Electronic Supplementary Information (ESI) for:

Methyl and Phenyl Substituent Effects on the Catalytic Behavior of NHC Ruthenium Complexes

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1. General Information

All reactions involving organometallic compounds were performed under nitrogen using standard Schlenk and glove-box techniques. Reagents were purchased from Sigma Aldrich Company and TCI chemicals and used without further purifications. Solvents were dried and distilled before use. Deuterated solvents were degassed under a N_2 flow and stored over activated 4 Å molecular sieves. 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 to the residual protons of the deuterated solvent in the NMR spectra. ^{31}P chemical shifts are referenced using H_3PO_4 as external standard. NMR spectra data are reported as follows: chemical shift (δ ppm), multiplicity, coupling costant in Hertz (Hz) and integration. Multiplicity are abbreviated as follows: singlet (s), doublet (d), triplet (t), quintuplet (quin), 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. Infrared spectra were recorded with a Bruker Vertex70 spectrometer. Electrochemical measurements were conducted with an AUTOLAB PG STAT 302N potentiostat. A three-electrode configuration was employed. The working electrode was a Pt disk (diameter 2 mm), the counter-electrode a Pt bar and the reference a quasi-reference electrode (Pt-QRE)[1], calibrated *vs*. octamethylferrocene as internal standard. All cyclic voltammograms were recorded in dry CH_2Cl_2 under a nitrogen atmosphere using NBu_4PF_6 (0.1 M) as supporting electrolyte at a scan rate of 100 mV/s. Potentials were referenced against the potential of octamethylferrocene.

[1] A. J. Bard, L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd ed., Wiley, New York, 2001, pp. 53–54.

2. Synthesis of ruthenium complex 3, 4, 7 and 8

Synthesis of N^2,N^3-di([1,1'-biphenyl]-2-yl)butane-2,3-diamine (**B**)

Meso-2,3-diaminebutane (**A**) was synthesized following literature procedure.[2] Diarylation to give compound **B** was accomplished by Pd-catalyzed Heck coupling reaction with 2-bromo-1,1'-biphenyl. Under nitrogen atmosphere, tris(dibenzylideneacetone)dipalladium(0) ($Pd_2(dba)_3$) (0.249 mmol, 228 mg), 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP) (0.600 mmol, 373 mg), sodium tert-butoxide (NaOtBu) (15.0 mmol, 1.44 g) and toluene (16.6 mL) were introduced in a flask equipped with a reflux condenser and stirred for 20 min. After this time, diamine **A** (4.99 mmol, 440mg) and 2-bromobiphenyl (9.98 mmol, 1.72 mL) were added and the solution was heated to 100°C for 20 hours. The reaction mixture was then cooled at room temperature, diluted with hexane and filtered through a plug of silica gel. The product was eluted from silica gel with methylene chloride. The solvent was removed under vacuum furnishing **B** as a yellow solid (2.80 mmol, 1.10 g, 56%).

^{1}H-NMR (300 MHz , CD_2Cl_2) δ: 7.43-7.13 (o m, 12H), 7.03 (dd, ^3J=1.35 Hz, ^3J=7.50 Hz, 2H), 6.74-6.64 (o m, 4H), 3.91 (d, ^3J=9.45 Hz, 2H), 3.80-3.68 (o m, 2H), 0.97 (d, ^3J=6.23 Hz 6H).

^{13}C-NMR (75 MHz, CD_2Cl_2) δ: 144.6, 130.6, 129.6, 129.1, 129.0, 127.4, 117.1, 111.4, 51.8, 16.2.

Anal. Calc. for $C_{28}H_{28}N_2$ (392.5): C 85.67; H 7.19; N 7.14. Found: C 85.74; H 7.26; N 7.19.

Synthesis of 1,3-di([1,1'-biphenyl]-2-yl)-4,5-dimethyl-4,5-dihydro-1H-imidazol-3-ium chloride (**C**)

Diamine **B** was introduced in a vial and dissolved in 9.0 mL of diethyl ether. A solution of hydrogen chloride (2.0 M in diethyl ether; 2.35 mmol, 1.2 ml) was added dropwise to precipitate the diamine hydrochloride salt as an off-white powder. The product was collected by filtration and washed with diethyl ether. Dried diamine salt (1.94 mmol, 902 mg) and a large excess of triethyl orthoformate (3.3 mL) were placed in a 50 ml round bottom flask equipped with a magnetic stirrer. The flask was fitted with a condenser and heated to 135 °C in an oil bath for four hours. Upon cooling to room temperature, the solid product was washed several times with hexane and then with Et_2O to give the desired imidazolinium chloride salt **C** as a faint yellow solid (0.389 mmol, 171 mg, 50% yield).

^{1}H-NMR (400MHz, $CDCl_3$) δ: 9.57 (br s, 1H), 8.38 (br s, 2H), 7.56 (br s, 2H), 7.52-7.48 (br m, 8H), 7.37-7.36 (br m, 6H), 3.80 (br s, 2H), 0.99 (br s, 6 H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ: 157.0, 137.6, 137.6, 131.2, 131.0, 129.9, 129.4, 129.1, 128.9, 128.5, 128.3, 61.3, 12.4.

Anal. Calc. for $C_{29}H_{27}ClN_2$ (439.0): C 79.34; H 6.20; N 6.38. Found: C 79.42; H 6.31; N 6.44.

[2] Chooi, S.Y.M.; Leung, P.-h.; Ng, S.-c.; Quek, G.H.; Sim, K.Y. *Tetrahedron: Asymmetry* **1991**, *2*, 981-982.

Synthesis of meso-N^1,N^2-di([1,1'-biphenyl]-2-yl)-1,2-diphenylethane-1,2-diamine (**E**)

Under nitrogen atmosphere, tris(dibenzylideneacetone)dipalladium(0) ($Pd_2(dba)_3$) (0.236 mmol, 216 mg), 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP) (0.565 mmol, 352 mg), sodium *tert*-butoxide (NaOtBu) (14.1 mmol, 1.36 g) and toluene (16.0 mL) were introduced in a flask equipped with a reflux condenser and stirred for 20 min. After this time, *meso*-1,2-diphenylethylenediamine (**D**) (4.71mmol, 1.00 g) and 2-bromobiphenyl (9.42 mmol, 1.60 mL) were added and the solution was heated to 105°C for 48 hours. The reaction mixture was then cooled at room temperature, diluted with hexane and filtered through a plug of silica gel. The product was eluted from silica gel with methylene chloride. The solvent was removed under vacuum to give **E** as a pale yellow solid (4.61 mmol, 2.38 g, 98%).

^{1}H-NMR (400 MHz, $CDCl_3$) δ: 7.41-7.35 (o m, 5H), 7.22 (d, ^3J=7.77 Hz, 5H), 7.12 (t, ^3J = 7.48 Hz, 2H), 7.06-6.97 (o m, 8H), 6.70-6.33 (o m, 6H), 6.30 (d, ^3J=8.39 Hz, 2H), 4.78 (d, ^3J=6.37 Hz, 2H), 4.66 (d, ^3J=6.95 Hz, 2H). ^{13}C-NMR (75 MHz, CD_2Cl_2) δ: 143.6, 139.6, 138.6, 130.2, 129.7, 129.4, 129.2, 128.7, 128.6, 128.5, 127.8, 127.6, 127.4, 117.6, 111.9, 62.3.

Anal. Calc. for $C_{38}H_{32}N_2$ (516.7) : C 88.34; H 6.24; N 5.42. Found: C 88.40; H 6.32; N 5.51.

Synthesis of 1,3-di([1,1'-biphenyl]-2-yl)-4,5-diphenyl-4,5-dihydro-1H-imidazol-3-ium tetrafluoroborate (**F**)

Triethyl orthoformate (2.40 mL, 13.9 mmol), diamine **E** (1.55 mmol, 800 mg) and ammonium tetrafluoroborate (1.91 mmol, 200 mg) were introduced in a 50 mL round-bottom flask equipped with a magnetic stirrer. The reaction mixture was heated at 120°C for 12 h. After cooling to room temperature, the product was precipitated and washed with diethylether (3 times x 10 mL). The solid obtained was dissolved in the minimum amount of methylene chloride and then filtered. The crude product was first washed with *n*-hexane and then eluted through a silica-gel chromatography column using *n*-hexane/ethylacetate = 1:3. The fractions containing the desired product were collected and the volatiles were removed in vacuo to afford **F** as a light yellow solid (0.770 mmol, 474 mg, 50% yield).

^{1}H-NMR (300 MHz in CD_2Cl_2) δ: 9.23 (s, 1H), 7.83 (dd, ^3J=1.60 Hz, ^3J=7.65 Hz, 2H), 7.65-7.63 (o m, 6H), 7.51-7,40 (o m, 6H), 7.34-7.27(o m, 6H), 7.01-6.93 (o m, 6H), 6.57-6.54 (o m, 4H), 4.88 (s, 2H). ^{13}C-NMR (75 MHz in CD_2Cl_2) δ: 158.7, 138.3, 137.5, 132.2,132.0, 130.3, 129.8, 129.7, 129.6, 129.5, 129.2, 129.1, 129.0, 128.6, 127.6, 71.2.

Anal. Calc. for $C_{39}H_{31}BF_4N_2$ (614.5): C 76.23; H 5.08; N 4.56. Found: C 76.31; H 5.17; N 4.53.

Synthesis of 1,3-di([1,1'-biphenyl]-2-yl)-4,5-dimethyl-4,5-dihydro-2-imidazolidinylidene] (dichloro)(benzilydene)(tricyclohexylphosphine)ruthenium (**3**)

In a glove box, to a suspension of **C** (0.442 mmol, 194 mg) in toluene (4.1 ml) was added KHMDS (0.455 mmol, 90.8 mg). The reaction mixture was stirred for 15 minutes at RT and then $(PCy_3)Ru(=CHPh)Cl_2$ (0.380 mmol, 312 mg) was added. The flask was removed from the glove box and stirred at 70°C for one hour. The reaction mixture was cooled at room temperature, and purified by column chromatography on TSI silica gel (n-hexane/diethylether = 95:5 to 4:1). The solvent was removed in vacuo to give **3** as a bright green powder (0.126 mmol, 119 mg, 33%). Complex **3** was observed to decompose in less than 1h in both CD_2Cl_2 and $CDCl_3$, therefore all the NMR data were acquired in C_6D_6.

^{1}H-NMR (400 MHz, C_6D_6) δ: 19.92 (s, 1H), 9.63 (d, ^3J=7.83 Hz, 1H); 8.51 (d, ^3J=7.21 Hz, 2H), 8.17 (br s, 2H), 7.95 (br s, 1H), 7.62-7.54 (o m, 3H), 7.46-7.41 (o m, 3H), 7.27 (t, ^3J=7.36 Hz, 1H), 7.22-7.16 (o m, 5H), 7.02-6.76 (o m, 3H), 6.65 (br s, 2H), 3.39 (br d, 2H), 2.12 (o m, 3H), 1.89 (o m, 3H), 1.77-1.68 (o m, 9H), 1.60-1.54 (o m, 10H), 1.19-1.02 (o m, 9H), 0.46 (d, ^3J=5.64 Hz 3H), 0.05 (d, ^3J=5.64 Hz, 3H). ^{13}C-NMR spectrum was not obtained due to the limited stability of complex **3** also in C_6D_6. The diagnostic carbene peak at 19.92 ppm in the ^{1}H NMR spectrum was indeed observed to disappear in C_6D_6 within four hours. ^{31}P NMR (161.97 MHz, C_6D_6) δ: 22.0 (s); 24,0 (br s).

Synthesis of 1,3-di([1,1'-biphenyl]-2-yl)-4,5-diphenyl-4,5-dihydro-2-imidazolidinylidene] (dichloro)(benzilydene) (tricyclohexylphosphine)ruthenium (**4**)

In a glove box, a solution of **F** (0.218 mmol, 134 mg) and potassium hexafluoro^{t}butoxide $[(CF_3)_2CH_3COK]$ (0.218 mmol, 48.0 mg) in 6.5 mL of toluene was stirred at room temperature for five minutes. $(PCy_3)_2Ru(=CHPh)Cl_2$ (0.148 mmol, 122 mg) was then added, the reaction flask was removed from the glove box and heated at 60°C for 1.30 hour in a oil bath. The mixture was then allowed to cool at room temperature and the crude product was purified by flash column chromatography on silica gel (n-hexane/diethylether = 95:5 to 3:1). The purification step allowed us to isolate **4** (104 mg, yield 66%) as a pastel green powder.

^{1}H-NMR (400 MHz,CD_2Cl_2) δ:19.40 (br s, 1 H), 9.38 (br t, 1H), 8.13-6.6 (o m, 30H), 6.21-6.10 (o m, 3H), 4.76-4.42 (o m, 2H), 1.75-0.87 (o m, 35 H).^{13}C NMR (100 MHz, C_6D_6) δ: 306.7, 220.5, 218.1, 151.3, 140.8, 139.9, 138.2, 138.1, 134.0, 133.3, 133.0, 132.7, 131.3, 130.4, 130.3, 129.7,

129.5, 129.1, 129.0, 127.0, 72.2, 71.7, 33.5, 33.4, 30.2, , 29.9, 29.2, 28.3, 28.1, 28.0, 27.9, 26.8. ^{31}P NMR (161.97 MHz, CD_2Cl_2) δ: 22.7, 20.4.

Anal. Calc. For $C_{64}H_{69}Cl_2N_2PRu$ (1069.2): C 71.89, H 6.50, N 2.62. Found: C 72.01, H 6.59, N 2.71.

Synthesis of 1,3-di([1,1'-biphenyl]-2-yl)-4,5-dimethyl-4,5-dihydro-2-imidazolidinylidene] (dichloro) (2-ipropoxyphenylmethylene)ruthenium (**7**)

A suspension of **C** (0.389 mmol, 171 mg) in toluene (2.5 mL) was prepared and stirred for couple of minutes in glove box. KHMDS (0.428 mmol, 85.3 mg) was added and the solution was stirred for five minutes at RT. $(PCy_3)Ru(=CH\text{-}o\text{-}OiPrC_6H_4)Cl_2$ (0,206 mmol, 123mg) was then added and the reaction was heated and stirred at 70°C for one hour. The crude product was first purified by column chromatography on TSI silica gel (pentane: diethyl ether = 7:1 to 1:1) to afford **7** as a deep green powder. Trace of impurities were removed by washing **7** with a mixture of *n*-hexane/acetonitrile. The pure desired complex was recuperated from the acetonitrile phase after removal of the solvent in vacuo (0.147 mmol, 107 mg, 72% yield).

