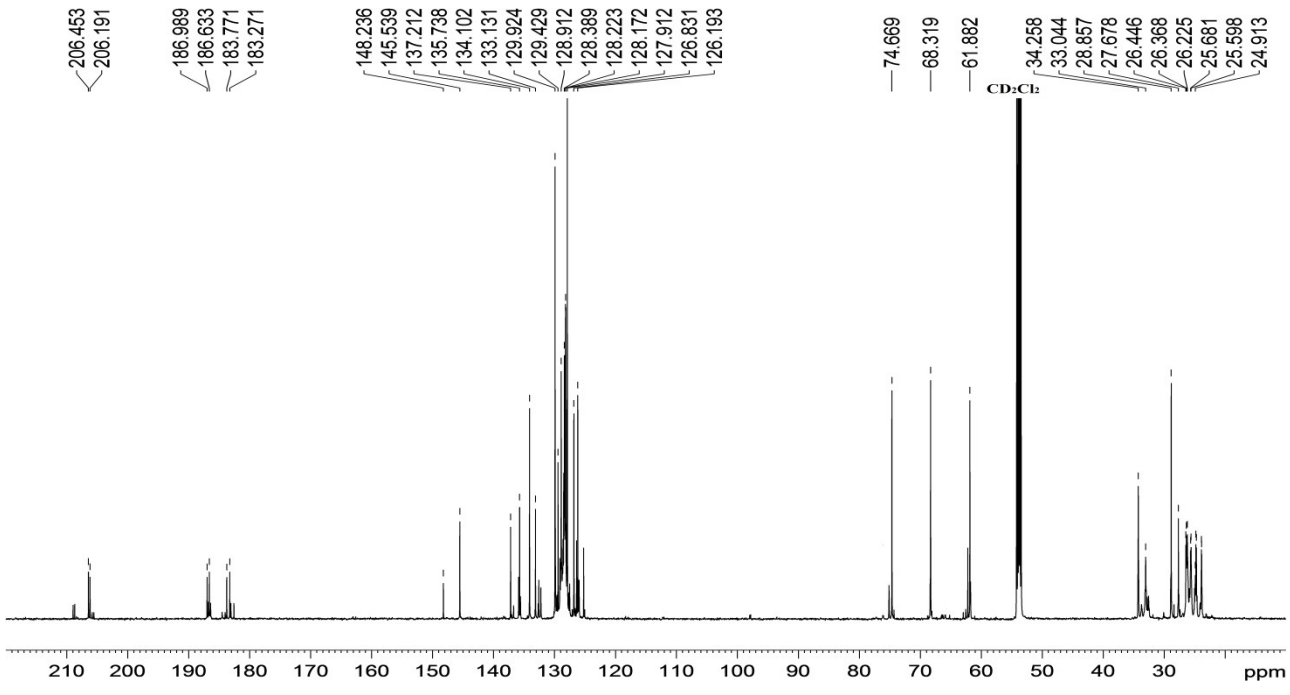


Figure S26: ^{13}C NMR $\{^{1}H\}$spectrum of **41** (CD_2Cl_2, 125MHz)

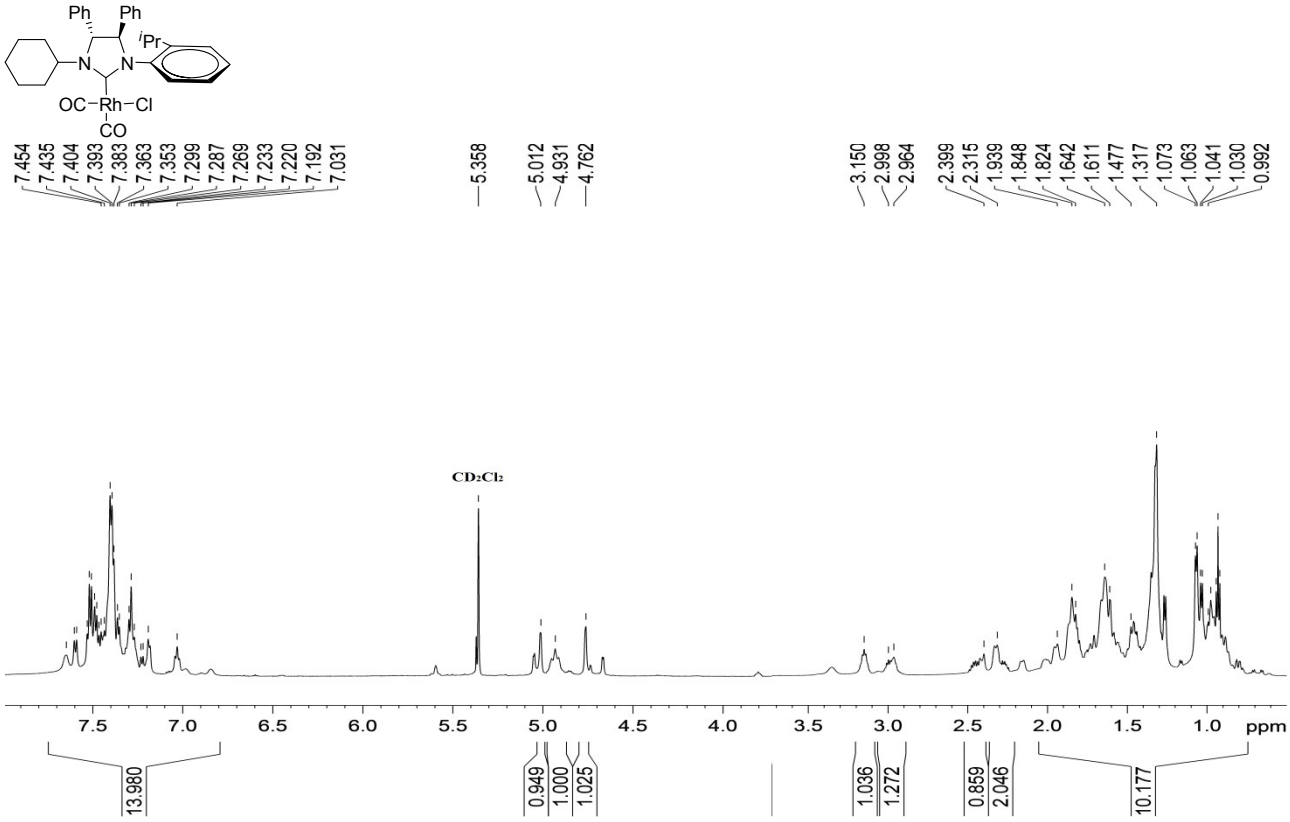


Figure S27: ^{1}H NMR spectrum of **42** (CD_2Cl_2, 600MHz**)**

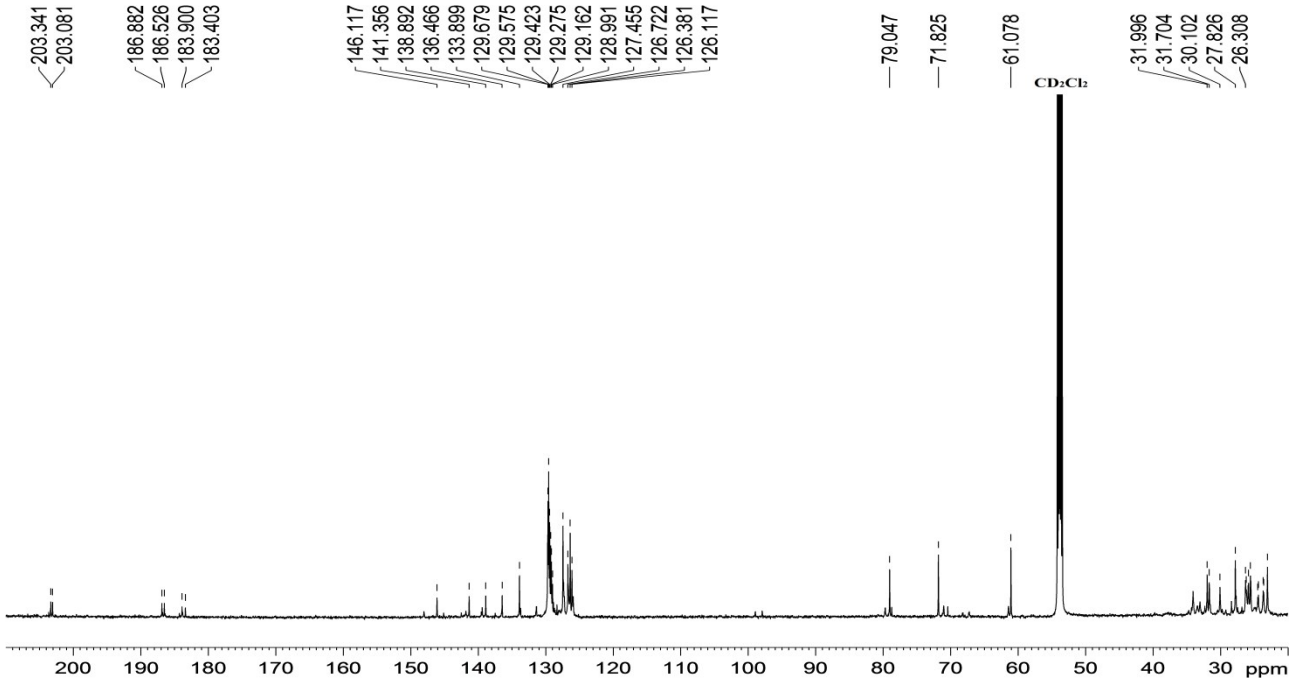
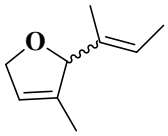


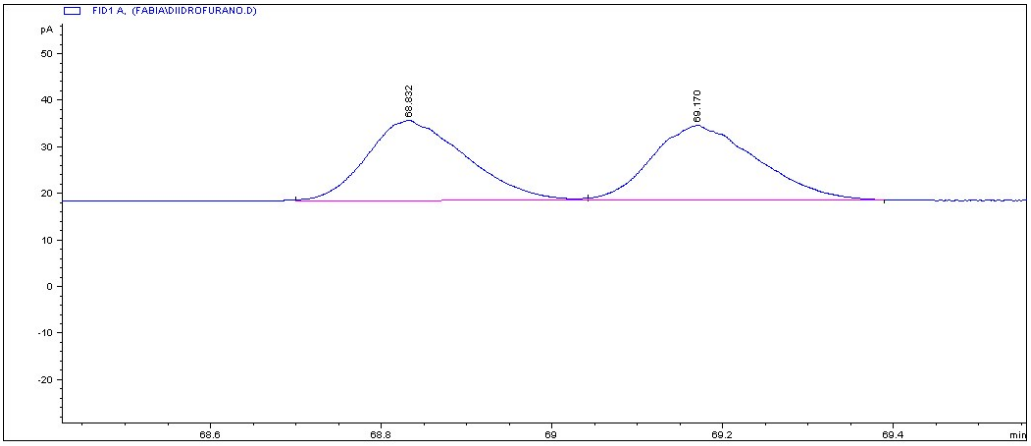
Figure S28: ^{13}C NMR $\{^{1}H\}$spectrum of **42** (CD_2Cl_2, 125MHz)

GC data analysis

Supelco β-DEX 120, 1mL/min, 40°C for 100min, then 1°C/ min up to 50°C for 120 min, then 1°C/ min up to 100°C for 10 min.



Racemic



35% *ee*

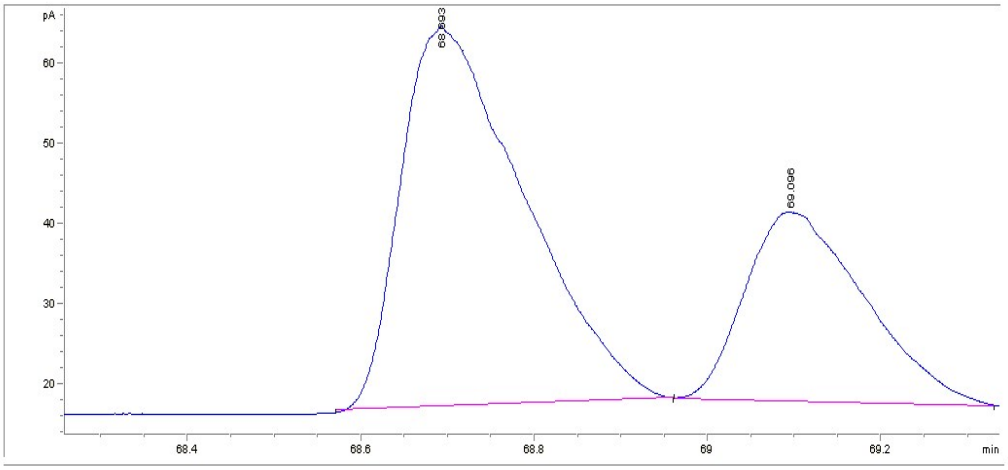
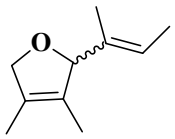
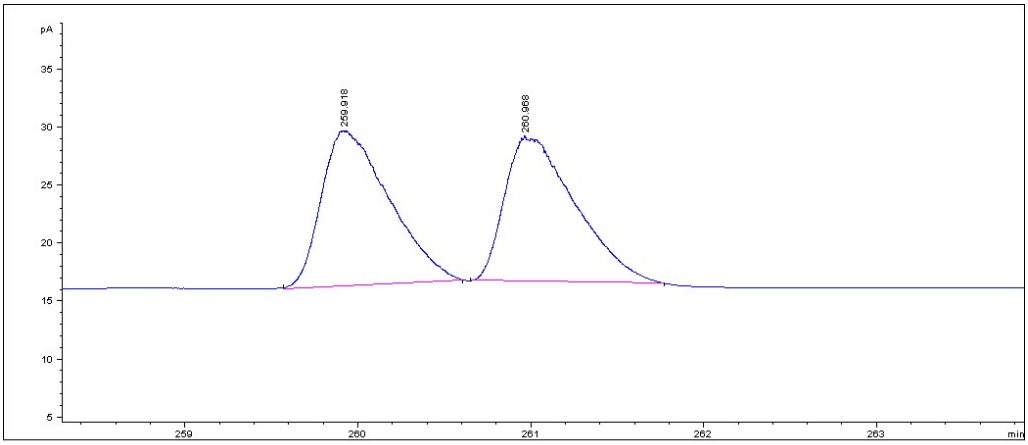


Figure S29: GC chromatogram of **33** obtained with catalyst **14**

Supelco β-DEX 120, 1mL/min, 40°C for 100min, then 1°C/ min up to 50°C for 120 min, then 1°C/ min up to 100°C for 10 min.



Racemic



25%*ee*

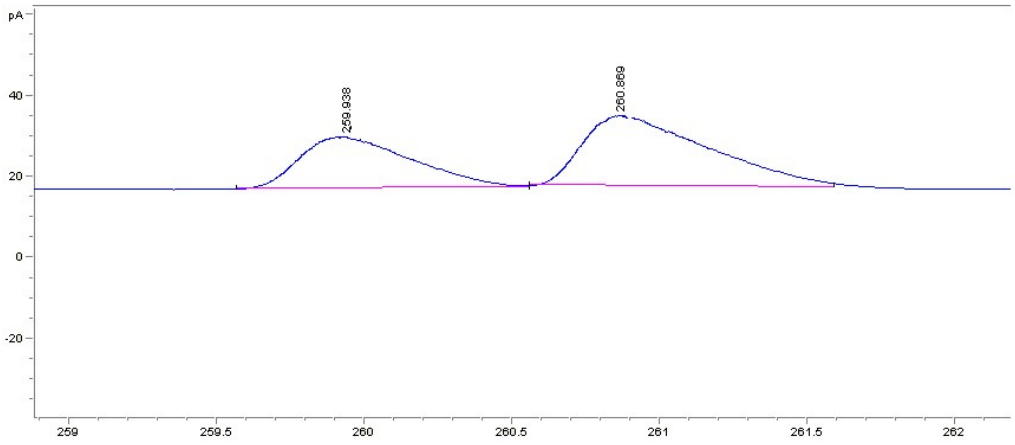
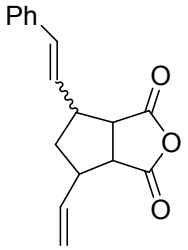


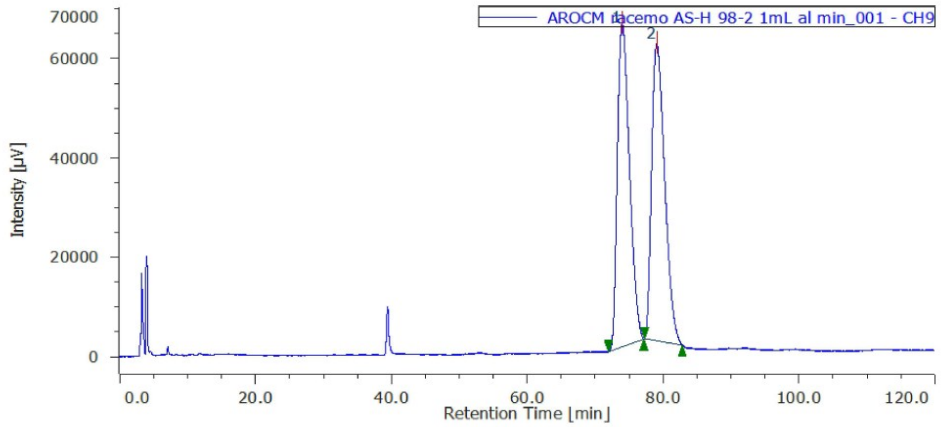
Figure S30: GC chromatogram of **34** obtained with catalyst **14**

HPLC data analysis

Column Chiralpak AS-H, Hexane:2-propanol 98:2, 1mL/min.



Racemic



29%*ee*

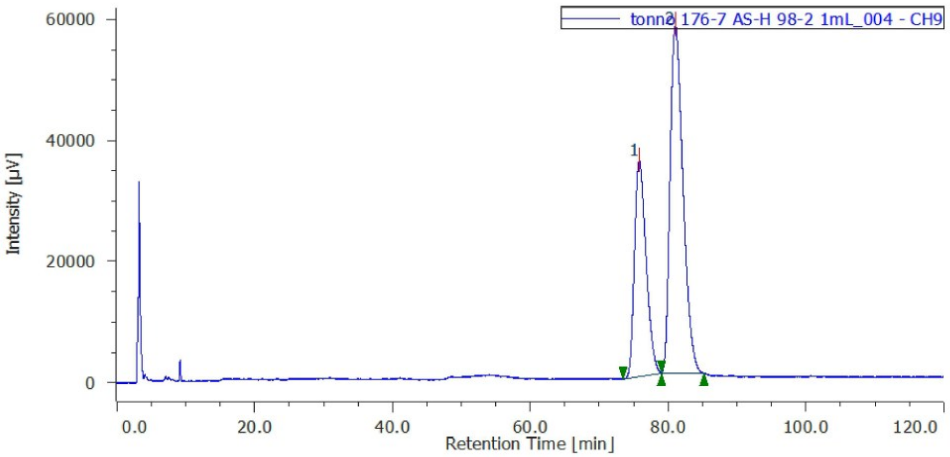


Figure S31: HPLC chromatogram of **36** obtained with catalyst **10**

Crystal structure determinations

The crystal data of compounds **39** and **40** were collected at room temperature using a Nonius Kappa CCD diffractometer with graphite monochromated Mo-Kα radiation. The data sets were integrated with the Denzo-SMN package[2] and corrected for Lorentz, polarization and absorption effects (SORTAV)[3]. The structure was solved by direct methods using SIR97[4] system of programs and refined using full-matrix least-squares with all non-hydrogen atoms anisotropically and hydrogens included on calculated positions, riding on their carrier atoms. The C7 and C10 atoms of the *COD* alkene molecule in the structure **40** were found disordered and refined isotropically over two independent positions.