^{1}H-NMR (400 MHz, CD_2Cl_2) δ: 17.11 (s, 1H), 9.28 (d, ^3J= 7.38 Hz, 1H), 7.83-7.78 (o m, 4H), 7.68-7.64 (o m, 2H), 7.60-7.49 (o m, 8H), 7.32-7.26 (o m, 4H), 7.01 (d, ^3J= 8.44 Hz, 1H), 6.93-6.87 (o m, 2 H), 5.12 (quin, ^3J = 6.14 Hz, 1H), 3.49 (quin, ^3J = 6.76 Hz, 1 H), 3.28 (quin, ^3J =6.08 Hz, 1H), 1.76 (d, ^3J= 6.18 Hz, 3H), 1.52 (d, ^3J= 5.90 Hz, 3H), 0.81 (d, ^3J= 6.50 Hz, 3H), 0.64 (d, ^3J = 6.70 Hz, 3H). ^{13}C-NMR (100 MHz, CD_2Cl_2) δ: 297.1, 209.4, 153.4, 144.4, 140.9, 140.3, 139.9, 139.7, 138.5, 138.1, 132.6, 132.1, 131.3, 130.6, 130.5, 129.7, 129.3, 129.1, 128.8, 128.5, 128.3, 128.1, 127.6, 127.2, 122.9, 122.5, 113.6, 75.2, 60.6, 60.4, 30.1, 22.9, 22.4, 13.9, 12.9.

Anal. Calc. For $C_{39}H_{38}Cl_2N_2ORu$ (722.7): C 64.81, H 5.30, N 3.88. Found: 64.89, H 5.41, N 3.84.

Synthesis of 1,3-di([1,1'-biphenyl]-2-yl)-4,5-diphenyl-4,5-dihydro-2-imidazolidinylidene] (dichloro) (2-ipropoxyphenylmethylene)ruthenium (**8**)

Ruthenium complex **4** (0.146 mmol, 156 mg) and CuCl (0.146 mmol, 14.5 mg) were weighted into a 50 mL round bottomed flask in a glovebox and dissolved in 5.0 mL of dry methylene chloride. A solution of 2-isopropoxystyrene (0.142 mmol, 24.7 mg) in methylene chloride (5.5 mL) was then added, the flask was removed from the glove box and stirred at 40°C for 1h. After cooling to room temperature, the solution was concentrated and filtered through a Pasteur pipette containing a plug

of cotton to remove the insoluble copper-phosphine before loading on column chromatography (TSI silica gel). Elution with *n*-hexane to *n*-hexane/methylene chloride= 1:1 led to isolate, after removal of solvent, the desired complex (containing traces of impurities) as a green powder. Further purification was effected by washing the product with a mixture of *n*-hexane/acetonitrile. The pure desired complex was recuperated from the acetonitrile phase after removal of the solvent in vacuo (0.142 mmol, 110 mg, 99%).

^{1}H-NMR (400 MHz, CD_2Cl_2) δ: 17.04 (s, 1H), 9.54 (d, 1 H), 7.83-7.78 (o m, 5H), 7.63 (o m, 8H), 7.44-7.37 (o m, 6H), 7.33 (d, ^3J=7.48 Hz, 1H), 7.16 (t, ^3J=7.48 Hz, 1H), 7.07 (d, ^3J=8.36 Hz 2H), 7.01 (t, ^3J=7.08 Hz, 1H), 6.93 (t, ^3J=7.40 Hz, 1H), 6.84 (t, ^3J=7.40 Hz, 3H), 6.72 (t, ^3J=7.56 Hz, 2H), 6.25 (d, ^3J=7.96 Hz, 2H), 5.20 (quin, ^3J=6.05 Hz, 1H), 4.78 (d, ^3J = 9.85 Hz, 1H), 4.37 (d, ^3J = 9.85 Hz, 1H), 1.85 (d, ^3J = 6.09 Hz, 3H,), 1.58 (d, ^3J = 6.09 Hz, 3H). ^{13}C NMR (100MHz, CD_2Cl_2) δ: 299.1, 213.3, 153.6; 144.2, 141.4, 140.2, 139.9, 139.8, 138.9, 137.6, 134.1, 132.8, 132.3, 131.6, 131.0, 130.8, 129.9; 129.7, 129.2, 129.2, 129.0, 129.0, 128.7, 128.3, 128.1, 128.0, 128.0, 127.8, 127.3, 126.2, 123.0, 122.8, 113.7, 75.4, 72.1, 70.7, 23.0, 22.5.

Anal. Calc. for $C_{49}H_{42}Cl_2N_2ORu$ (846.8): C 69.50, H 5.00, N 3.31. Found: C 69.59, H5.12, N 3.29.

3. General procedure for the synthesis of rhodium complexes 21-24

In a glove box the imidizolidinium salt (1 eq.), potassium bis(trimethylsilyl)amide (KHMDS, 1 eq.) and dry toluene (5 mL) were introduced in a vial and stirred for 15 min at room temperature. A solution of $[RhCl(COD)]_2$ (0.4 eq.) in 2.5 mL of dry toluene was then added. After two hours at room temperature the reaction mixture was concentrated and purified by column chromatography on silica gel (methylene chloride:ethanol 98:2).

Synthesis of *syn*-[1,3-bis(2-methylphenyl)-4,5-dimethyl-2-imidazolidinylidene] chloro(η^4-1,5-cyclooctadiene)rhodium (**21**)

The product was obtained as a yellow solid (yield= 83%).

^{1}H NMR (CD_2Cl_2, 600 MHz): δ 8.41 (br s, 2H), 7.37-7.29 (o m, 8H), 4.51 (br s, 2H), 4.38 (br s, 2H), 2.82 (br s, 2H), 2.32 (br s, 6H), 1.63-1.59 (o m, 2H), 1.48-1.42 (o m, 6H), 1.07 (overlapped signals, 6H), ^{13}C NMR (CD_2Cl_2, 150 MHz): δ 214.1 (br s), 139.1, 134.6, 133.9, 131.3, 130.6, 128.5, 128.2, 126.4, 97.5, 66.7, 61.3, 32.5, 28.4, 18.7, 13.4.

Anal. Calc. for $C_{27}H_{34}ClN_2Rh$ (524.9): C, 61.78, H, 6.53, N, 5.34. Found: C, 61.86, H, 6.62, N, 5.26.

Synthesis of *syn*-[1,3-bis(2-methylphenyl)-4,5-diphenyl-2-imidazolidinylidene] chloro(η^4-1,5-cyclooctadiene)rhodium (**22**)

The product was obtained as a yellow solid (yield= 73%). ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 8.67 (br s, 2H), 7.31 (t, ^3J=7.5Hz ,2H), 7.24-7.17 (o m, 8H), 7.03-6.98 (o m, 6H), 5.83 (s, 2H), 4.70 (br s, 2H), 2.84 (br s, 2H), 2.43 (s, 6H), 1.70-1.64 (o m, 2H), 1.55-1.50 (o m, 2H), 1.50-1.43 (o m, 2H), 1.39-1.34 (o m, 2H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 218.3 (J_{Rh-C}=46.6 Hz), 139.4, 134.0, 133.6, 130.8, 129.5, 128.2, 128.1, 128.0, 126.5, 98.3 (J_{Rh-C}=6.9Hz), 72.1, 67.3 (J_{Rh-C}=15.1Hz), 32.5, 28.4, 19.5.

Anal. Calc. for $C_{37}H_{38}ClN_2Rh$ (649.1): C, 68.47, H, 5.90, N, 4.32. Found: 68.52, H, 5.98, N, 4.27.

Synthesis of *syn*-[1,3-bis(2-biphenyl)-4,5-dimethyl-2-imidazolidinylidene] chloro(η^4-1,5-cyclooctadiene)rhodium (**23**)

The product was obtained as a yellow solid (yield= 67%). ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 9.34 (d, ^3J=8.0Hz, 2H), 7.56 (t, ^3J=7.6Hz, 2H), 7.46-7.39 (o m, 8H), 7.32-7.28 (o m, 6H), 4.87 (br s, 2H), 3.32-3.30 (o s, 4H), 1.89 (b s, 2H), 1.64-1.54 (o m, 6H), 0.75-0.74 (o d, 2H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 214.1 (J_{Rh-C}=46.5Hz), 140.9, 138.2, 137.4, 133.0, 131.4, 129.4, 128.9, 128.1, 128.0, 97.7 (J_{Rh-C}=6.7Hz), 66.9 (J_{Rh-C}=14.9Hz), 60.5, 33.0, 28.9, 13.9.

Anal. Calc. for $C_{37}H_{38}ClN_2Rh$ (649.1): C, 68.47, H, 5.90, N, 4.32. Found: 68.58, H, 5.97, N, 4.37.

Synthesis of *syn*-[1,3-bis(2-biphenyl)-4,5-diphenyl-2-imidazolidinylidene] chloro(η^4-1,5-cyclooctadiene)rhodium (**24**)

The product was obtained as a yellow solid (yield= 73%). ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 9.70 (d, 2H, ^3J=8.2Hz), 7.55-7.50 (o m, 8H), 7.32 (t, ^3J=7.5Hz, 2H), 7.20-7.18 (o m, 4H), 7.09 (dd, ^3J=7.6Hz, 2H), 6.82 (o m, 6H), 6,64 (br s, 4H), 5.06 (br s, 2H), 4.56 (s, 2H), 3.44 (br s, 2H), 1.98 (m, 2H), 1.72-1.67 (o m, 2H), 1.64-1,61 (o m, 4H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 217.3 (J_{Rh-C}=46.9Hz), 140.9, 138.4, 136.6, 134.2, 131.3, 129.4, 129.3, 128.8, 128.0, 127.8, 127.7, 127.5, 98.2 (J_{Rh-C}=6.6Hz), 70.9, 67.4 (J_{Rh-C}=15.5Hz), 32.7, 28.7.

Anal. Calc. for $C_{47}H_{42}ClN_2Rh$ (773.2): C, 73.01, H, 5.48, N, 3.62. Found: 73.12, H, 5.41, N, 3.75.

4. General procedure for the synthesis of complexes 25-28

Complexes **21**-**24** were dissolved in dry methylene chloride (C=0.013M) and exposed to a bubbling of carbon monoxide 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 *syn*-[1,3-bis(2-methylphenyl)-4,5-dimethyl-2-imidazolidinylidene] dicarbonylchloro rhodium (**25**)

The product was obtained as a pale yellow solid (yield= 92%). ^{1}H NMR (CD_2Cl_2, 600 MHz):), δ 7.59-7.31 (o s, 8H), 4.46 (br s, 2H), 2.42 (s, 6H), 1.17 (s, 6H). ^{13}C NMR (CD_2Cl_2, 150 MHz): δ 204.3 (br s), 186.5 (J_{Rh-C} =75.9Hz), 184.4 (J_{Rh-C} =72.9Hz),183.3 (J_{Rh-C} =54.5Hz), 138.0, 137.4, 136.0, 135.2, 135.6, 133.5, 131.3, 129.1, 129.4, 128.6, 128.4, 128.1, 127.7, 127.3, 126.8, 62.3, 18.5, 18.1, 13.4. IR (CH_2Cl_2): νCO 2078, 1997 cm^{-1}.

Anal. Calc. for $C_{21}H_{22}ClN_2O_2Rh$ (472.8): C, 53.35, H, 4.69, N, 5.93. Found: C, 53.43, H, 4.76, N, 5.86.

Synthesis of *syn*-[1,3-bis(2-methylphenyl)-4,5-diphenyl-2-imidazolidinylidene] dicarbonylchloro rhodium (**26**)

The product was obtained as a pale yellow solid (yield= 94%) . ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 7.80 (br s, 2H), 7.44-6.99 (o m, 16H), 5.84 (br s, 2H), 2.53 (br s, 6H). ^{13}C NMR (CD_2Cl_2, 150 MHz): δ 208.3 (J_{Rh-C}=41.3Hz), 186.4 (J_{Rh-C}=53.5Hz), 182.9 (J_{Rh-C}=74.9Hz), 138.3, 135.3, 133.0, 131.4, 129.5, 129.2, 129.0, 128.7, 128.3, 128.1, 126.7, 126.5, 73.4, 18.6.

IR (CH_2Cl_2): νCO 2080, 1999 cm^{-1}. Anal. Calc. for $C_{31}H_{26}ClN_2O_2Rh$ (596.9): C, 62.38, H, 4.39, N, 4.69. Found: C, 62.49, H, 4.46, N, 4.59.

Synthesis of *syn*-[1,3-bis(2-biphenyl)-4,5-dimethyl-2-imidazolidinylidene] dicarbonylchloro rhodium (**27**)

The product was obtained as a pale yellow solid (yield= 84%). ^{1}H NMR (CD_2Cl_2, 600 MHz): δ 8.32 (br s, 1H), 7.80-7.38 (o m, 17H), 3.36 (br s, 2H), 0.75 br (s, 6H).

^{13}C NMR (CD_2Cl_2, 150 MHz): δ 202.9 (br s), 186.2 (J_{Rh-C}=53.5Hz), 184.0 (J_{Rh-C}=73.9Hz), 139.6, 139.0, 136.7, 133.8, 131.3, 129.7, 129.1, 128.9, 128.1, 61.5, 13.2.

IR (CH_2Cl_2): νCO 2081, 1997 cm^{-1}.

Anal. Calc. for $C_{31}H_{26}ClN_2O_2Rh$ (596.9): C, 62.38, H, 4.39, N, 4.69. Found: C, 62.47, H, 4.47, N, 4.75.

Synthesis of *syn*-[1,3-bis(2-biphenyl)-4,5-diphenyl-2-imidazolidinylidene] dicarbonylchloro rhodium (**28**)

The product was obtained as a pale yellow solid (yield= 84%) and as a mixture of two isomers (major:minor 1:0.2). ^{1}H NMR (CD_2Cl_2, 600 MHz): (only major isomer signals are shown below) δ 8.75 (d, ^{3}J=8.1Hz, 2H), 7.54 (o s, 8H), 7.40 (t, 7.8Hz, 2H), 7.34-7.30 (o m, 6H), 7.15 (d, 7.6Hz, 2H), 6.92-6.87 (o m, 6H), 6.60 (d, ^{3}J=6.9Hz, 4H), 4.54 (s, 2H). ^{13}C NMR (CD_2Cl_2, 150 MHz): δ 206.1 (J_{Rh-C}=40.6Hz), 186.1 (J_{Rh-C}=53.6Hz), 184.0 (J_{Rh-C}=74.4Hz), 140.0, 138.2, 137.1, 133.5, 132.6, 131.4, 129.4, 129.3, 129.2, 128.9, 128.5, 128.3, 128.2, 127.9, 127.8., 71.9.

IR (CH_2Cl_2): νCO 2084, 2000 cm^{-1}.

Anal. Calc. for $C_{41}H_{30}ClN_2O_2Rh$ (721.0): C, 68.29, H, 4.19, N, 3.89. Found: C, 68.37, H, 4.29, N, 4.08.

5. RCM catalytic tests

RCM of Diethyldiallyl malonate (**9**) (**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, 19.3 μL (0.080 mmol) of **9** were injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **10** 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.

RCM of N-Tosyl diallylamine (**11**) (**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, 17.2 μL (0.080 mmol) of **11** was injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **12** 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.

RCM of Diethyldiallylmethallylmalonate (**13**) (**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 (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 **13** were injected and the reaction was monitored as a function of time, determining the conversion to the cyclic product **14** 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.

RCM of N-tosyl allylmethallylamine (**15**) (**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 (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 **15** was injected and the reaction was monitored as a

function of time, determining the conversion to the cyclic product **16** 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.