All calculations were performed using SHELXL-97[5] and PARST[6] implemented in WINGX[7] system of programs. The crystal data are given in Table S4.

Crystallographic data (excluding structure factors) have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers CCDC 1414525-1414526. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html or on application to CCDC, Union Road, Cambridge, CB2 1EZ, UK [fax: (+44)1223-336033, e-mail: deposit@ccdc.cam.ac.uk]

[2] Otwinowski, Z.;Minor, W. *Methods in Enzymology*, C.W. Carter, R.M. Sweet Editors, Vol. 276, Part A, Academic Press, London, **1997**, 307-326.
[3] Blessing, R. H. *Acta Crystallogr. Sect A* **1995**, 51, 33-38.
[4] Altomare, A.; Burla, M. C.; Camalli,M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G.; Polidori G.; Spagna, R. *J. Appl. Crystallogr*. **1999**, 32, 115-119.
[5] Sheldrick, G. M. SHELX-97, *Program for Crystal Structure Refinement*, University of Gottingen, Germany, **1997**.
[6] Nardelli, M. *J. Appl. Crystallogr*. **1995**, *28*, 659-659.
[7] Farrugia, L. J. *J. Appl. Crystallogr*. **1999**, 32, 837-838.

Table S4. Crystallographic data.

Compound	**39**	**40**
Formula	$C_{38}H_{46}ClN_2Rh$	$C_{38}H_{46}ClN_2Rh$
M	669.13	669.13
Space group	*C2/c*	$P2_12_12_1$
Crystal system	Monoclinic	Orthorhombic
a/Å	23.2672(6)	15.1213(5)
b/Å	14.4735(2)	11.1057(3)
c/Å	22.2443(7)	20.3596(7)
α/°	90.00	90.00
β/°	114.730(1)	90.00
γ/°	90.00	90.00
U/Å^3	6803.9(3)	3419.0(2)
Z	8	4
T/K	295	295
D_c/g cm^{-3}	1.306	1.300
F(000)	2800	1400
μ(Mo-Kα)/mm^{-1}	0.608	0.605
Measured Reflections	27353	14007
Unique Reflections	9786	7166
R_{int}	0.0500	0.1111
Obs. Refl.ns [I≥2σ(I)]	6641	5908
θ_{min}- θ_{max}/°	3.22– 30.00	3.52 – 27.00
hkl ranges	-32,32;-20,20;-31,30	-16,19;-14,14;-25,26
R(F^2) (Obs.Refl.ns)	0.0501	0.0724
wR(F^2) (All Refl.ns)	0.1393	0.1807
No. Variables/Constraints	381/0	379/8
Goodness of fit	1.042	1.051
$\Delta\rho_{max}$; $\Delta\rho_{min}$ /e Å^{-3}	1.135; -1.217	2.783; -1.197
CCDC Deposition N.	1414525	1414526

Cartesian coordinates and energies of calculated structures

```
124
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  C      5.923647     0.190221     2.953624
  C      5.891322    -1.258988     3.466800
  C      4.486813    -1.866710     3.321234
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97

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C	-1.903914	-3.866961	2.553164
C	5.891856	0.096335	-2.110685
C	6.207941	0.653242	0.362491
C	7.695575	0.879539	0.292939
C	8.571655	0.589635	1.273918
H	8.082554	1.334685	-0.638222
H	3.169334	-0.963609	-2.358269
H	0.180227	-2.991730	-2.158385
H	-1.681131	2.272657	1.837882
H	-2.624184	0.190000	2.030089
H	-0.161787	-3.471339	-0.357609
H	-3.959262	-4.646493	0.538908
H	-4.111597	-4.861712	-1.931076
H	-3.102435	-3.083769	-3.413623
H	-2.008520	-1.079036	-2.356694
H	-2.256601	-1.771743	2.319053
H	7.333494	-1.725753	-0.562319
H	6.027596	-2.125664	0.597349
H	5.827889	-2.508405	-1.143970
H	5.691574	1.628970	0.200135
H	5.935831	0.319558	1.388290
H	6.981383	0.154205	-2.311691
H	5.463584	-0.610319	-2.850747
H	5.453708	1.098291	-2.308818
H	2.705917	-3.325116	-1.830082
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H	3.696404	0.644842	-0.500256
H	3.899265	-0.703869	0.665927
H	9.649552	0.793146	1.165565
H	8.241499	0.141457	2.227574
H	-4.728610	0.851911	2.610379
H	-7.114776	1.303390	2.024647
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H	-6.111208	1.053754	-2.195111
H	-3.728758	0.631704	-1.608261
H	-3.115480	4.044536	1.162267
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H	0.309489	2.314639	2.999035
H	1.033871	0.672061	2.911572
H	2.577771	2.358957	4.024601
H	3.295894	1.640869	2.566789
H	1.944167	4.421191	2.740982
H	3.689244	4.112777	2.563938
H	2.615095	4.687275	0.338761
H	3.318210	3.054855	0.328900
H	0.332719	3.771340	0.712123
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  C      1.089270     1.827865     2.444980
  C      2.435967     2.496999     2.773946
  C      2.534787     3.912123     2.180497
  C      2.267950     3.895244     0.666089
  N     -0.457108     1.147696     0.612558
  C     -1.795460     1.712545     0.883928
  C     -2.646296     0.390868     0.988843
  N     -1.805425    -0.559327     0.194396
  C     -0.516389    -0.113585     0.120625
  C     -2.259144     2.715740    -0.169669
  C     -1.905312     2.585999    -1.530324
  C     -2.389582     3.507550    -2.475375
  C     -3.227657     4.564605    -2.078335
  C     -3.580085     4.700545    -0.724220
  C     -3.096359     3.781316     0.221698
  Ru     1.120234    -1.039880    -0.590947
  Cl     0.647310     0.013817    -2.729982
  C     -2.292965    -1.815726    -0.305816
  C     -2.418424    -1.956466    -1.707635
  C     -2.942004    -3.130651    -2.265271
  C     -3.354893    -4.171788    -1.416332
  C     -3.205576    -4.039329    -0.027932
  C     -2.660167    -2.876982     0.565346
  C     -4.106338     0.499324     0.599848
  C     -5.070851     0.617891     1.624351
  C     -6.433752     0.775105     1.319940
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  C     -5.901877     0.685003    -1.048835
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  C     -2.451186    -2.829171     2.079372
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  C      3.269728    -1.021605    -1.357323
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  C      6.288559     0.572405     0.538159
  C      7.783986     0.746227     0.488505
  H      8.188754     1.300239    -0.379455
  C      6.226633    -1.693403    -0.609985
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  H      3.940732    -0.746169     0.678835
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  H      1.071650     0.778023     2.806033
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  H      3.260285     1.867925     2.367420
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P3 E(gas)=-2679.13913821 G(gas)=-2678.417023 E(CH2Cl2)=-2679.15387148
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  C     -2.170286    -2.088801    -1.657229
  C     -2.544228    -3.327330    -2.195145
  C     -2.893864    -4.378046    -1.330251
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  N     -1.765425    -0.583484     0.220444
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C	-6.489897	0.553119	1.115921
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C	0.975585	1.920396	2.487672
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  C      2.367416     2.836851     2.761660
  C      2.267587     4.287309     2.261820
  C      1.986515     4.330214     0.750612
  N     -0.374941     1.274413     0.552143
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  Ru     1.082639    -1.191819    -0.693867
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97
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  C      2.112866     3.055272     2.784941
  C      0.917582     2.162207     2.407604
  C     -2.515127     2.582815    -0.215212
  C     -2.151441     2.505040    -1.576481
  C     -2.770399     3.343619    -2.520170
  C     -3.755945     4.263325    -2.120533
  C     -4.119932     4.346368    -0.765097
  C     -3.500426     3.511891     0.180037
  C     -1.755609    -1.974586    -0.161066
  C     -1.686979    -2.229459    -1.551405
  C     -1.869249    -3.527614    -2.053269
  C     -2.142857    -4.576676    -1.162572
  C     -2.206042    -4.320163     0.216258
  C     -2.001467    -3.032846     0.760927
  Ru     1.184987    -1.066263    -0.696905
  C      2.675624     0.000778    -0.610504
  C      3.864109    -0.095005     0.301223
  C      5.241915     0.294026    -0.330781
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C	5.509895	-0.574287	-1.578682
C	-2.045731	-2.846629	2.278236
C	-3.495511	-2.925460	2.807980
Cl	1.426029	-1.760793	1.640988
Cl	0.539013	0.174508	-2.727376
C	2.113573	-3.056057	-0.981042
C	1.887908	-2.502458	-2.251113
C	-1.140453	-3.852707	3.019255
C	5.262954	1.789406	-0.714083
C	6.322824	-0.000561	0.763443
C	7.746901	0.320657	0.392147
C	8.744736	-0.578208	0.290313
H	7.980388	1.385738	0.204076
H	2.720912	0.791848	-1.397415
H	2.697960	-2.036244	-2.832985
H	-1.965605	2.165872	1.822134
H	-2.556696	-0.042771	2.041508
H	0.995431	-2.777390	-2.835638
H	-2.403408	-5.157360	0.904418
H	-2.304275	-5.599861	-1.537612
H	-1.814390	-3.707328	-3.138432
H	-1.484220	-1.388564	-2.233420
H	-1.634828	-1.839119	2.496910
H	6.514871	-0.367166	-2.000822
H	5.469402	-1.656193	-1.329676
H	4.759070	-0.378465	-2.372876
H	6.047837	0.585256	1.672332
H	6.250665	-1.072736	1.050745
H	6.225278	2.072660	-1.187987
H	4.462240	2.035416	-1.442153
H	5.120259	2.437234	0.178017
H	3.112661	-3.054497	-0.517397
H	1.404971	-3.781537	-0.546624
H	3.668430	0.583704	1.169116
H	3.918368	-1.105595	0.756262
H	9.771383	-0.275615	0.026711
H	8.572798	-1.653272	0.474422
H	-4.802186	0.345751	2.487944
H	-7.190724	0.290253	1.760068
H	-7.757711	0.020221	-0.674196
H	-5.910282	-0.178053	-2.364964
H	-3.528154	-0.097560	-1.638376
H	-3.787302	3.585069	1.242630
H	-4.885978	5.068392	-0.440067
H	-4.236504	4.919845	-2.863465
H	-2.472924	3.276321	-3.578881
H	-1.367129	1.800372	-1.905842
H	1.504758	1.759695	0.362400
H	0.013656	2.513855	2.957840
H	1.098330	1.108556	2.709208
H	2.259913	3.041987	3.886224
H	3.041870	2.622925	2.346579
H	1.080863	4.972028	2.803441
H	2.833061	5.105184	2.515839
H	1.509501	5.550928	0.400815
H	2.569877	4.134528	0.222157

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  H     -0.465056     4.091444     0.821207
  H      0.302644     3.640235    -0.719068
  H     -1.132945    -3.623503     4.105705
  H     -1.503284    -4.896646     2.908551
  H     -0.098422    -3.790561     2.648478
  H     -3.524548    -2.725061     3.900128
  H     -4.167385    -2.202632     2.303089
  H     -3.919376    -3.939407     2.643988
91
P6 E(gas)=-2600.60340065 G(gas)=-2599.927293 E(CH2Cl2)=-2600.61740889
  C      1.046691    -2.389730    -1.516474
  C      1.149855    -2.090080    -0.138086
  C      1.236375    -3.137148     0.825382
  C      1.248122    -4.462134     0.335547
  C      1.150312    -4.760679    -1.032238
  C      1.035672    -3.718864    -1.965360
  N      1.172740    -0.696503     0.239702
  C      0.055051     0.096418     0.238637
  N      0.395769     1.326375     0.704682
  C      1.865862     1.489501     0.800425
  C      2.336251    -0.011406     0.867192
  C     -0.538541     2.357107     1.180514
  Ru    -1.662204    -0.673803    -0.475265
  C     -2.843348     0.736684    -0.341138
  C     -4.170889     0.752200     0.350286
  C     -5.329794     0.149163    -0.523823
  C     -6.631729     0.174898     0.301429
  C      3.696660    -0.305481     0.266655
  C      2.452631     2.324087    -0.335990
  C      1.324413    -2.893551     2.332537
  C     -2.731669    -2.500068    -1.243749
  C     -3.675722    -1.542160    -1.596084
  C     -4.961626    -1.326335    -0.845504
  Cl    -2.161919    -1.571914     1.711768
  Cl    -1.007989     0.088129    -2.699225
  C     -5.524846     0.972802    -1.815329
  H     -3.562773    -1.045155    -2.575595
  H     -2.576899     1.651859    -0.924179
  H     -4.443484     1.803948     0.599136
  H     -4.106580     0.162679     1.289894
  H     -5.786934    -1.747948    -1.468354
  H     -4.939485    -1.911502     0.098069
  H     -1.966584    -2.806884    -1.978995
  H     -2.898508    -3.164249    -0.379269
  H      2.373637    -0.295907     1.943824
  H      2.131968     1.977724     1.759467
  H      1.320167    -5.290836     1.057361
  H      1.158218    -5.810703    -1.365821
  H      0.950735    -3.931220    -3.042684
  H      0.951369    -1.557934    -2.230760
  C      0.328196    -3.758812     3.131423
  C      2.766241    -3.113652     2.844906
  H      1.035905    -1.835750     2.509912
  H     -7.473397    -0.265203    -0.274834
  H     -6.524590    -0.402341     1.243692
  H     -6.915881     1.214467     0.568718
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H	-6.349765	0.551494	-2.428754
H	-5.791975	2.023804	-1.575070
H	-4.611914	0.998696	-2.445289
C	3.556555	3.161386	-0.070563
C	4.144805	3.922955	-1.094397
C	3.629907	3.857978	-2.400754
C	2.527809	3.027947	-2.672575
C	1.939297	2.263950	-1.649859
H	3.962278	3.219042	0.953619
H	5.005190	4.573176	-0.868948
H	4.084884	4.457468	-3.205465
H	2.113986	2.973109	-3.692190
H	1.067605	1.627902	-1.884909
C	4.819146	-0.354541	1.122153
C	6.109836	-0.566505	0.608932
C	6.294572	-0.742734	-0.773036
C	5.183704	-0.697554	-1.633313
C	3.895319	-0.476188	-1.119815
H	4.679152	-0.224335	2.208508
H	6.972517	-0.602005	1.293118
H	7.303484	-0.917809	-1.179279
H	5.319458	-0.833369	-2.717928
H	3.035900	-0.434547	-1.803227
C	-0.494184	3.670698	0.374218
H	-1.540876	1.898929	1.041986
C	-1.551897	4.664961	0.888544
H	0.516852	4.127720	0.459476
H	-0.646519	3.451934	-0.703410
C	-1.402974	4.931054	2.396262
H	-1.485394	5.614656	0.315746
H	-2.568646	4.254181	0.687944
C	-1.432237	3.619771	3.199896
H	-0.436226	5.454183	2.581562
H	-2.201017	5.619323	2.749364
C	-0.375005	2.620761	2.694890
H	-1.275993	3.819108	4.281834
H	-2.441379	3.155708	3.113841
H	0.638354	3.037682	2.898372
H	-0.450480	1.657379	3.242367
H	2.842434	-2.864488	3.924763
H	3.065367	-4.177013	2.725368
H	3.507868	-2.502501	2.292057
H	0.358075	-3.475376	4.204590
H	-0.705947	-3.607247	2.764769
H	0.578757	-4.839482	3.072917

91

P7 E(gas)=-2600.60266195 G(gas)=-2599.927687 E(CH2Cl2)=-2600.61685866

C	0.972679	-2.345112	-1.518125
C	1.115308	-2.078589	-0.136369
C	1.194686	-3.145062	0.804332
C	1.176866	-4.459097	0.287010
C	1.046083	-4.727451	-1.084753
C	0.925275	-3.664857	-1.993048
N	1.161348	-0.694448	0.264304
C	0.078227	0.132200	0.168005
N	0.425889	1.373377	0.586457

C	1.886786	1.492894	0.800956
C	2.312555	-0.022038	0.928502
C	-0.526454	2.422502	0.985927
Ru	-1.644152	-0.565873	-0.600586
C	-2.996944	0.716152	-0.608126
C	-4.189960	0.832766	0.295383
C	-5.438397	0.108358	-0.326970
C	-6.548422	-0.006319	0.735197
C	3.688146	-0.368863	0.393535
C	2.588027	2.280188	-0.304040
C	1.277171	-2.931011	2.316092
C	-2.693104	-2.256128	-1.522445
C	-3.725698	-1.300034	-1.625210
C	-4.940706	-1.304406	-0.731053
Cl	-2.197428	-1.505016	1.566265
Cl	-0.975508	0.252727	-2.793069
C	-5.979746	0.886225	-1.546737
H	-3.792523	-0.747146	-2.579968
H	-2.943157	1.454704	-1.445704
H	-4.439622	1.909721	0.436597
H	-3.977346	0.373153	1.280748
H	-5.759201	-1.836261	-1.270514
H	-4.710345	-1.891571	0.182830
H	-2.073659	-2.467866	-2.409600
H	-2.762249	-3.038409	-0.746255
H	2.294164	-0.282414	2.011536
H	2.090035	1.992782	1.770775
H	1.245160	-5.304010	0.990380
H	1.030141	-5.770275	-1.439856
H	0.811424	-3.853346	-3.072145
H	0.885525	-1.497085	-2.215566
C	0.230222	-3.767130	3.080991
C	2.700027	-3.213921	2.847859
H	1.027158	-1.866132	2.507076
H	-7.434518	-0.537265	0.326193
H	-6.195383	-0.565715	1.626428
H	-6.885616	0.996599	1.072042
H	-6.847626	0.357754	-1.995912
H	-6.325804	1.897403	-1.244694
H	-5.220454	1.023018	-2.343846
C	4.774196	-0.424007	1.294160
C	6.076947	-0.687113	0.838284
C	6.309469	-0.909663	-0.529808
C	5.234644	-0.858762	-1.434465
C	3.934500	-0.585675	-0.978676
H	4.595799	-0.258407	2.369963
H	6.911366	-0.726495	1.556460
H	7.327741	-1.125381	-0.890585
H	5.408262	-1.031456	-2.508361
H	3.103178	-0.539638	-1.696155
C	3.735196	3.036699	0.013948
C	4.428551	3.744080	-0.982272
C	3.977545	3.705175	-2.313242
C	2.832674	2.956024	-2.637145
C	2.138583	2.246032	-1.641607
H	4.092069	3.073135	1.057076

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  H      5.321292     4.332432    -0.716299
  H      4.515857     4.262636    -3.096452
  H      2.468369     2.922689    -3.676375
  H      1.234703     1.673412    -1.914737
  C     -0.096831     3.842057     0.571242
  H     -1.461274     2.175065     0.438610
  C     -1.151121     4.879794     1.001666
  H      0.877384     4.095659     1.046882
  H      0.069691     3.883641    -0.524450
  C     -1.446021     4.810897     2.509809
  H     -0.809552     5.897659     0.715740
  H     -2.093781     4.700532     0.434719
  C     -1.868817     3.392444     2.926982
  H     -0.531746     5.104010     3.076281
  H     -2.231107     5.547986     2.785006
  C     -0.830346     2.339999     2.500106
  H     -2.035560     3.336703     4.024149
  H     -2.847363     3.147394     2.454060
  H      0.114650     2.502248     3.069843
  H     -1.183975     1.314095     2.736866
  H      2.764125    -2.994333     3.934926
  H      2.966652    -4.283422     2.707706
  H      3.470611    -2.612585     2.324599
  H      0.252334    -3.506604     4.160214
  H     -0.788692    -3.562933     2.697012
  H      0.434028    -4.856381     3.003494
91
P8 E(gas)=-2600.61098419 G(gas)=-2599.935038 E(CH2Cl2)=-2600.62450627
  C      1.170443    -2.264073    -1.673864
  C      1.239493    -2.081630    -0.274328
  C      1.314687    -3.197274     0.604028
  C      1.377078    -4.478281     0.009411
  C      1.327525    -4.663628    -1.380264
  C      1.204671    -3.550761    -2.228599
  N      1.227133    -0.725170     0.215292
  C      0.142008     0.088322     0.157593
  N      0.446298     1.310034     0.641114
  C      1.899266     1.454835     0.885478
  C      2.342056    -0.061370     0.957749
  C     -0.571833     2.326798     0.965658
  Ru    -1.650798    -0.426887    -0.562137
  Cl    -0.951880     0.439812    -2.713325
  C      3.744416    -0.369784     0.476121
  C      2.609139     2.298736    -0.169654
  C      1.297765    -3.072120     2.127921
  C     -2.468400    -2.017953    -1.450866
  C     -3.672775    -1.037067    -1.463173
  C     -3.381284     0.474672    -0.888293