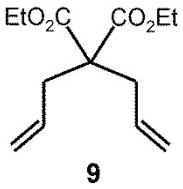
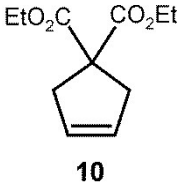
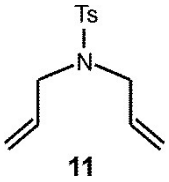
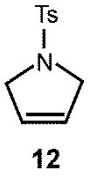
RCM of Diethyldimethallylmalonate (**17)** (**Figure 4**)

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 **17** 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 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.

RCM of N-tosyl dimethallylamine (**19**) (**Figure 4**).

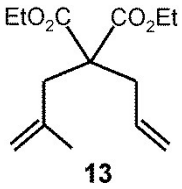
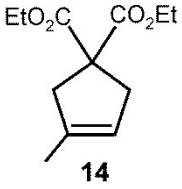
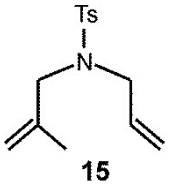
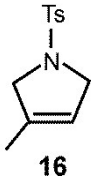
An NMR tube with a screw-cap septum top was charged with 0.8 mL of a CD_2Cl_2 or C_6D_6 solution of catalyst (5%mol in CD_2Cl_2, 1%mol in C_6D_6) and then was equilibrated at the appropriate temperature (30°C for Grubbs second generation catalysts and 60°C for Hoveyda-Grubbs second generation catalysts) in the NMR probe. After that, 20.2 μL (0.080 mmol) of **19** 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 **9** and **11**

Entry[a]	Substrate	Product	Catalyst (mol%)	Time (min)	Yield[b] (%)
1	 **9**	 **10**	**1** (1)	30	97
2			**2** (1)	30	>98
3			**3** (1)	5	>99
4			**4** (1)	8	95
5			**5** (1)	4	>99
6			**6** (1)	5	>99
7			**7** (1)	2	>99
8			**8** (1)	3	>99
9	 **11**	 **12**	**1** (1)	28	98
10			**2** (1)	25	>99
11			**3** (1)	3	>99
12			**4** (1)	6	98
13			**5** (0.1)	8	98
14			**6** (0.1)	6	>99
15			**7** (0.1)	4	>99
16			**8** (0.1)	7	>99

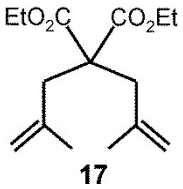
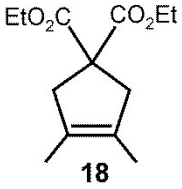
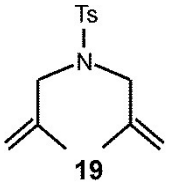
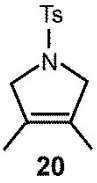
[a]Runs with catalysts **1**, **2**, **3** and **4** were carried out in CD_2Cl_2 at 30°C; while runs with catalyst **5**, **6**, **7** and **8** were performed in C_6D_6 at 60°C. [b]Yields based on NMR analysis.

Table S2. RCM of **13** and **15**

Entry[a]	Substrate	Product	Catalyst (mol%)	Time (min)	Yield[b] (%)
1	 **13**	 **14**	**1** (1)	35	89
2			**2** (1)	35	>95
3			**3** (1)	9	>99
4			**4** (1)	16	86
5			**5** (1)	5	>99
6			**6** (1)	6	>99
7			**7** (1)	4	>99
8			**8** (1)	6	>99
9	 **15**	 **16**	**1** (1)	28	99
10			**2** (1)	30	99
11			**3** (1)	3	>99
12			**4** (1)	10	93
13			**5** (0.1)	12	99
14			**6** (0.1)	10	>99
15			**7** (0.1)	6	>99
16			**8** (0.1)	8	>99

[a]Runs with catalysts **1**, **2**, **3** and **4** were carried out in CD_2Cl_2 at 30°C; while runs with catalyst **5**, **6**, **7** and **8** were performed in C_6D_6 at 60°C. [b]Yields based on NMR analysis.

Table S3. RCM of **17** and **19**

Entry[a]	Substrate	Product	Catalyst (mol%)	Time (min)	Yield[b] (%)
1	 **17**	 **18**	**1** (5)	60	82
2			**2** (5)	30	92
3			**3** (5)	60	61
4			**4** (5)	60	45
5			**5** (5)	60	97
6			**6** (5)	30	99
7			**7** (5)	60	86
8			**8** (5)	60	78
9	 **19**	 **20**	**1** (5)	60	87
10			**2** (5)	60	97
11			**3** (5)	60	82
12			**4** (5)	60	61
13			**5** (1)	30	97
14			**6** (1)	30	99
15			**7** (1)	30	98
16			**8** (1)	30	98

[a]Runs with catalysts **1**, **2**, **3** and **4** were carried out in CD_2Cl_2 at 30°C; while runs with catalyst **5**, **6**, **7** and **8** were performed in C_6D_6 at 60°C. [b]Yields based on NMR analysis.