  C     -4.464008     0.765196     0.150584
  C     -5.646543    -0.201996    -0.181978
  C     -4.887907    -1.483399    -0.625780
  C     -6.538505    -0.461429     1.043836
  C     -6.501731     0.361051    -1.338374
  Cl    -2.181573    -1.291682     1.627175
  H     -3.300059     1.202836    -1.720959
  H     -3.888500    -0.837926    -2.533360
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H	-4.774582	1.831379	0.115189
H	-4.095129	0.542091	1.171745
H	-5.529258	-2.185558	-1.200627
H	-4.516110	-2.017499	0.273692
H	-2.053252	-2.254307	-2.447872
H	-2.603590	-2.888522	-0.780111
H	2.273195	-0.371040	2.025478
H	2.075354	1.914368	1.879738
H	1.446189	-5.362667	0.662951
H	1.373572	-5.681554	-1.799211
H	1.145332	-3.677679	-3.320892
H	1.061803	-1.377366	-2.317725
C	0.169437	-3.913221	2.761254
C	2.669033	-3.428778	2.743049
H	1.065066	-2.013575	2.367871
H	-7.344433	-1.188330	0.804865
H	-5.946940	-0.872127	1.888688
H	-7.027715	0.473966	1.390496
H	-7.294815	-0.359721	-1.631422
H	-7.001807	1.306051	-1.037063
H	-5.897151	0.580612	-2.243329
C	4.779137	-0.480593	1.430506
C	6.107047	-0.707645	1.031514
C	6.416384	-0.839164	-0.333087
C	5.392539	-0.735468	-1.290963
C	4.067240	-0.497666	-0.891505
H	4.540505	-0.386806	2.503227
H	6.900802	-0.790392	1.790871
H	7.454762	-1.025939	-0.649973
H	5.626088	-0.838726	-2.362364
H	3.276583	-0.411442	-1.649965
C	3.716442	3.084176	0.213471
C	4.421763	3.843028	-0.735436
C	4.023089	3.827005	-2.083295
C	2.917912	3.049489	-2.472156
C	2.212249	2.287802	-1.524447
H	4.031885	3.102864	1.270287
H	5.282756	4.453231	-0.418993
H	4.570601	4.424937	-2.829321
H	2.593603	3.035972	-3.524971
H	1.335393	1.698861	-1.846973
C	-0.323441	3.692634	0.298303
H	-1.518967	1.909911	0.548521
C	-1.449383	4.685564	0.642137
H	0.650184	4.103531	0.648418
H	-0.235670	3.561908	-0.799424
C	-1.637749	4.834821	2.161073
H	-1.232644	5.670190	0.175385
H	-2.401795	4.330443	0.185511
C	-1.878925	3.469465	2.826999
H	-0.725855	5.302709	2.599489
H	-2.478703	5.527184	2.381615
C	-0.762166	2.463865	2.492216
H	-1.968635	3.578820	3.929068
H	-2.852447	3.055765	2.477715
H	0.193202	2.810604	2.950551

H	-0.992703	1.464834	2.917664
H	2.655690	-3.277299	3.843309
H	2.922169	-4.494565	2.557527
H	3.489852	-2.816275	2.317248
H	0.145420	-3.749335	3.859356
H	-0.816882	-3.617827	2.351148
H	0.320401	-5.000752	2.593638

91

P9 E(gas)=-2600.58390812 G(gas)=-2599.912511 E(CH2Cl2)=-2600.59710554

C	-3.886392	-0.951578	-1.588888
C	-3.757987	0.407369	-1.260735
C	-4.732643	0.765902	-0.142543
C	-5.725054	-0.449897	-0.073408
C	-4.873730	-1.630730	-0.657665
Ru	-1.677032	-0.314984	-0.602501
Cl	-0.942070	0.544662	-2.750089
C	-6.208679	-0.729757	1.358015
C	-6.927596	-0.180376	-1.002711
C	0.149637	0.049973	0.100642
N	0.427688	1.271737	0.618862
C	1.865889	1.452292	0.898758
C	2.327361	-0.053972	0.977065
N	1.269368	-0.727007	0.160320
C	-0.624607	2.259322	0.914711
C	1.387627	-2.060843	-0.362386
C	1.433412	-3.198292	0.488102
C	1.621348	-4.457485	-0.128232
C	1.729631	-4.600776	-1.519114
C	1.637554	-3.468748	-2.347094
C	1.472041	-2.204657	-1.766022
C	3.766527	-0.334826	0.597601
C	2.586104	2.313406	-0.136216
C	1.250608	-3.120674	2.004494
C	-1.676442	-2.036913	-1.224235
Cl	-2.372232	-1.017694	1.605808
H	-3.386605	1.143601	-1.993107
H	-3.619111	-1.345490	-2.581400
H	-5.257030	1.720379	-0.368229
H	-4.212883	0.896202	0.829600
H	-5.492695	-2.385987	-1.187719
H	-4.336919	-2.149033	0.166251
H	-1.373697	-2.282258	-2.267618
H	-1.993148	-2.889290	-0.579500
H	2.193395	-0.375738	2.035477
H	2.010462	1.910068	1.899281
H	1.669242	-5.357306	0.506136
H	1.874976	-5.600875	-1.957895
H	1.699367	-3.566047	-3.442353
H	1.374633	-1.303246	-2.390798
C	0.022166	-3.931716	2.469908
C	2.527337	-3.555835	2.756291
H	1.038567	-2.062288	2.261786
H	-6.878251	-1.615945	1.389613
H	-5.346463	-0.919377	2.029890
H	-6.781584	0.132958	1.760845
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  C      2.926191     3.090135    -2.425928
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  H      3.977158     3.116418     1.334936
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  H      4.571592     4.484580    -2.741831
  H      2.618989     3.084718    -3.483991
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  C      4.714853    -0.494642     1.631666
  C      6.074880    -0.695993     1.341196
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  C      5.568357    -0.598645    -1.033011
  C      4.211145    -0.387304    -0.740963
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  C     -0.390150     3.638116     0.269798
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  C     -0.887574     2.367165     2.432487
  H     -2.163883     3.441810     3.837737
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  H      0.044390     2.717609     2.933881
  H     -1.123093     1.355236     2.824099
  H     -0.099771    -3.841928     3.569953
  H     -0.906571    -3.550448     1.999825
  H      0.128455    -5.011829     2.233239
  H      2.397750    -3.430103     3.852120
  H      2.757547    -4.626823     2.571178
  H      3.413223    -2.967437     2.440891
91
P10 E(gas)=-2600.58464910 G(gas)=-2599.914959 E(CH2Cl2)=-2600.59775922
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  C     -3.936760     0.543482    -1.089298
  C     -4.901615     0.651869     0.077579
  C     -5.835196    -0.602989    -0.069410
  C     -4.962994    -1.600243    -0.910623
  Ru    -1.669205    -0.283905    -0.593402
  Cl    -1.075848     0.712542    -2.711941
  C     -6.246995    -1.190578     1.290030
  C     -7.086995    -0.212262    -0.884135
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C	-0.616951	2.253363	0.939880
C	1.420247	-2.043472	-0.398657
C	1.514596	-3.193892	0.431922
C	1.718170	-4.437620	-0.208813
C	1.795060	-4.557871	-1.604610
C	1.655675	-3.416770	-2.412295
C	1.474457	-2.165427	-1.807444
C	3.774178	-0.332576	0.603204
C	2.582920	2.308746	-0.149607
C	1.348455	-3.148532	1.951657
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Cl	-2.326349	-1.036114	1.606770
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H	-5.471082	1.606880	0.042436
H	-4.359251	0.624160	1.047533
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H	-1.389870	-2.225906	-2.272332
H	-1.390792	-2.861368	-0.488935
H	2.190968	-0.372766	2.030351
H	2.020232	1.912404	1.891234
H	1.801126	-5.346001	0.409632
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H	1.694400	-3.495730	-3.510003
H	1.354491	-1.256406	-2.416999
C	0.109594	-3.951436	2.405448
C	2.622349	-3.620881	2.684861
H	1.154579	-2.094045	2.236377
H	-6.876540	-2.097006	1.159643
H	-5.352174	-1.469034	1.883988
H	-6.839360	-0.457542	1.878705
H	-7.736062	-1.095335	-1.067341
H	-7.692960	0.546163	-0.343709
H	-6.812185	0.216288	-1.872202
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C	4.013124	3.855220	-2.037473
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H	5.274132	4.445908	-0.361082
H	4.566686	4.460341	-2.773204
H	2.577963	3.100349	-3.492856
H	1.302440	1.752427	-1.837669
C	4.713742	-0.500911	1.643857
C	6.075288	-0.705971	1.363058
C	6.515505	-0.756761	0.029616
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C	4.229354	-0.378952	-0.732172
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  C     -2.009111     3.328854     2.783913
  H     -0.878675     5.184034     2.629924
  H     -2.628126     5.387281     2.368352
  C     -0.869295     2.346581     2.460375
  H     -2.132766     3.410874     3.885015
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  H      2.502688    -3.511760     3.783512
  H      2.831109    -4.692906     2.481447
  H      3.516450    -3.043165     2.373222
  H     -0.000164    -3.892553     3.508882
  H     -0.817930    -3.540209     1.957853
  H      0.194712    -5.025341     2.134426
97
NP1 E(gas)=-2679.12037082 G(gas)=-2678.403781 E(CH2Cl2)=-2679.13302907
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  C     -1.310437    -2.113999    -0.356173
  C     -1.057746    -2.127473    -1.748038
  C     -0.886963    -3.337960    -2.432969
  C     -0.988161    -4.549463    -1.728598
  C     -1.240241    -4.532563    -0.348180
  N     -1.479143    -0.835882     0.271683
  C     -2.744952    -0.404680     0.953220
  C     -2.691575     1.147734     0.737850
  N     -1.230253     1.334957     0.626867
  C     -0.574950     0.198132     0.254155
  C     -4.020585    -1.112300     0.552412
  C     -4.370088    -1.360530    -0.793413
  C     -5.588848    -1.981848    -1.109681
  C     -6.481743    -2.358423    -0.090704
  C     -6.147007    -2.113092     1.251810
  C     -4.922634    -1.499761     1.567519
  C     -3.489051     1.688896    -0.445996
  C     -2.976906     1.692038    -1.761041
  C     -3.766577     2.157413    -2.827148
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  C     -5.587941     2.627471    -1.288885
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  C     -0.559651     2.615945     0.918936
  C     -0.977755     3.774848    -0.007074
  C     -0.177341     5.049280     0.320581
  C     -0.306141     5.445643     1.800904
  C      0.101887     4.284507     2.722854
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C	3.773413	0.473015	-0.938544
C	4.706249	-0.377393	-0.113824
C	6.230487	-0.210831	-0.445360
C	6.982156	-1.252094	0.451677
C	8.485318	-1.245543	0.359992
C	9.241514	-2.257888	-0.106524
C	-1.537542	-3.373712	1.900721
C	-0.151894	-3.539445	2.567872
Cl	1.910034	0.435168	2.131343
Cl	0.742365	1.117994	-2.385397
C	1.655367	-1.424182	-0.467880
C	-2.526271	-4.451367	2.387004
C	6.502694	-0.515043	-1.933722
C	6.694420	1.221955	-0.110858
H	8.996711	-0.333067	0.720504
H	3.625953	0.190831	-1.996875
H	2.438185	-1.821796	-1.151972
H	-3.067527	1.633805	1.660906
H	-2.600584	-0.564757	2.046528
H	1.075289	-2.198705	0.074020
H	-1.301452	-5.489810	0.192962
H	-0.868247	-5.511097	-2.252386
H	-0.683391	-3.330612	-3.515231
H	-0.975758	-1.165745	-2.278144
H	-1.934850	-2.394800	2.234423
H	7.592237	-0.510615	-2.144440
H	6.111904	-1.515639	-2.219550
H	6.028061	0.236718	-2.598028
H	6.686542	-1.056236	1.509123
H	6.603219	-2.268678	0.204085
H	7.765681	1.369174	-0.359736
H	6.116486	1.972724	-0.688333
H	6.559172	1.449864	0.968487
H	2.842603	2.394164	-1.264730
H	3.527559	2.085723	0.469071
H	4.455626	-1.452556	-0.258501
H	4.544775	-0.155755	0.962824
H	10.341602	-2.193433	-0.135007
H	8.786850	-3.195465	-0.472129
H	-4.658764	-1.319892	2.623283
H	-6.837224	-2.406475	2.058678
H	-7.437041	-2.845523	-0.343266
H	-5.843219	-2.171574	-2.164381
H	-3.684293	-1.068290	-1.600718
H	-5.209030	2.171043	0.800884
H	-6.607657	2.996848	-1.095282
H	-5.686600	2.991270	-3.434907
H	-3.349505	2.161280	-3.846909
H	-1.943253	1.359560	-1.957239
H	0.526356	2.421775	0.742455
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H	-0.314030	2.154772	3.026134
H	-0.039710	4.560508	3.789855
H	1.188813	4.075324	2.599667

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  H     -0.823212     3.476736    -1.064174
  H     -0.252898    -3.566767     3.673557
  H      0.333156    -4.485989     2.247352
  H      0.527093    -2.699099     2.315820
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  C     -5.074353    -1.520902     1.286538
  C     -6.290314    -2.085053     0.865000
  C     -6.532123    -2.284813    -0.504736
  C     -5.554900    -1.912058    -1.444429
  C     -2.826280    -0.476830     0.864280
  C     -2.766769     1.096397     0.762869
  N     -1.308214     1.294912     0.651545
  C     -0.664949     0.181651     0.221704
  N     -1.543273    -0.861499     0.196249
  C     -0.587550     2.532336     0.996661
  C     -1.090780     3.783399     0.253000
  C     -0.259455     5.022431     0.634357
  C     -0.226895     5.249724     2.155150
  C      0.282076     3.999227     2.891085
  C     -0.533311     2.746654     2.524604
  C     -3.559128     1.716628    -0.385902
  C     -3.045975     1.778962    -1.699948
  C     -3.825410     2.321088    -2.736916
  C     -5.119850     2.806020    -2.479042
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  C     -0.841347    -3.654435    -2.180307
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  C     -1.124049    -3.119390     2.159754
  C     -2.297172    -3.902641     2.787787
  Cl     0.595372     0.954077    -2.517516
  C      1.810833    -1.337198    -0.850999
  C      3.096433     1.559983    -0.549539
  C      3.640419     0.371940    -1.058275
  C      4.667886    -0.457574    -0.320866
  C      6.154099     0.008596    -0.519051
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H	-3.143631	1.518738	1.717268
H	-2.734009	-0.729868	1.945702
H	2.247560	-2.078984	-0.144142
H	-0.730779	-5.416687	0.751088
H	-0.541260	-5.760696	-1.703167
H	-0.733506	-3.788654	-3.268079
H	-1.172451	-1.502595	-2.315041
H	-1.270840	-2.042311	2.380428
H	7.600799	0.252784	-2.154738
H	6.321959	-0.951711	-2.498888
H	5.946925	0.802773	-2.568790
H	6.678783	-1.096771	1.283409
H	6.812780	-2.057867	-0.212727
H	7.433624	1.730949	-0.030526
H	5.747376	2.171327	-0.400757
H	6.142807	1.417561	1.178795
H	2.707372	2.314251	-1.254108
H	3.377502	1.886723	0.466316
H	4.611386	-1.512696	-0.662958
H	4.420474	-0.450770	0.762786
H	10.503029	-1.407337	-0.336431
H	9.118780	-2.539620	-0.917035
H	-4.884665	-1.374725	2.363242
H	-7.046927	-2.376717	1.610636
H	-7.480563	-2.733775	-0.840126
H	-5.736464	-2.065580	-2.519915
H	-3.591675	-1.045453	-1.766719
H	-5.266352	2.169620	0.889032
H	-6.645335	3.132255	-0.957289
H	-5.724929	3.233649	-3.294449
H	-3.408903	2.369146	-3.755780
H	-2.022698	1.427212	-1.921113
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H	-1.574013	2.857474	2.908618
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H	0.260057	4.152459	3.991289
H	1.349840	3.821966	2.627359
H	-1.254319	5.494912	2.511572
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H	1.043061	-2.861060	2.429716
H	-2.344799	-3.722289	3.882594
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97
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C	-0.490134	-2.331523	-1.467485
C	0.064471	-3.541509	-1.906219
C	0.309125	-4.565283	-0.975938
C	0.028632	-4.354124	0.382146
N	-1.374321	-0.865439	0.269595
C	-2.741228	-0.679902	0.845723
C	-2.927797	0.882828	0.691357
N	-1.517237	1.325961	0.607086
C	-0.699131	0.312445	0.257845
C	-3.833459	-1.551159	0.261534
C	-3.921324	-1.835909	-1.117942
C	-4.976530	-2.615860	-1.617956
C	-5.964937	-3.114686	-0.751403
C	-5.890485	-2.832876	0.623352
C	-4.828156	-2.061537	1.124052
C	-3.771893	1.330788	-0.498877
C	-3.228494	1.440296	-1.797316
C	-4.049751	1.811960	-2.875986
C	-5.415687	2.078160	-2.674553
C	-5.961137	1.974652	-1.382982
C	-5.141871	1.604126	-0.303493
C	-1.029129	2.668021	0.978113
C	-1.768570	3.814918	0.264738
C	-1.190555	5.181612	0.677478
C	-1.207593	5.375613	2.203156
C	-0.468380	4.229788	2.913914
C	-1.024096	2.851712	2.512123
Ru	1.217509	0.524260	-0.238570
C	2.683097	-0.632158	-0.891918
C	3.420120	0.770270	-0.928806
C	4.747307	0.755545	-0.128541
C	5.981185	0.061115	-0.784394
C	7.147012	0.221972	0.254588
C	8.494160	-0.305206	-0.164727
C	9.156736	-1.313337	0.434179
C	-0.723802	-2.953888	2.365658
C	0.573846	-3.184062	3.169509
Cl	1.857593	0.181709	2.046985
Cl	0.521690	0.948404	-2.514700
C	2.517157	1.994742	-0.424696
C	-1.868479	-3.854247	2.880926
C	5.750378	-1.439781	-1.054201
C	6.349507	0.771625	-2.106686
H	8.974484	0.197218	-1.025699
H	3.554398	0.987145	-2.008024
H	2.877797	2.428219	0.529099
H	-3.393950	1.268967	1.621104
H	-2.685266	-0.896010	1.936949
H	2.312188	2.728778	-1.227383
H	0.247189	-5.157590	1.103738
H	0.728938	-5.529118	-1.305445
H	0.294296	-3.682923	-2.973872

```
  H     -0.676645    -1.510464    -2.176887
  H     -1.008944    -1.894611     2.534858
  H      6.686946    -1.916645    -1.411380
  H      5.435030    -1.974952    -0.133793
  H      4.974428    -1.605307    -1.829259
  H      7.247572     1.309880     0.479267
  H      6.839505    -0.266637     1.205271
  H      7.240183     0.310437    -2.580741
  H      5.525209     0.705904    -2.847281
  H      6.569914     1.848564    -1.942286
  H      2.518901    -1.076782    -1.891137
  H      3.078975    -1.325876    -0.127251
  H      4.538316     0.306773     0.867225
  H      5.042504     1.809683     0.065975
  H     10.150260    -1.639869     0.085720
  H      8.732201    -1.846678     1.302816
  H     -4.768082    -1.852444     2.205349
  H     -6.657344    -3.221882     1.311885
  H     -6.791115    -3.726592    -1.147060
  H     -5.026409    -2.834418    -2.696310
  H     -3.157506    -1.447325    -1.805901
  H     -5.574428     1.526109     0.708164
  H     -7.028426     2.188483    -1.212932
  H     -6.054288     2.372686    -3.522670
  H     -3.611773     1.897663    -3.883254
  H     -2.154973     1.250943    -1.973774
  H      0.031519     2.682785     0.634346
  H     -2.067133     2.749041     2.892612
  H     -0.419229     2.038655     2.966078
  H     -0.523133     4.349199     4.017206
  H      0.613861     4.271565     2.653672
  H     -2.264108     5.410244     2.557145
  H     -0.756972     6.354774     2.473940
  H     -1.757278     5.992712     0.172248
  H     -0.141943     5.261554     0.308862
  H     -2.850429     3.778792     0.525103
  H     -1.703957     3.676172    -0.833654
  H      0.387510    -3.006049     4.249746
  H      0.944153    -4.226135     3.065437
  H      1.370024    -2.485213     2.842889
  H     -2.059412    -3.666604     3.958867
  H     -2.812816    -3.683376     2.324531
  H     -1.610253    -4.929303     2.771724
52
pcy3 E(gas)=-1046.56037777 G(gas)=-1046.141425 E(CH2Cl2)=-1046.56258699
  P      0.004987    -0.006533    -1.260465
  C      1.627679    -0.695914    -0.547442
  C     -0.210394     1.744249    -0.548571
  C     -1.411423    -1.056601    -0.552105
  H     -2.276604    -0.663782    -1.140523
  H      0.559675     2.303679    -1.134185
  H      1.730371    -1.638805    -1.138698
  C     -1.816305    -0.981538     0.935503
  C     -1.219992    -2.527649    -0.999782
  C      1.777967    -1.090395     0.939638
  C      2.792284     0.222427    -0.993549
```

C	-1.583373	2.300945	-1.000094
C	0.047979	2.063643	0.941058
C	-3.056549	-1.851069	1.228034
H	-0.973282	-1.316493	1.578035
H	-2.027504	0.069019	1.223607
C	-2.855569	-3.309149	0.784403
H	-3.307989	-1.802736	2.310262
H	-3.933239	-1.425041	0.686527
C	-2.462851	-3.386884	-0.700760
H	-2.049040	-3.771662	1.399999
H	-3.774058	-3.905228	0.977196
H	-2.279304	-4.441455	-1.002154
H	-3.313419	-3.027462	-1.325156
H	-0.345849	-2.966160	-0.464538
H	-0.971849	-2.563238	-2.083335
C	-0.094132	3.573126	1.226921
H	-0.666503	1.500538	1.580880
H	1.062901	1.726842	1.236912
C	-1.460439	4.116720	0.777541
H	0.069367	3.772831	2.308668
H	0.711170	4.121624	0.684709
C	-1.719669	3.806564	-0.706538
H	-2.261996	3.647052	1.394377
H	-1.525347	5.210671	0.965042
H	-2.727472	4.165093	-1.010482
H	-0.987085	4.367292	-1.332118
H	-2.396369	1.758002	-0.464079
H	-1.734768	2.099929	-2.083441
C	3.160200	-1.716145	1.220499
H	1.643596	-0.197225	1.588097
H	0.983594	-1.808421	1.231053
C	4.308962	-0.795461	0.776351
H	3.253002	-1.963504	2.300779
H	3.238053	-2.684261	0.672826
C	4.167296	-0.407604	-0.705008
H	4.298196	0.129620	1.398919
H	5.291520	-1.282219	0.960112
H	4.978259	0.291385	-1.005564
H	4.290272	-1.318174	-1.336065
H	2.723987	1.194402	-0.451793
H	2.692880	0.460291	-2.075474

25

Model of substrate **15** E(gas)=-352.27643243 G(gas)=-352.094685 E(CH2Cl2)=-352.277946504

C	-3.637620	-0.273775	-0.184025
C	-2.544741	0.512529	-0.147514
C	-1.235316	0.217103	-0.830423
C	0.000000	0.000019	0.106813
C	-0.235193	-1.240921	0.993340
H	-2.602242	1.463176	0.415531
C	1.235314	-0.217143	-0.830410
C	2.544731	-0.512563	-0.147483
H	2.602208	-1.463179	0.415615
C	0.235195	1.241028	0.993242
C	3.637629	0.273712	-0.184039
H	1.170334	1.132703	1.580605