6. NMR spectra

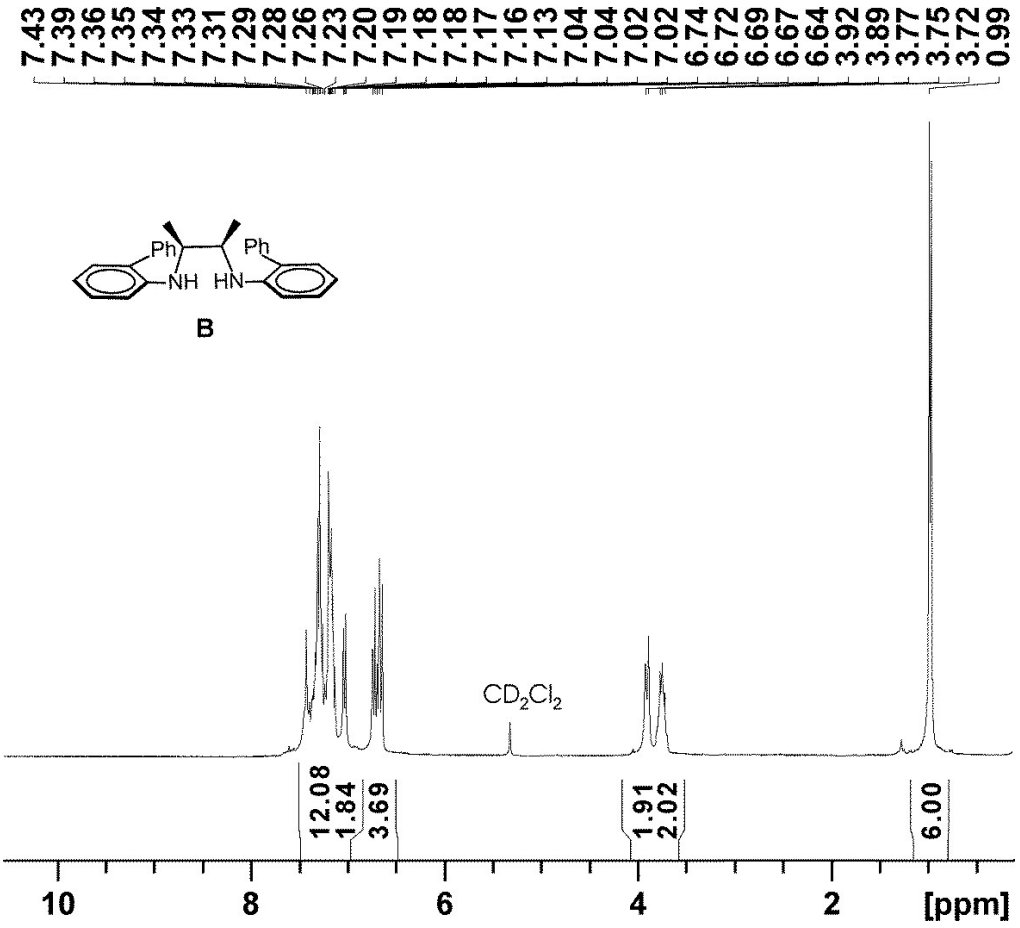


Figure S1. ^{1}H NMR (300 MHz, CD_2Cl_2) of **B**

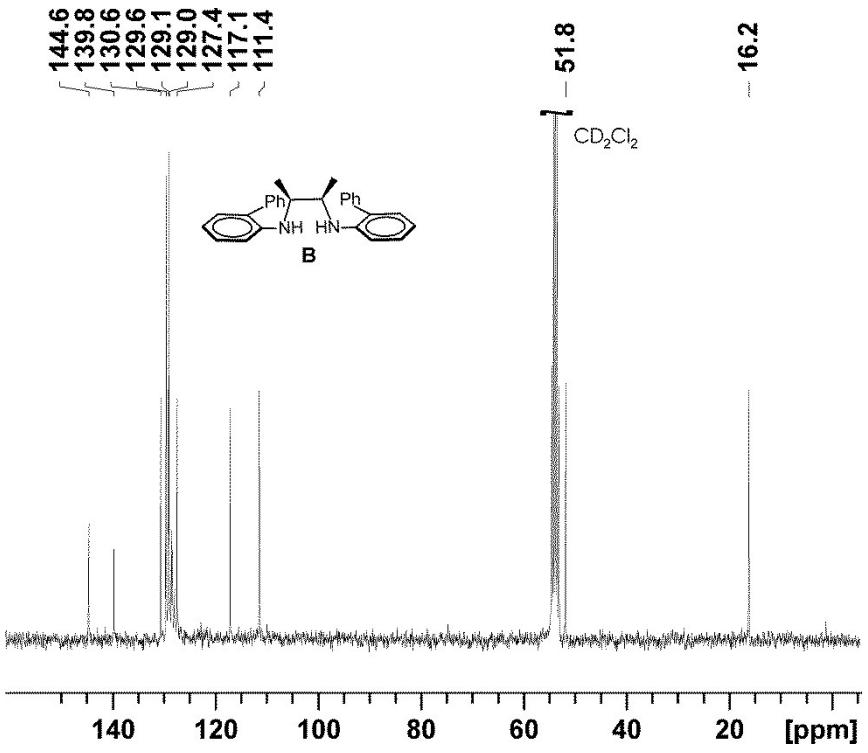


Figure S2. ^{13}C NMR (75MHz, CD_2Cl_2) of **B**

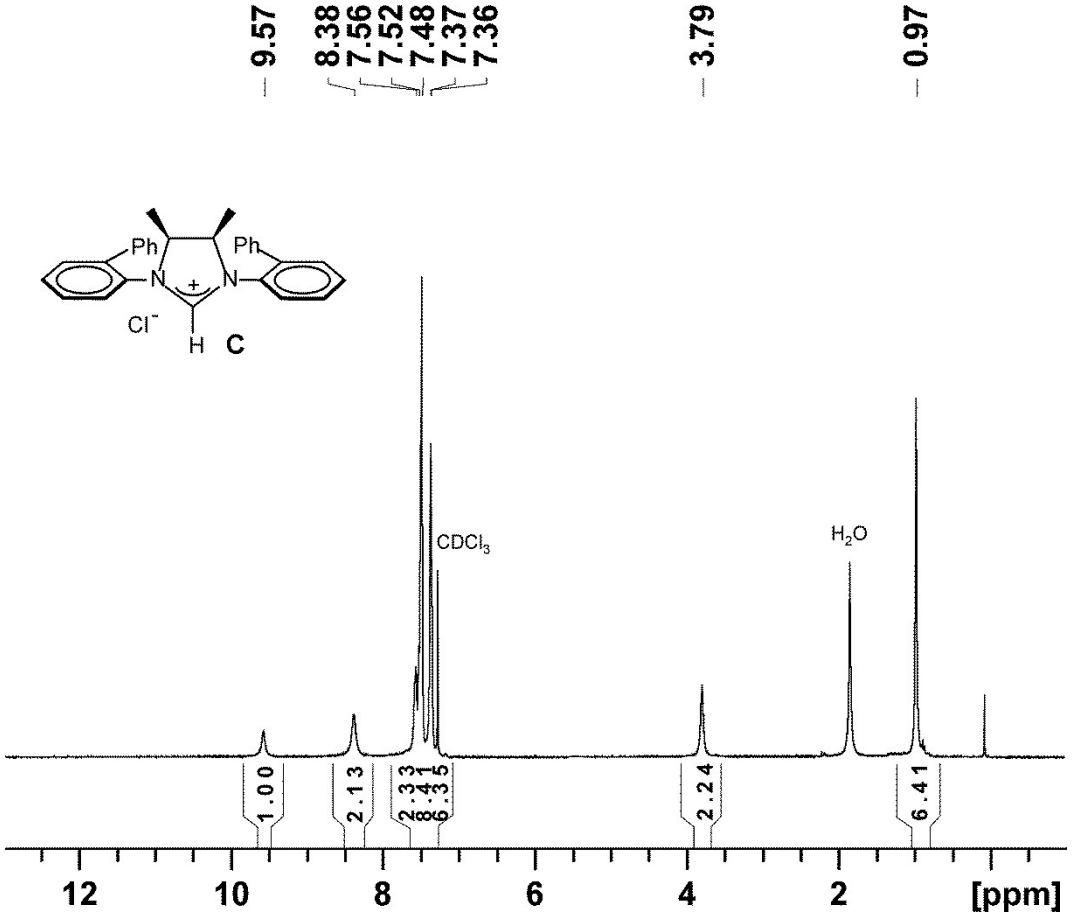


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) of **C**

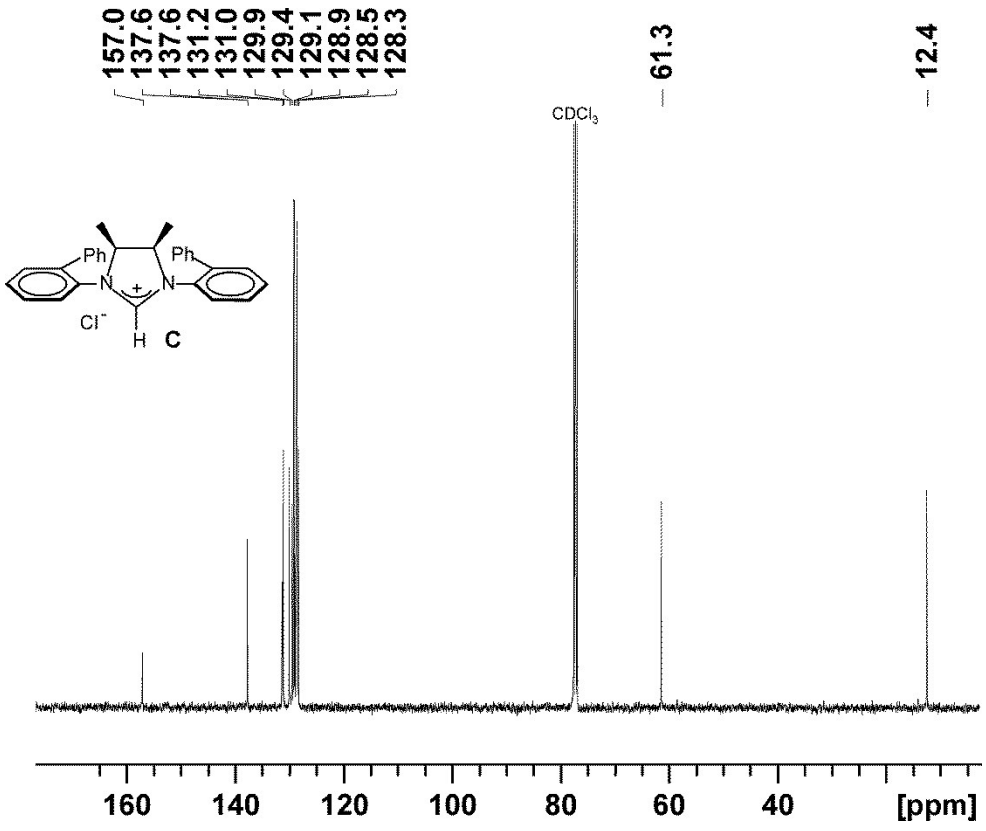


Figure S4. ^{13}C NMR (100MHz, $CDCl_3$) of **C**

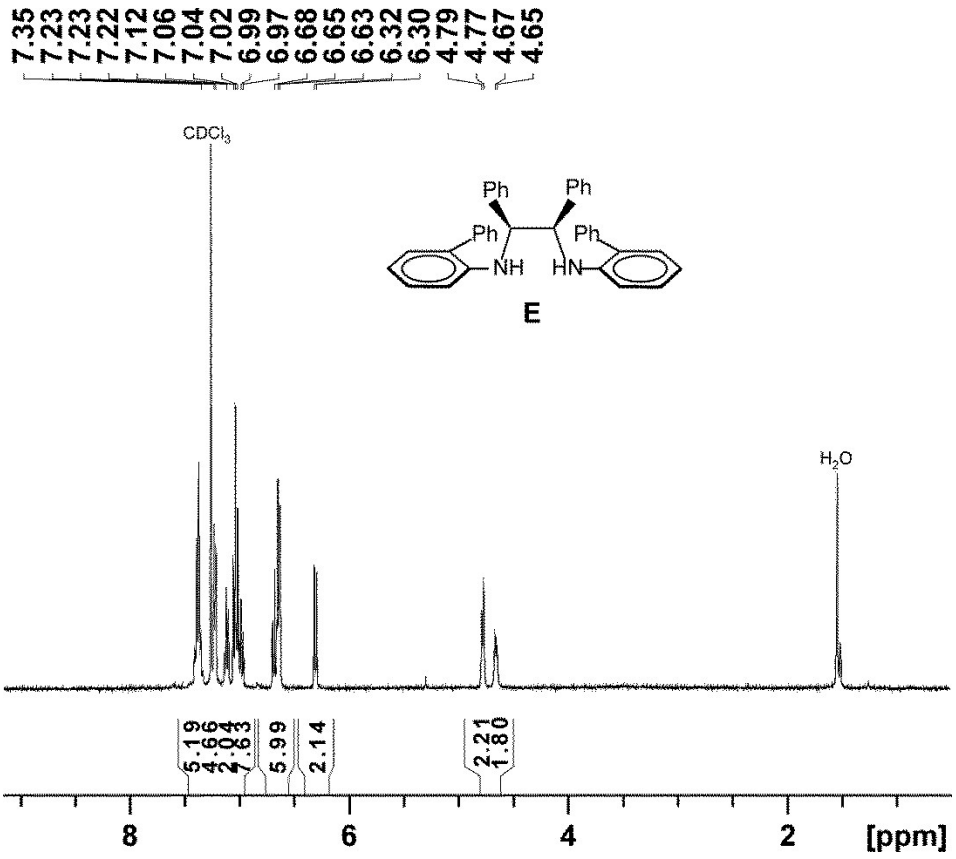


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) of **E**

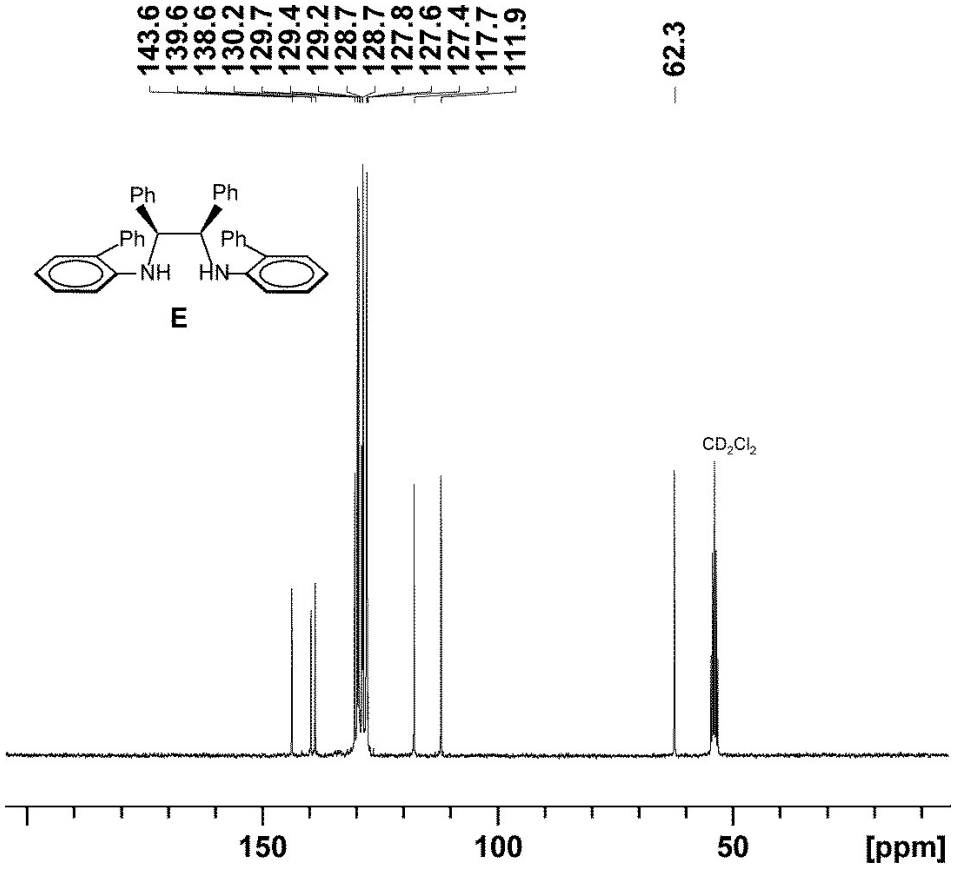


Figure S6. ^{13}C NMR (75MHz, CD_2Cl_2) of **C**

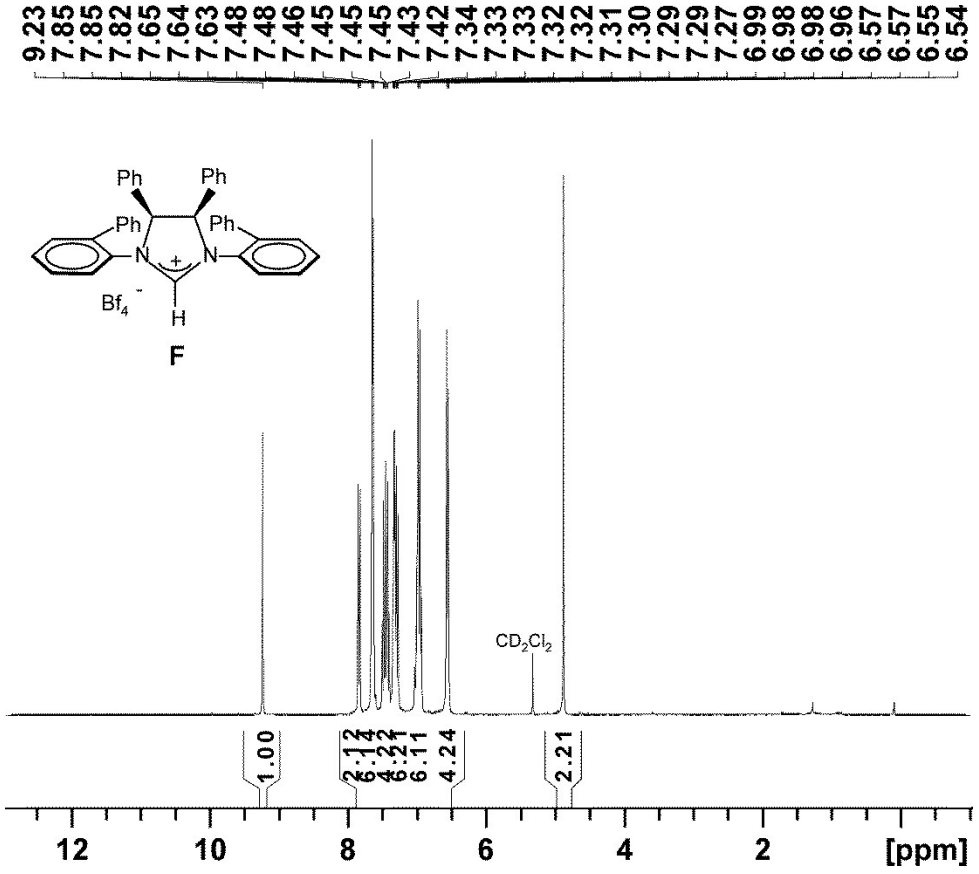