```
  H      0.331908     2.163367     0.380360
  H     -0.596827     1.394877     1.711129
  H      0.990555    -1.064558    -1.513356
  H      1.351486     0.682229    -1.475460
  H      0.596829    -1.394713     1.711238
  H     -1.170332    -1.132550     1.580694
  H     -0.331906    -2.163308     0.380529
  H     -4.571139     0.008724     0.329572
  H     -3.641974    -1.229593    -0.737064
  H     -1.351468    -0.682308    -1.475423
  H     -0.990576     1.064486    -1.513415
  H      4.571141    -0.008781     0.329573
  H      3.642008     1.229497    -0.737134
6
ethylene E(gas)=-78.5245851448 G(gas)=-78.496235 E(CH2Cl2)=-78.5254875623
  C      0.000000     0.000000     0.670834
  C      0.000000     0.000000    -0.670834
  H      0.000000     0.938061    -1.251855
  H      0.000000    -0.938061    -1.251855
  H      0.000000    -0.938061     1.251855
  H      0.000000     0.938061     1.251855
72
Anti Rh (42) E(gas)=-2071.27094193
  C     -3.145075     0.173677     1.678504
  C     -2.616056    -0.011805     0.249031
  C     -3.549065     0.636448    -0.782105
  C     -4.969965     0.071558    -0.649400
  C     -5.516852     0.244209     0.771418
  C     -4.572038    -0.376142     1.805781
  N     -1.204898     0.414078     0.123776
  C     -0.735274     1.789708     0.405917
  C      0.803648     1.572662     0.596481
  N      0.977112     0.198423     0.053475
  C     -0.196803    -0.440237    -0.076619
  H     -1.166862     2.134403     1.344554
  Rh    -0.414743    -2.492647    -0.414306
  C     -0.254449    -2.243187    -2.243667
  C      2.279536    -0.403102    -0.072857
  C      2.642406    -1.391879     0.844141
  C      3.894264    -1.985191     0.780593
  C      4.797943    -1.576379    -0.194091
  C      4.432434    -0.594622    -1.104585
  C      3.169177     0.008595    -1.078442
  C      1.274105     1.728630     2.028448
  C      2.044159     2.838708     2.376911
  C      2.442918     3.041887     3.695464
  C      2.077037     2.129845     4.679213
  C      1.312599     1.016100     4.338179
  C      0.911038     0.815074     3.022484
  C      2.808716     1.039558    -2.139364
  C      2.879057     0.447570    -3.557961
  C      3.679296     2.303204    -2.030508
  C     -0.656565    -4.399106    -0.529269
  Cl    -0.667280    -2.692613     1.977593
  C     -1.055425     2.806451    -0.674721
  H      1.348948     2.279930    -0.026124
```

H	5.142071	-0.296982	-1.867398
H	5.782835	-2.024559	-0.249975
H	4.160687	-2.755819	1.493187
H	1.930369	-1.697067	1.598112
H	1.772869	1.336084	-1.975525
H	2.336047	3.550431	1.612202
H	3.043601	3.906910	3.949916
H	2.389888	2.281289	5.705325
H	1.030678	0.296855	5.097667
H	0.328116	-0.065018	2.773685
H	-2.582504	-1.085003	0.045331
H	-3.576158	1.719850	-0.635682
H	-3.164356	0.463768	-1.789789
H	-5.626744	0.558641	-1.374843
H	-4.960487	-0.993758	-0.906267
H	-5.637911	1.313031	0.983952
H	-6.511537	-0.202591	0.851144
H	-4.943543	-0.200102	2.818589
H	-4.546082	-1.462640	1.671680
H	-3.148112	1.238106	1.939811
H	-2.479954	-0.339437	2.374728
H	2.558581	1.190175	-4.292801
H	3.896249	0.145710	-3.816154
H	2.235438	-0.427606	-3.657048
H	3.354160	3.054890	-2.753545
H	3.625972	2.744278	-1.033008
H	4.728980	2.078923	-2.232711
O	-0.153443	-2.074752	-3.374575
O	-0.785206	-5.528156	-0.555239
C	-0.930235	2.507064	-2.032982
C	-1.170085	3.480228	-2.996602
C	-1.536332	4.769222	-2.616450
C	-1.662975	5.077140	-1.266109
C	-1.424254	4.100241	-0.303120
H	-0.665245	1.503213	-2.341643
H	-1.076363	3.230501	-4.046662
H	-1.726516	5.525359	-3.368386
H	-1.953589	6.074938	-0.960160
H	-1.529935	4.345815	0.748025

72

Syn Rh (**41**) E(gas)=-2071.26262662 A.U.

C	2.287884	2.907692	0.171172
C	1.975840	1.654065	0.996521
C	2.104448	1.926135	2.502980
C	3.495979	2.474739	2.846298
C	3.831099	3.718912	2.018575
C	3.683779	3.441673	0.519580
N	0.680561	1.017252	0.677838
C	-0.638781	1.646601	0.924400
C	-1.575153	0.384656	0.914839
N	-0.713121	-0.612762	0.213862
C	0.572526	-0.219302	0.187882
C	-0.989457	2.748553	-0.059136
C	-0.646500	2.676978	-1.410116
C	-1.014012	3.696752	-2.280688
C	-1.729479	4.796829	-1.816880

C	-2.072968	4.875726	-0.471659
C	-1.701590	3.857179	0.399650
Rh	2.163507	-1.300094	-0.642343
C	2.424966	-2.229243	0.938143
C	-1.179581	-1.886495	-0.270762
C	-1.157013	-2.092937	-1.651691
C	-1.613601	-3.282226	-2.197417
C	-2.115911	-4.269577	-1.357744
C	-2.119831	-4.069161	0.014820
C	-1.638815	-2.890712	0.597398
C	-2.969981	0.578617	0.371053
C	-4.008889	0.794050	1.279177
C	-5.307744	1.026303	0.840123
C	-5.587819	1.032717	-0.521540
C	-4.561550	0.812134	-1.434597
C	-3.262515	0.590761	-0.993290
C	-1.604007	-2.772459	2.115499
C	-0.820870	-3.925521	2.766458
C	-3.018862	-2.679500	2.712827
C	3.607713	-2.183429	-1.565692
Cl	1.798858	-0.016554	-2.650644
H	-0.658506	2.071852	1.927220
H	-1.677777	0.056887	1.952892
H	-2.491482	-4.858124	0.657017
H	-2.490491	-5.199405	-1.768306
H	-1.581693	-3.430765	-3.269339
H	-0.754811	-1.317037	-2.288988
H	-1.069175	-1.854802	2.365104
H	-3.800933	0.779313	2.343612
H	-6.098929	1.192630	1.560960
H	-6.598868	1.205204	-0.869541
H	-4.771156	0.813383	-2.497152
H	-2.476633	0.427519	-1.715911
H	-1.969212	3.927574	1.448543
H	-2.624317	5.730245	-0.098539
H	-2.011207	5.590440	-2.498182
H	-0.733154	3.631664	-3.324866
H	-0.068316	1.840362	-1.784764
H	2.710584	0.891291	0.725401
H	1.348993	2.656742	2.813420
H	1.910360	1.004700	3.059290
H	3.549487	2.698263	3.915086
H	4.244943	1.698641	2.653029
H	3.158668	4.536414	2.304388
H	4.845938	4.057452	2.244242
H	3.879837	4.349333	-0.056645
H	4.437968	2.709593	0.209592
H	1.544010	3.683781	0.369744
H	2.228759	2.663421	-0.890079
H	-0.744990	-3.764355	3.844490
H	-1.318699	-4.885064	2.612852
H	0.189540	-4.002070	2.365289
H	-2.969265	-2.516039	3.792356
H	-3.594209	-1.867792	2.266475
H	-3.572730	-3.605880	2.544134
O	2.598348	-2.791635	1.923349

```
  O      4.454297    -2.683887    -2.136530
66
nhc-anti E(gas)=-1273.55138855 A.U.
  C     -3.091388    -2.056227    -0.714379
  C     -2.573666    -0.766420    -1.370744
  C     -3.647450     0.330651    -1.338086
  C     -4.941506    -0.151422    -2.007999
  C     -5.463150    -1.442771    -1.370259
  C     -4.389659    -2.535300    -1.376357
  N     -1.268327    -0.355490    -0.833074
  C     -1.026685    -0.050579     0.603204
  C      0.530632    -0.134964     0.682399
  N      0.885281    -0.164392    -0.770076
  C     -0.161321    -0.400664    -1.589838
  H     -1.465298    -0.828050     1.229111
  C      2.245731    -0.221948    -1.213232
  C      2.703650    -1.412143    -1.783530
  C      4.012244    -1.536900    -2.222288
  C      4.885939    -0.463925    -2.080384
  C      4.428485     0.723693    -1.528438
  C      3.105864     0.882244    -1.098490
  C      1.048372    -1.327636     1.460589
  C      1.753081    -1.130503     2.647768
  C      2.206220    -2.212072     3.398481
  C      1.959129    -3.509749     2.967277
  C      1.258173    -3.718642     1.781740
  C      0.808522    -2.637212     1.034885
  C      2.640251     2.239122    -0.590880
  C      2.745692     3.311513    -1.689088
  C      3.389226     2.676314     0.678225
  C     -1.559049     1.293168     1.065418
  H      0.920274     0.769430     1.148172
  H      5.112146     1.560480    -1.447208
  H      5.915187    -0.547774    -2.407886
  H      4.349170    -2.466762    -2.663784
  H      2.008287    -2.233777    -1.885429
  H      1.583215     2.153655    -0.342262
  H      1.949463    -0.120603     2.990128
  H      2.755552    -2.038689     4.315955
  H      2.313407    -4.353811     3.546286
  H      1.066955    -4.727629     1.436453
  H      0.275029    -2.809454     0.107874
  H     -2.350784    -0.987759    -2.416572
  H     -3.861515     0.615933    -0.303963
  H     -3.268833     1.223450    -1.840439
  H     -5.700191     0.633784    -1.951778
  H     -4.753480    -0.325857    -3.073788
  H     -5.765907    -1.238591    -0.336490
  H     -6.358144    -1.789736    -1.894155
  H     -4.755213    -3.432512    -0.869368
  H     -4.178004    -2.827508    -2.411223
  H     -3.279880    -1.882718     0.351036
  H     -2.322699    -2.830531    -0.781758
  H      2.335605     4.260621    -1.334420
  H      3.783944     3.486615    -1.980057
  H      2.194075     3.013195    -2.582296
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  H      2.986619     3.619173     1.056446
  H      3.304987     1.929011     1.469921
  H      4.453311     2.825528     0.480505
  C     -1.411399     2.444785     0.288723
  C     -1.853200     3.675910     0.758461
  C     -2.451784     3.776394     2.012172
  C     -2.606238     2.635629     2.791404
  C     -2.161856     1.403812     2.318922
  H     -0.965702     2.370534    -0.695843
  H     -1.735489     4.559487     0.142565
  H     -2.798900     4.736082     2.375056
  H     -3.075287     2.701407     3.765789
  H     -2.287747     0.517602     2.931413
66
nhc-syn E(gas)=-1273.54399617 A.U.
  C      3.789923    -0.810861    -0.697067
  C      2.547147    -1.634348    -0.332965
  C      2.763694    -2.397775     0.985308
  C      4.019974    -3.275126     0.930589
  C      5.260904    -2.460295     0.554031
  C      5.040626    -1.697701    -0.755826
  N      1.293196    -0.869054    -0.307918
  C      1.066580     0.325580     0.549362
  C     -0.491609     0.280769     0.661659
  N     -0.822854    -0.503521    -0.570094
  C      0.207755    -1.281172    -0.981022
  C      1.657293     1.603109    -0.023467
  C      1.719635     1.838094    -1.397942
  C      2.241752     3.029239    -1.889756
  C      2.713006     4.004122    -1.014995
  C      2.658792     3.778235     0.356077
  C      2.135162     2.585586     0.844320
  C     -2.180920    -0.801260    -0.932767
  C     -2.767595    -0.053293    -1.953153
  C     -4.075417    -0.287197    -2.352158
  C     -4.811561    -1.282581    -1.719846
  C     -4.225374    -2.037787    -0.713889
  C     -2.905519    -1.825399    -0.300727
  C     -1.227469     1.581492     0.871946
  C     -1.752806     1.853845     2.137327
  C     -2.418522     3.046969     2.399427
  C     -2.578588     3.988006     1.389225
  C     -2.068001     3.725200     0.121346
  C     -1.398696     2.534965    -0.134257
  C     -2.295379    -2.728735     0.760679
  C     -2.151143    -4.169740     0.242629
  C     -3.077733    -2.686046     2.083013
  H      1.491754     0.170654     1.541598
  H     -0.724554    -0.355214     1.523885
  H     -4.805027    -2.823874    -0.244474
  H     -5.835558    -1.477535    -2.015194
  H     -4.513827     0.300706    -3.149065
  H     -2.175093     0.708291    -2.441164
  H     -1.286391    -2.369946     0.961507
  H     -1.642726     1.119851     2.928249
  H     -2.817329     3.235545     3.388873
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  H     -3.101409     4.916199     1.585352
  H     -2.191441     4.450854    -0.673489
  H     -1.002303     2.347915    -1.121642
  H      2.096573     2.417763     1.915170
  H      3.026847     4.527784     1.046268
  H      3.123759     4.929692    -1.399653
  H      2.285296     3.194965    -2.959707
  H      1.367651     1.078066    -2.084275
  H      2.378559    -2.369485    -1.122982
  H      2.862200    -1.683695     1.811468
  H      1.880196    -3.007299     1.191353
  H      4.166979    -3.773825     1.892601
  H      3.871240    -4.068856     0.189481
  H      5.482474    -1.745915     1.355866
  H      6.132753    -3.115066     0.470182
  H      5.914552    -1.084282    -0.990987
  H      4.935929    -2.416182    -1.577203
  H      3.944290    -0.019308     0.043038
  H      3.633839    -0.314813    -1.656626
  H     -1.666687    -4.798470     0.994350
  H     -3.124698    -4.611023     0.015925
  H     -1.546492    -4.193067    -0.664839
  H     -2.571464    -3.284787     2.844339
  H     -3.170991    -1.664734     2.458464
  H     -4.086768    -3.088252     1.966814
6
rh-co-relax E(gas)=-797.629609638 A.U.
  Rh     0.021873    -0.291625    -0.000283
  C     -1.837303    -0.620817    -0.000068
  C     -0.285986     1.505252    -0.000025
  Cl     2.292279    -0.377045     0.000399
  O     -2.952526    -0.854275     0.000657
  O     -0.449136     2.632559     0.000157
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