Figure S7. ^{1}H NMR (300 MHz, CD_2Cl_2) of **F**

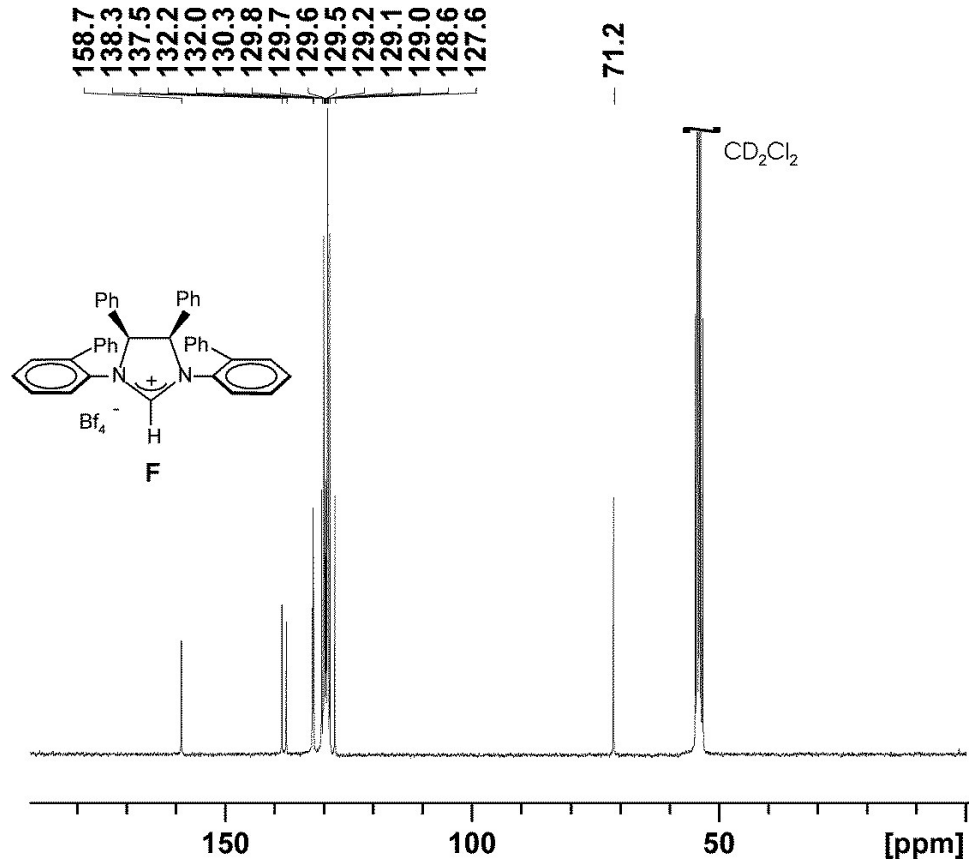


Figure S8. ^{13}C NMR (75MHz, CD_2Cl_2) of **F**

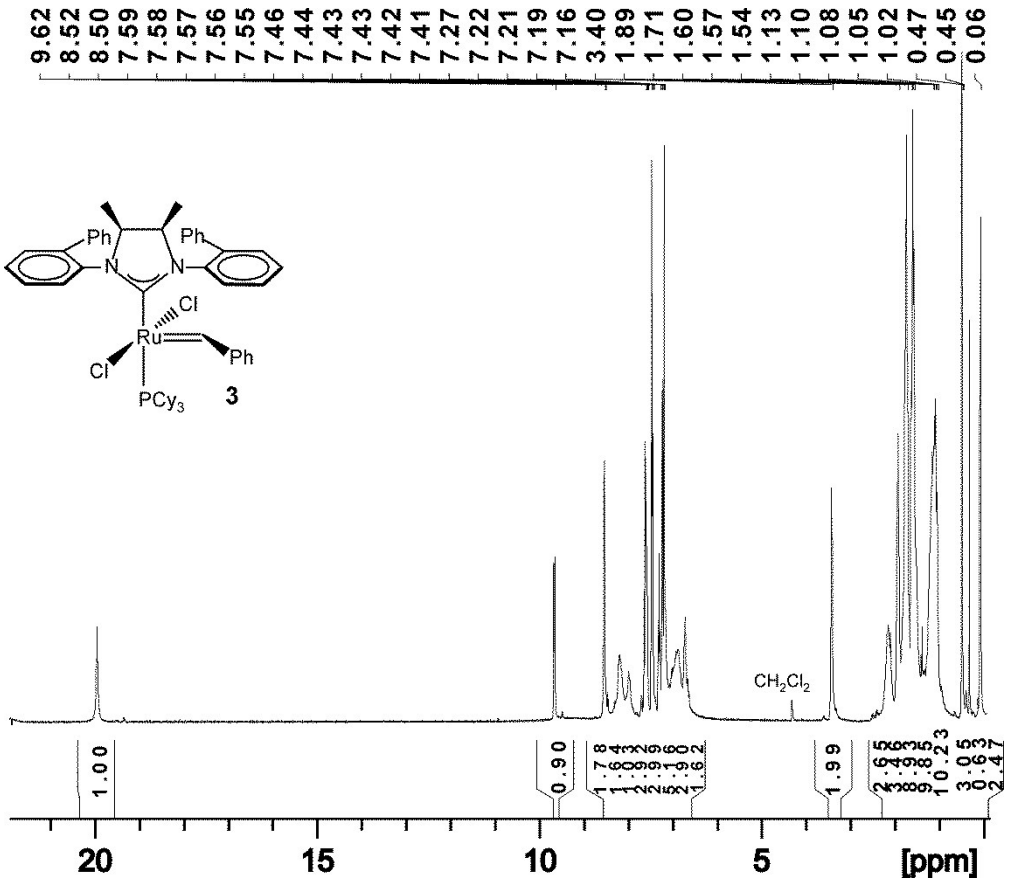


Figure S9. ^{1}H NMR (400 MHz, C_6D_6) of **3**

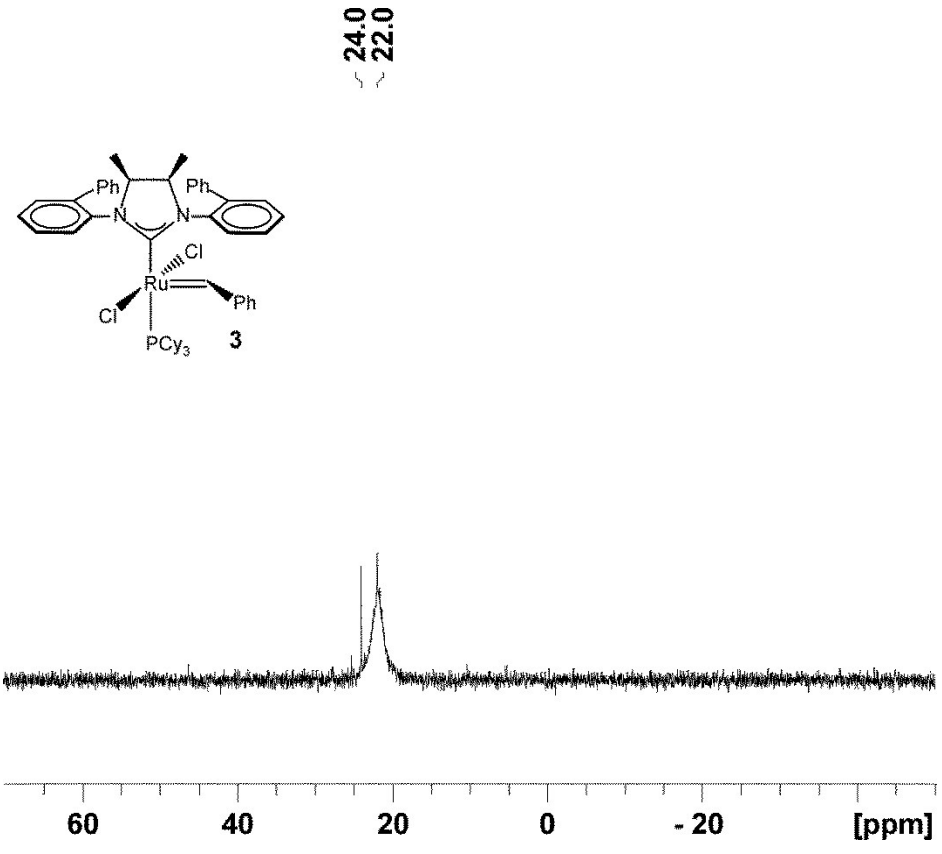


Figure S10. ^{31}P NMR (161.97MHz, C_6D_6) of **3**

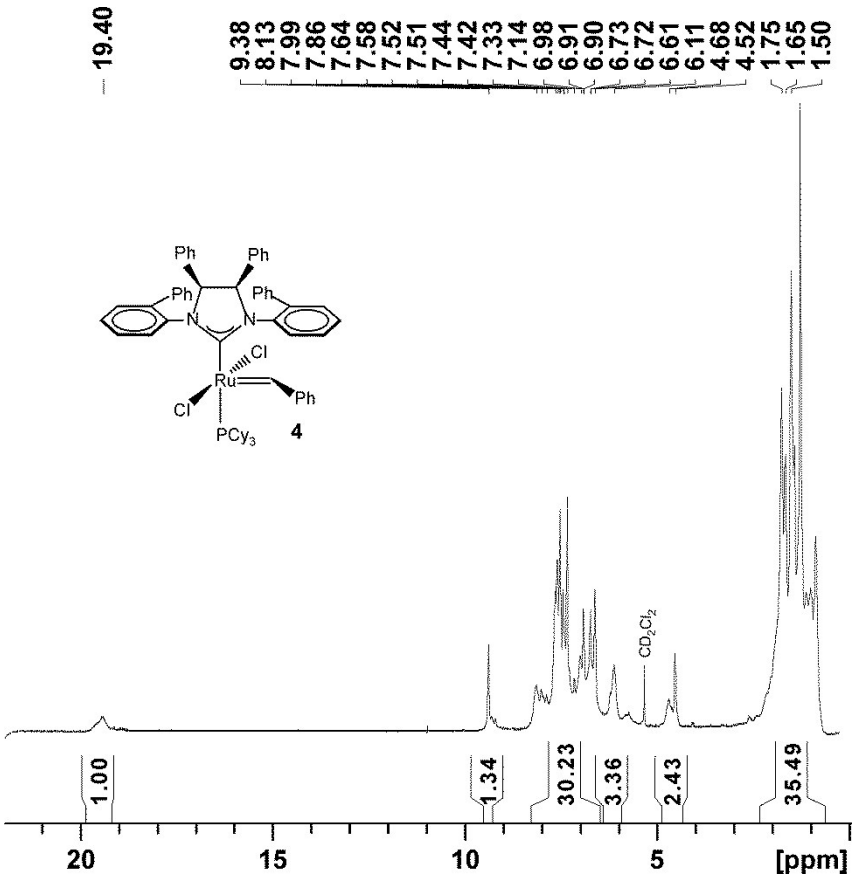


Figure S11. ^{1}H NMR (400MHz, CD_2Cl_2) of **4**

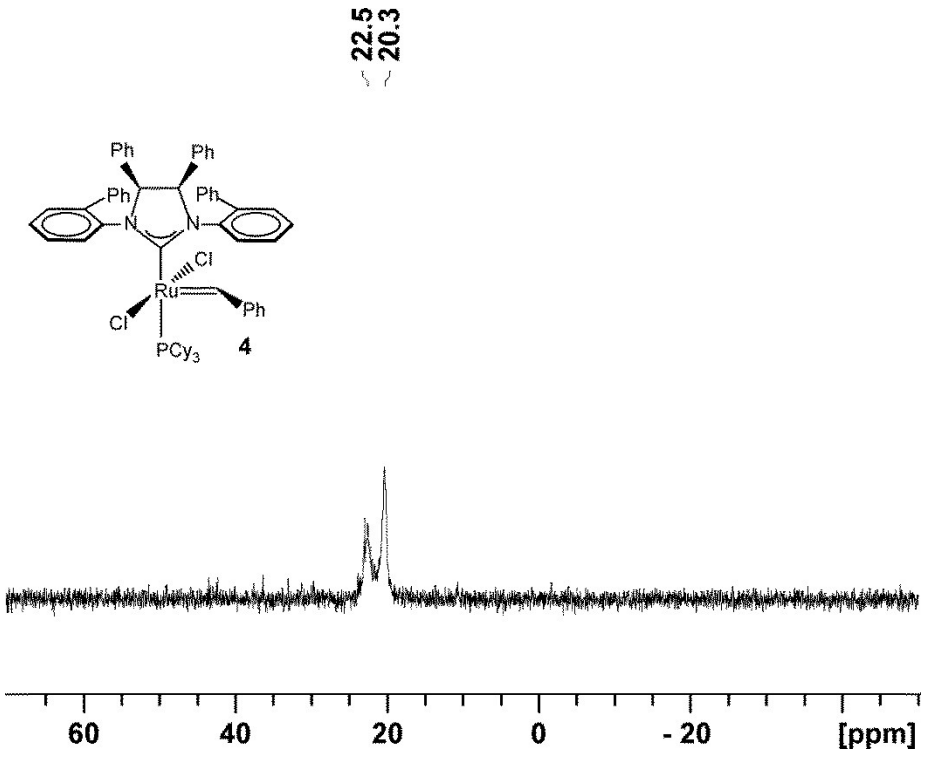


Figure S12. ^{31}P NMR (161.97MHz, CD_2Cl_2) of **4**

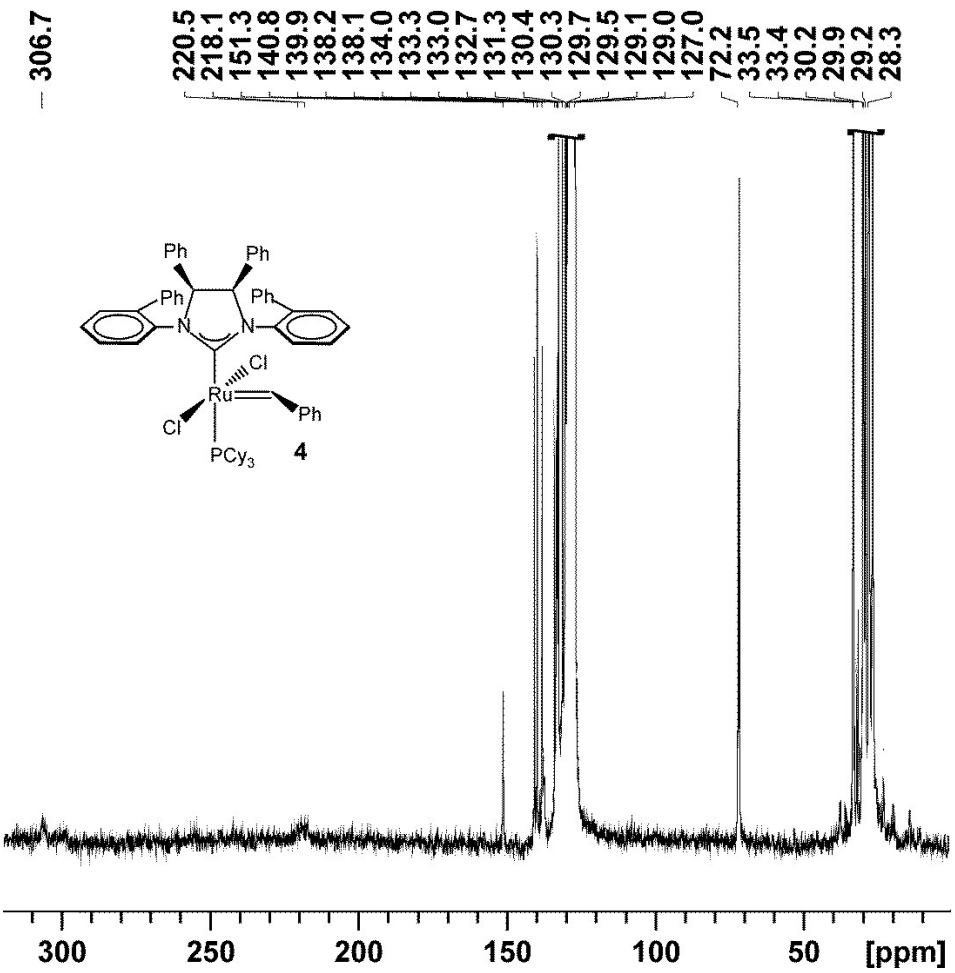


Figure S13. ^{13}C NMR (100MHz, C_6D_6) of **4**

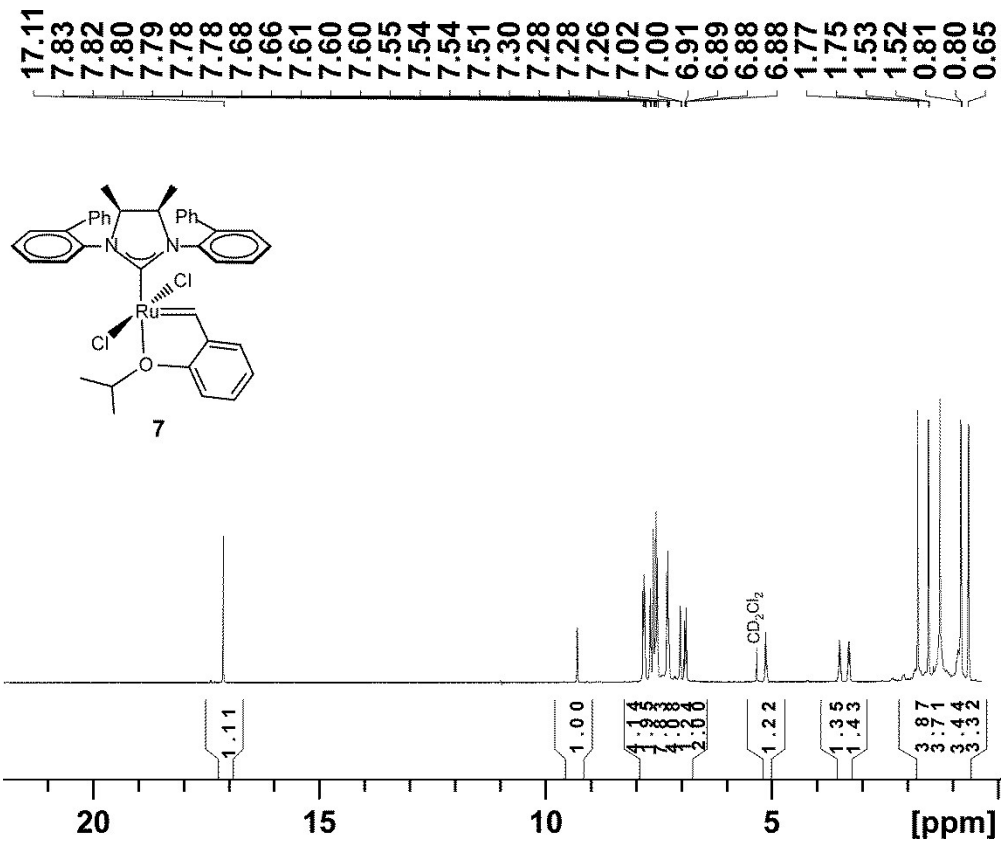


Figure S14. ^{1}H NMR (400MHz, CD_2Cl_2) of **7**

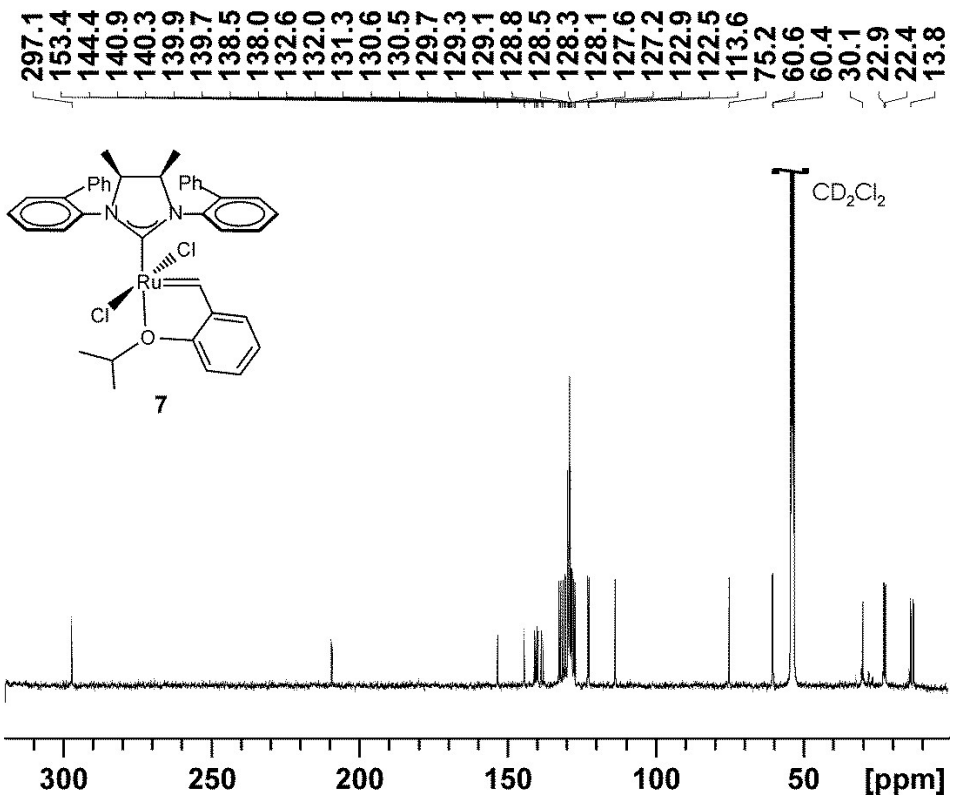


Figure S15. ^{13}C NMR (100MHz, CD_2Cl_2) of **7**

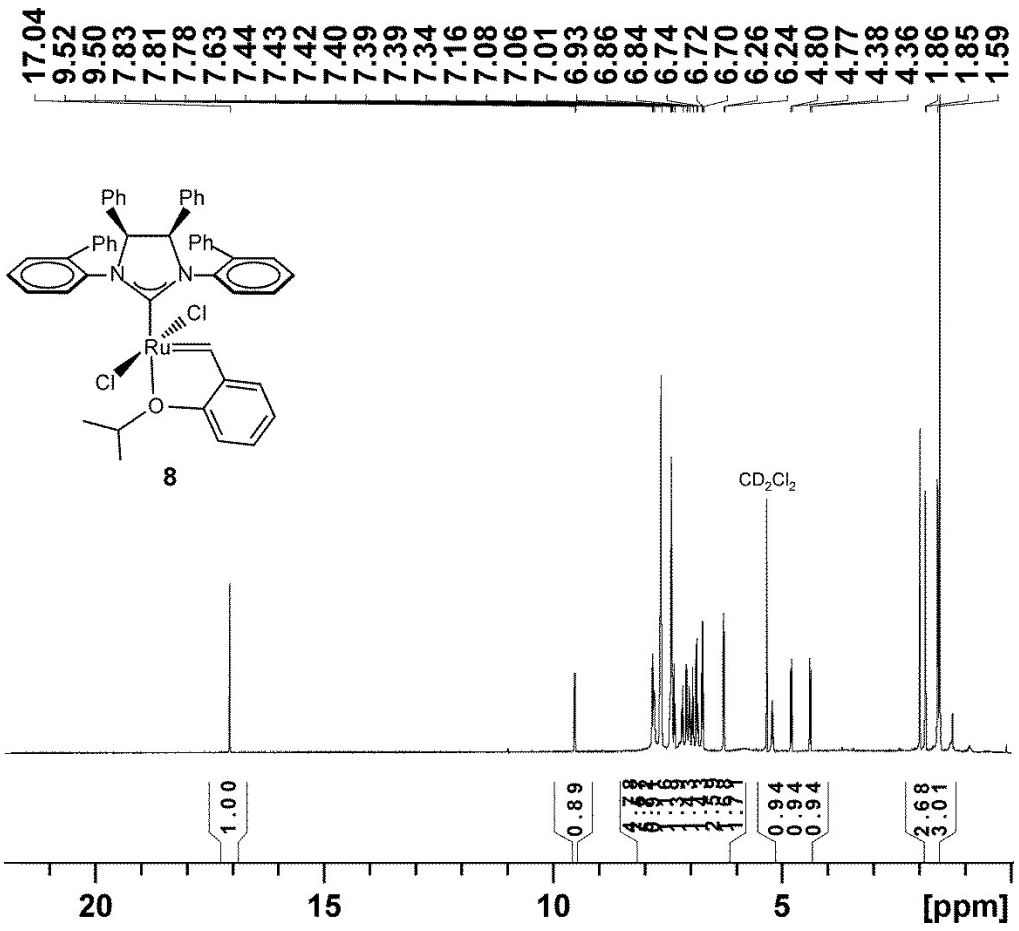


Figure S16. ^{1}H NMR (400MHz, CD_2Cl_2) of **8**

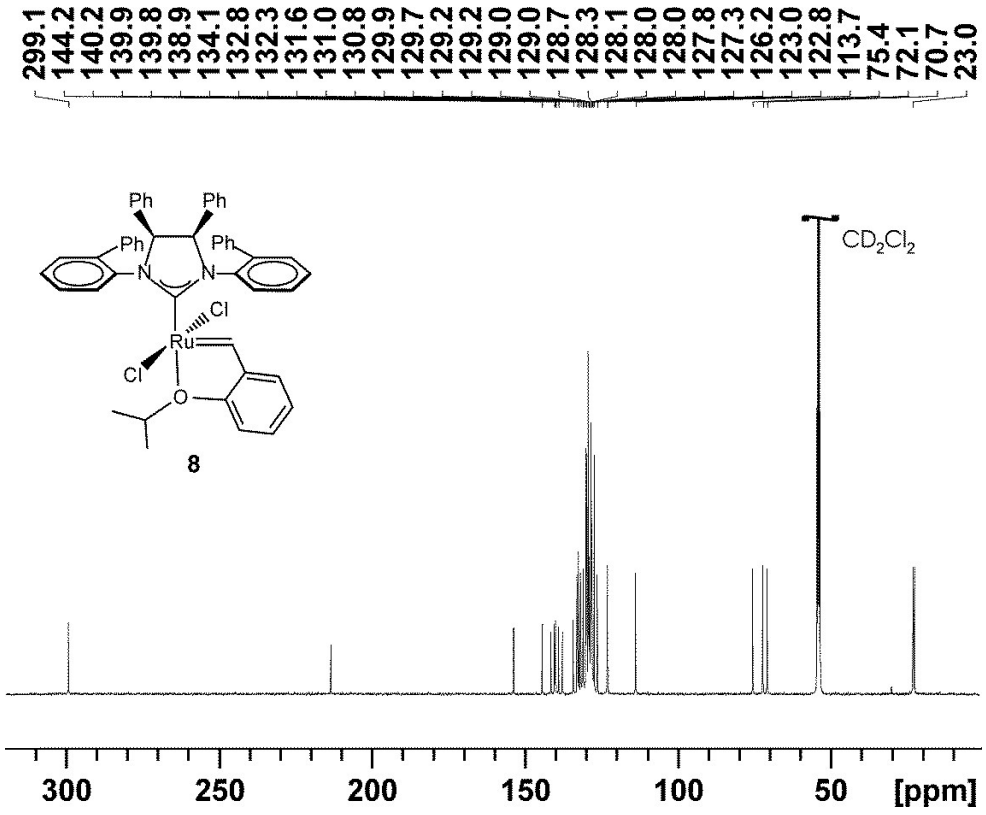


Figure S17. ^{13}C NMR (100MHz, CD_2Cl_2) of

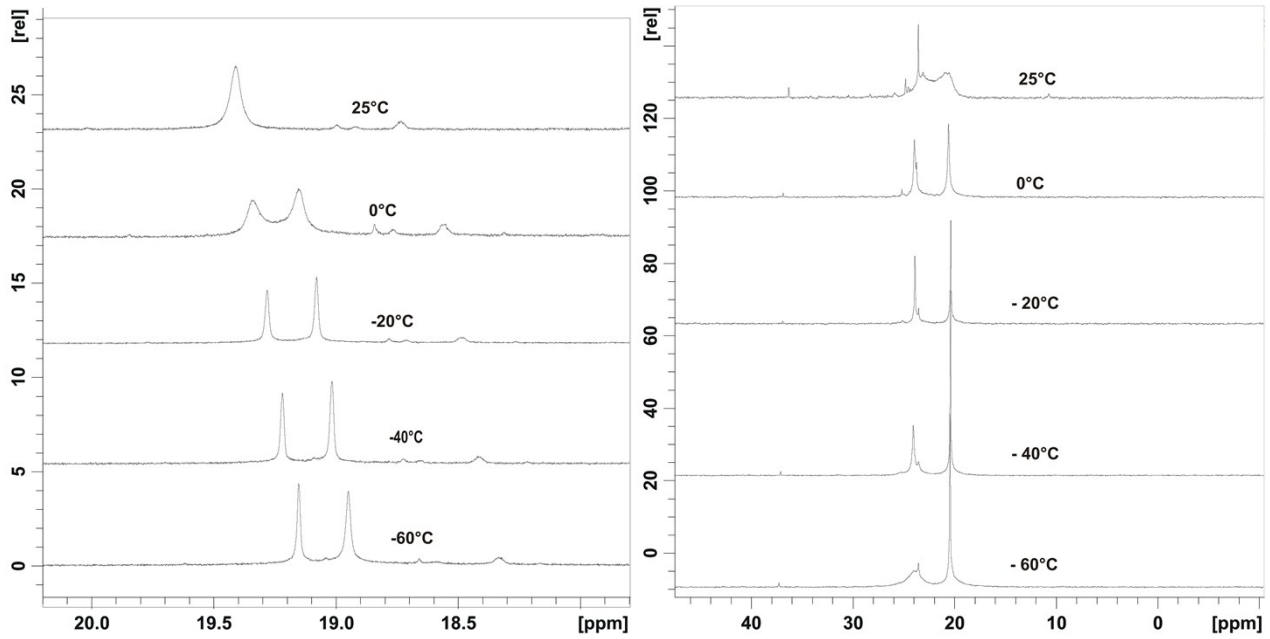


Figure S18. Variable Temperature NMR spectra of **3** (C_6D_6):^{1}H NMR carbenic region (left) and ^{31}P NMR (right).

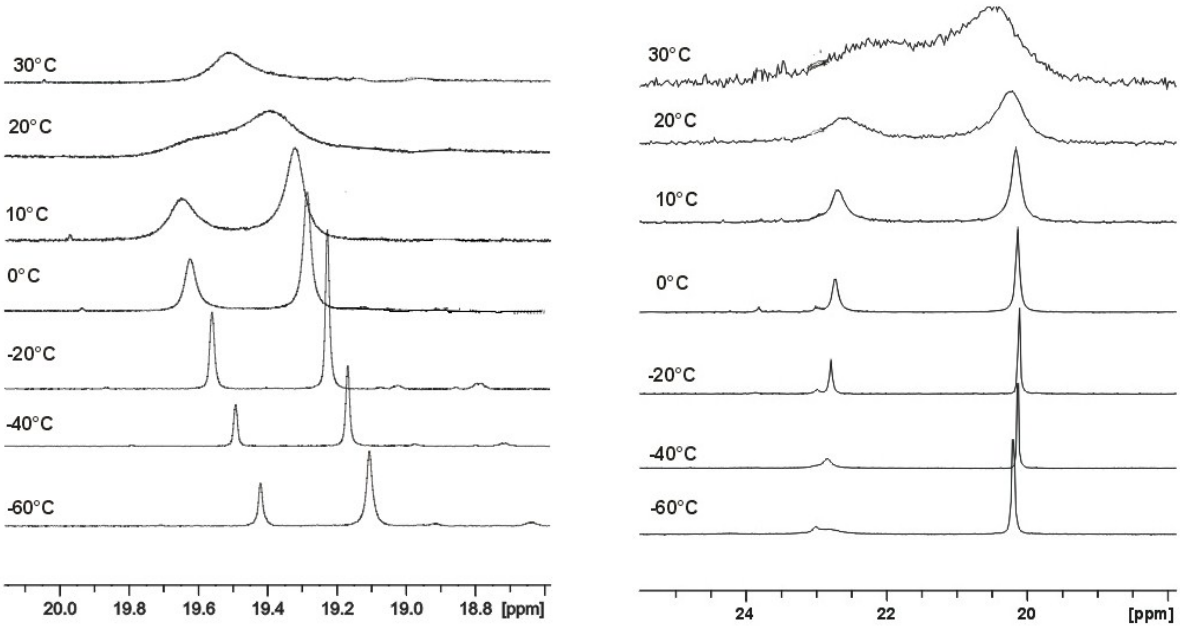


Figure S19. Variable Temperature NMR spectra of **4** (CD_2Cl_2):^{1}H NMR carbenic region (left) and ^{31}P NMR (right).

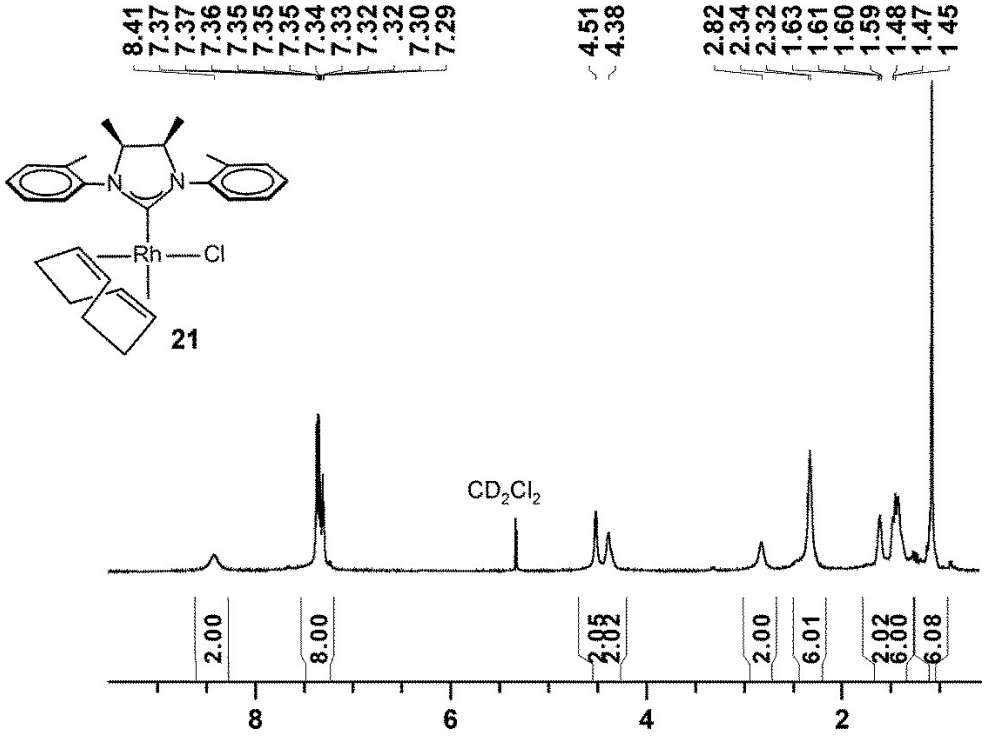


Figure S20. ^{1}H NMR (600 MHz, CD_2Cl_2) of **21**

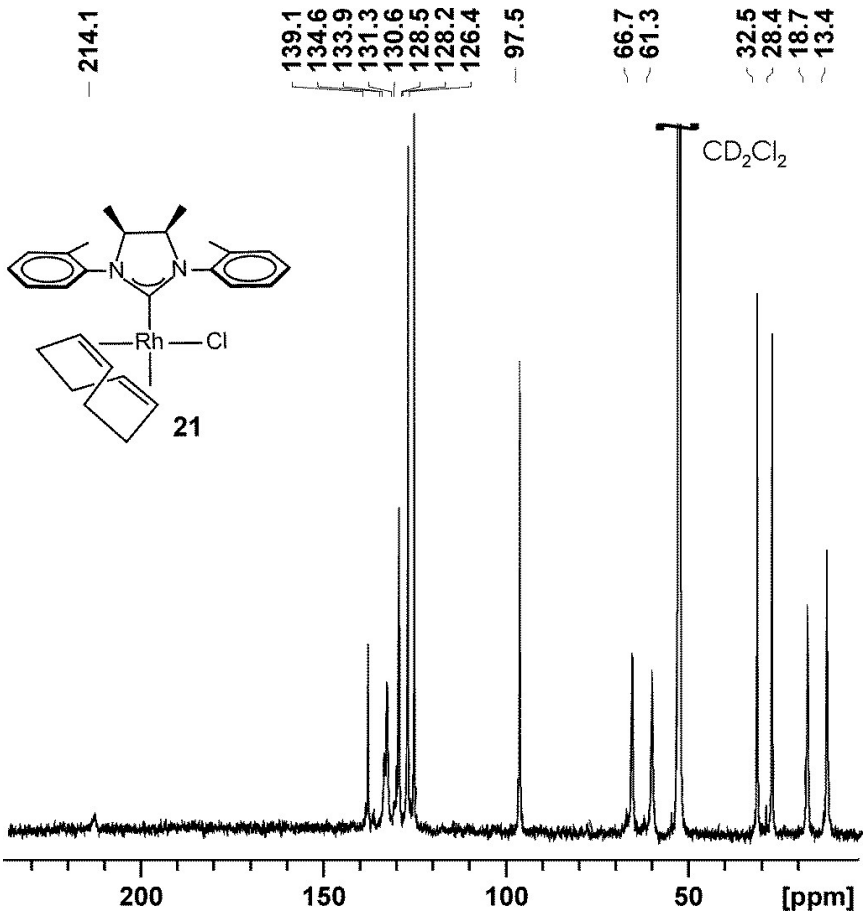


Figure S21. ^{13}C NMR (150 MHz, CD_2Cl_2) of **21**

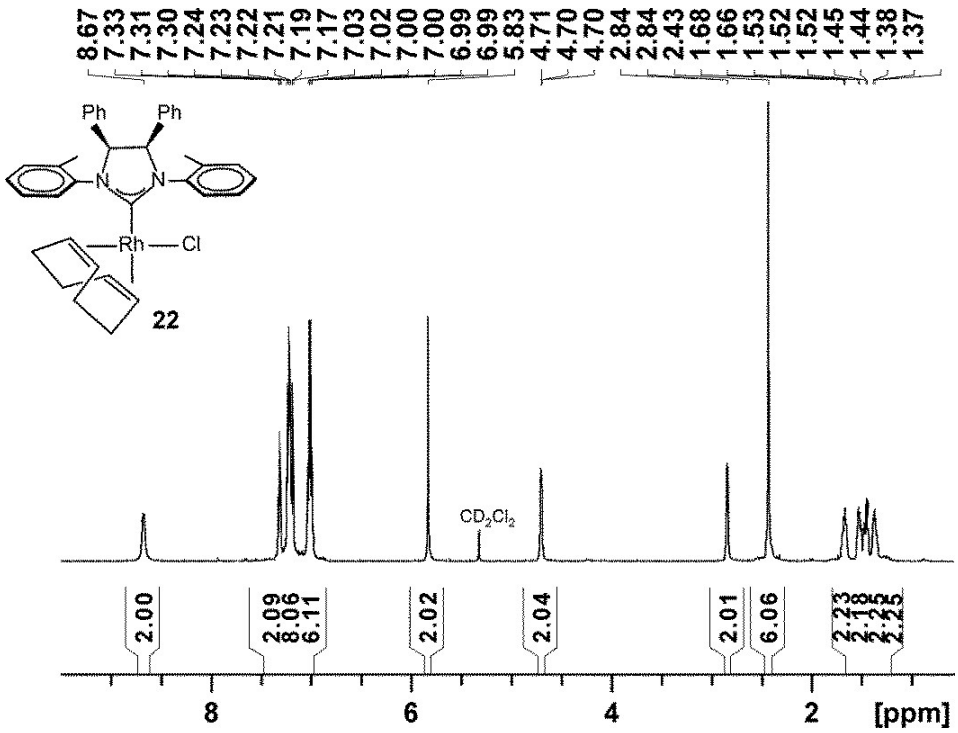


Figure S22. ^{1}H NMR (600 MHz, CD_2Cl_2) of **22**

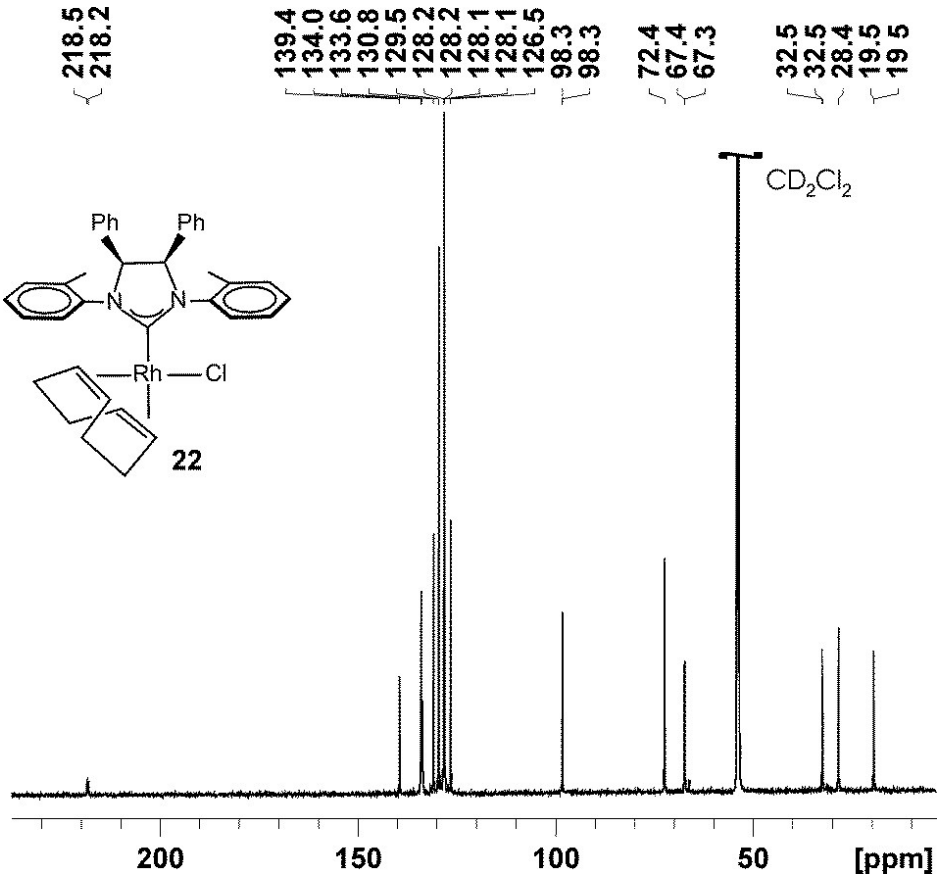


Figure S23. ^{13}C NMR (150 MHz, CD_2Cl_2) of **22**

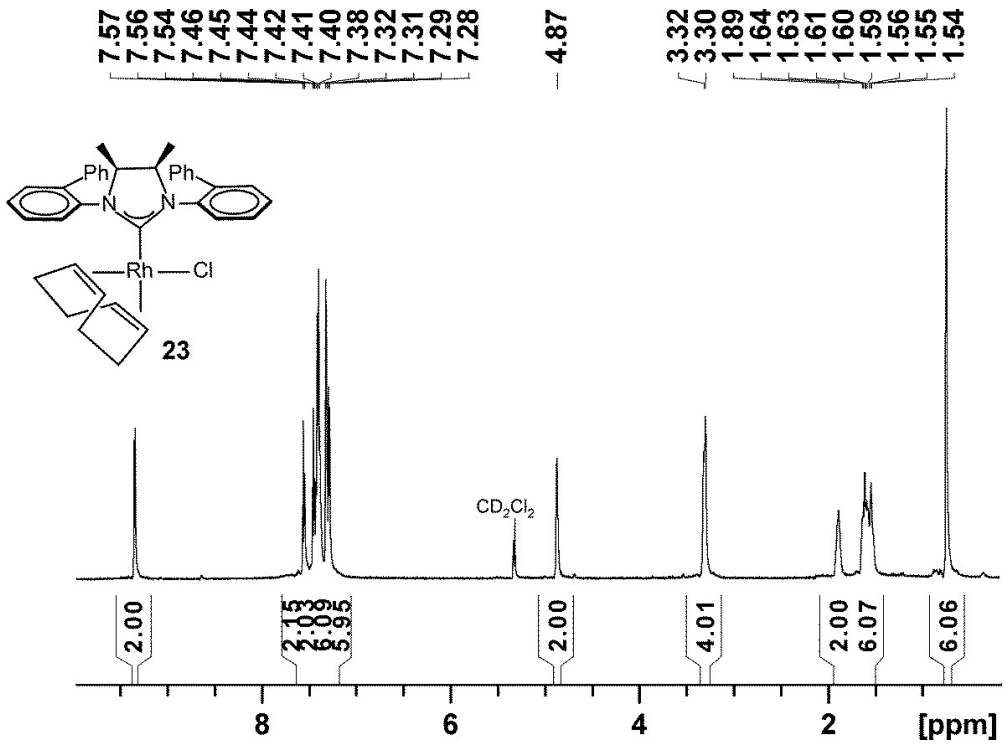


Figure S24. ^{1}H NMR (600 MHz, CD_2Cl_2) of **23**

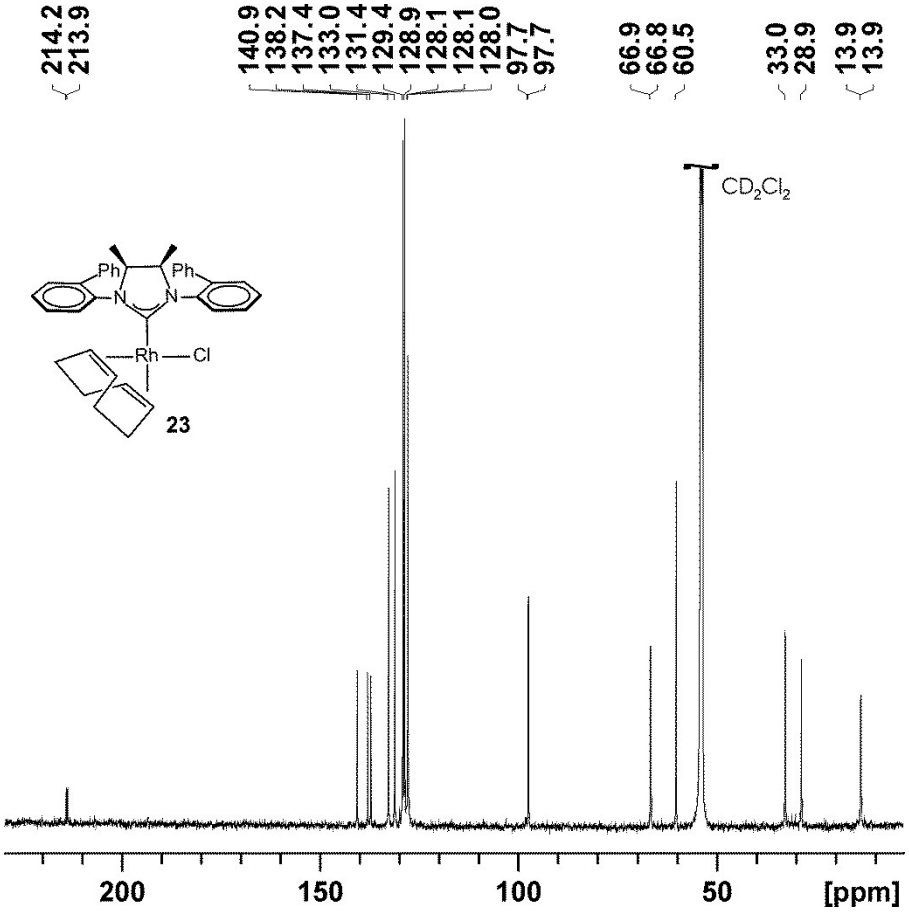


Figure S25. ^{13}C NMR (150 MHz, CD_2Cl_2) of **23**

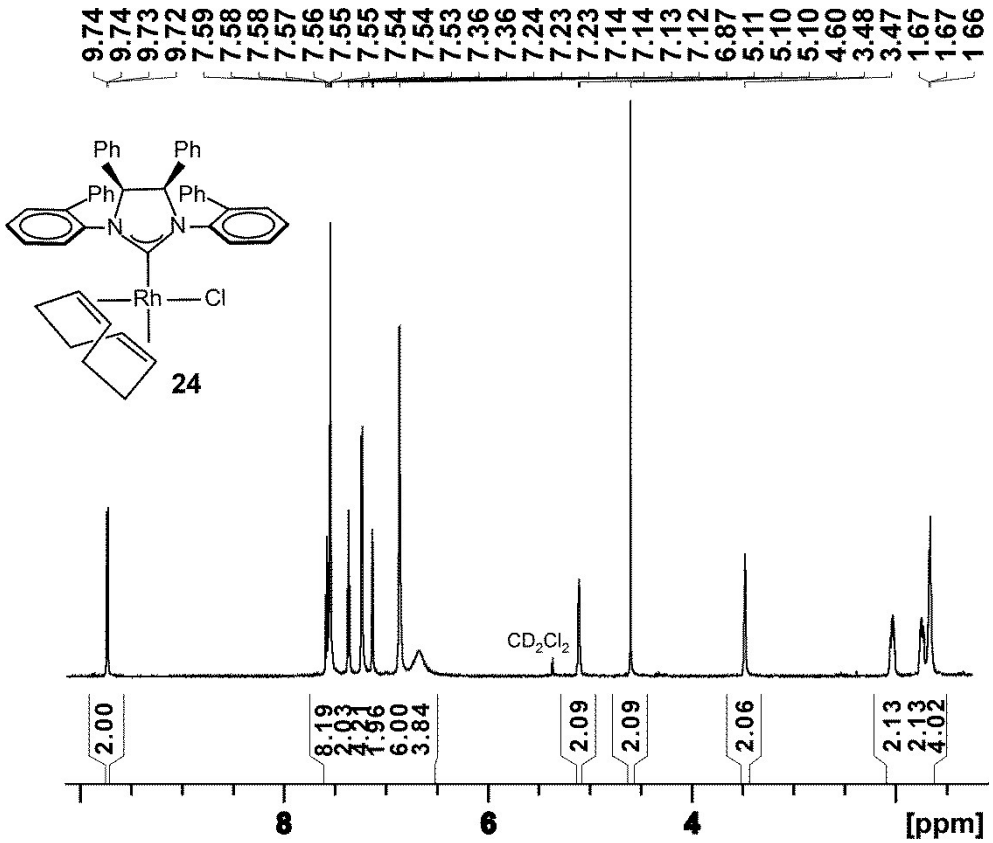


Figure S26. ^{1}H NMR (600 MHz, CD_2Cl_2) of **24**

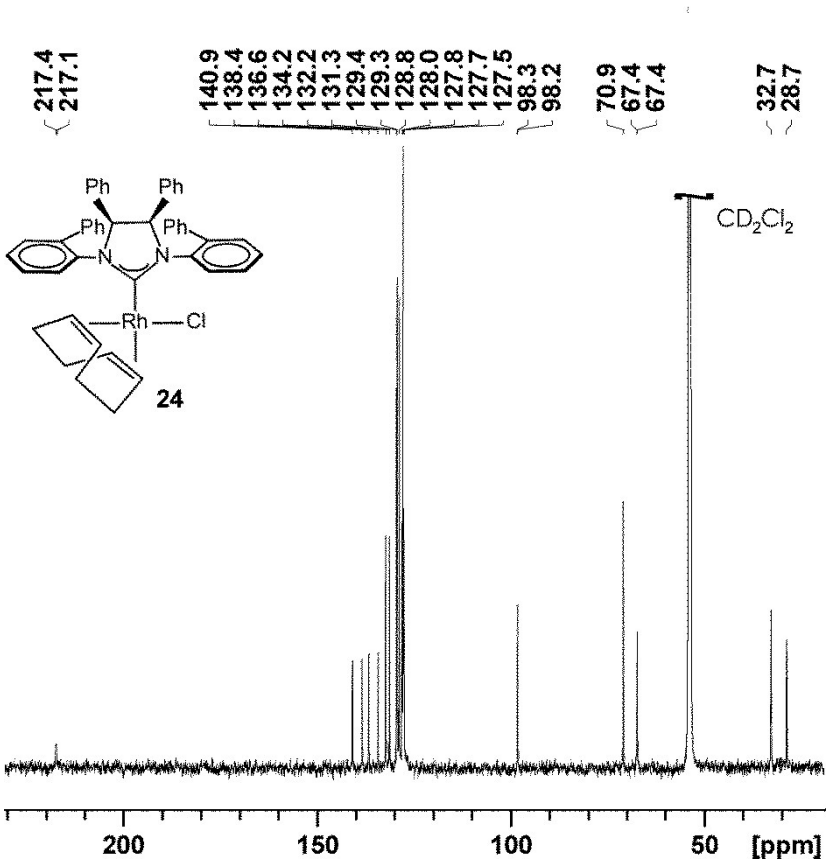


Figure S27. ^{13}C NMR (150 MHz, CD_2Cl_2) of **24**

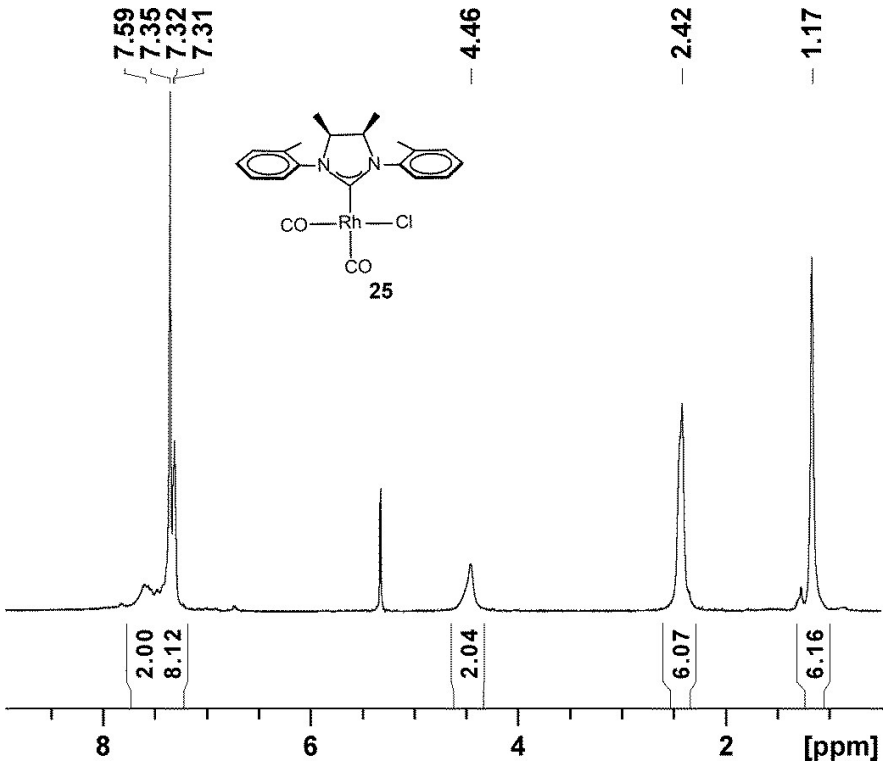


Figure S28. ^{1}H NMR (600 MHz, CD_2Cl_2) of **25**

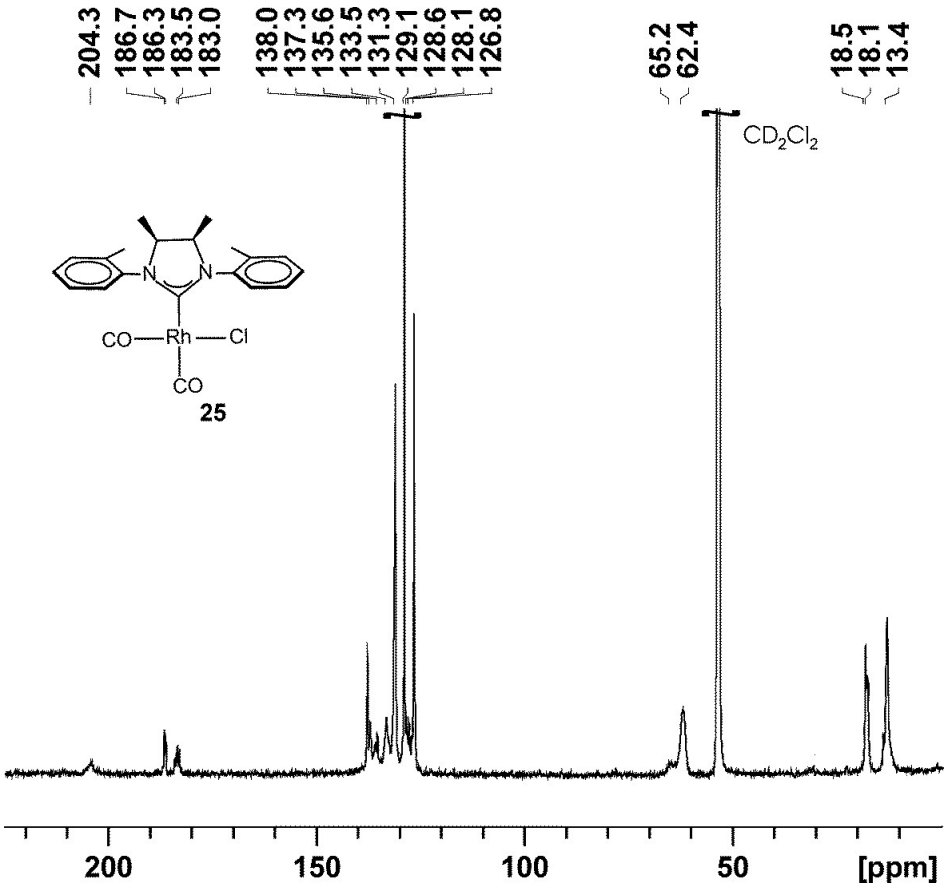


Figure S29. ^{13}C NMR (150 MHz, CD_2Cl_2) of **25**

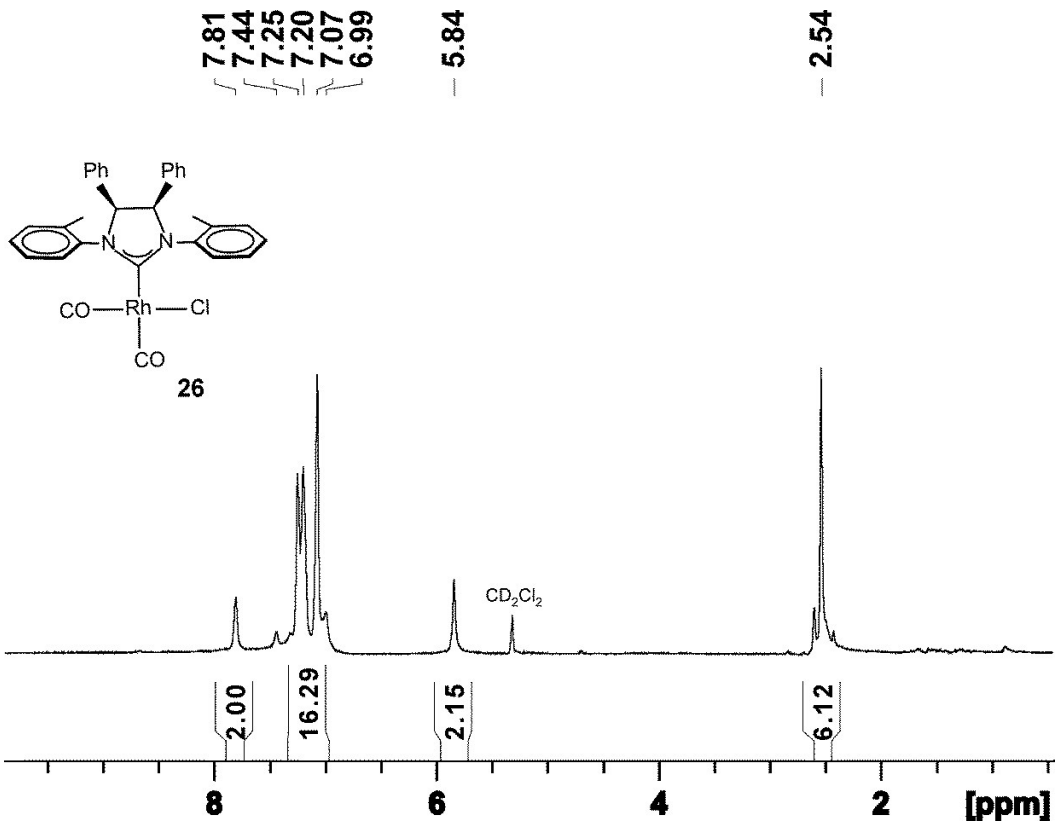


Figure S30. ^{1}H NMR (600 MHz, CD_2Cl_2) of **26**

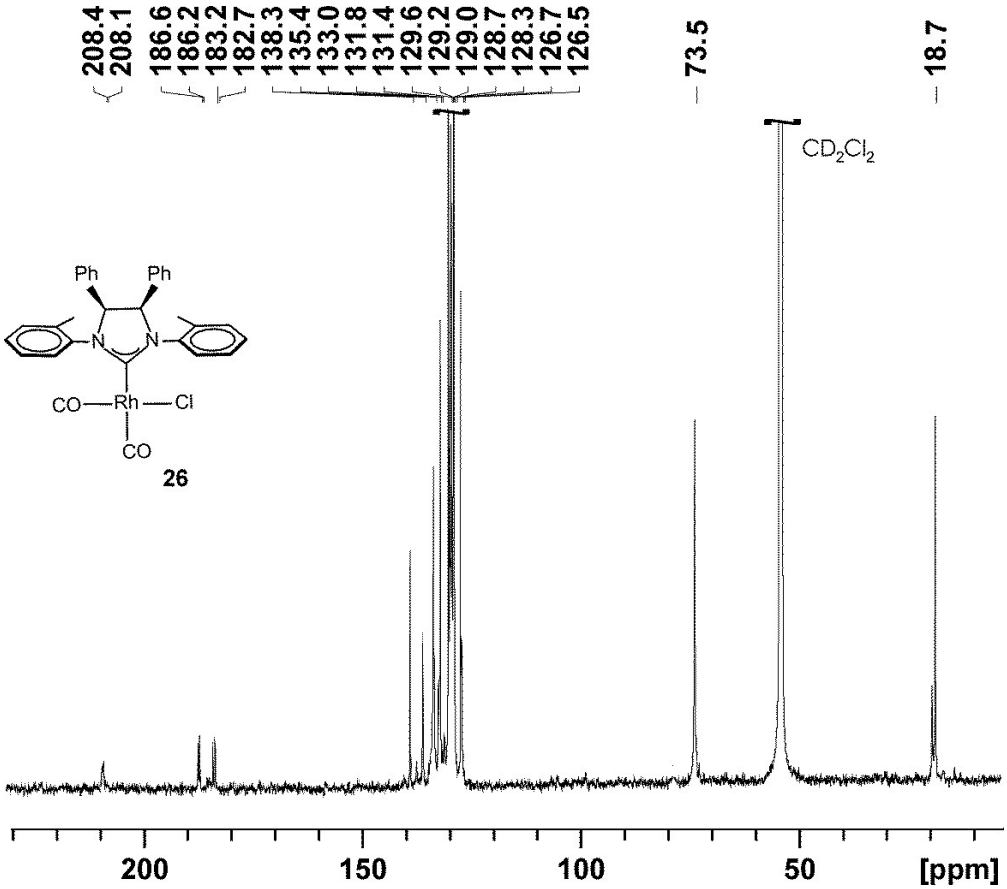


Figure S31. ^{13}C NMR (150 MHz, CD_2Cl_2) of **26**

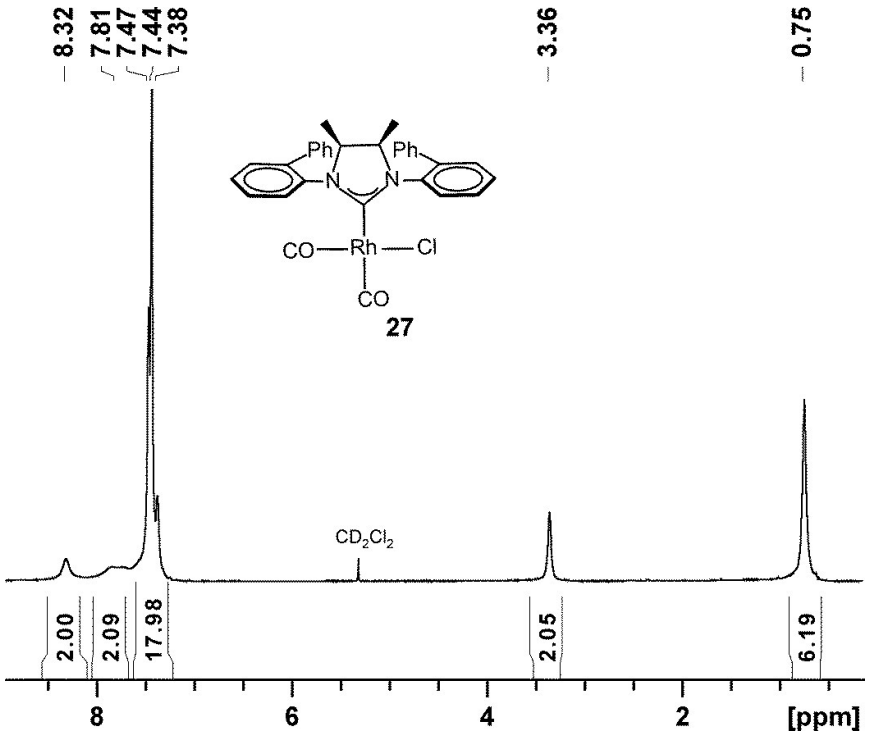


Figure S32. ^{1}H NMR (600 MHz, CD_2Cl_2) of **27**

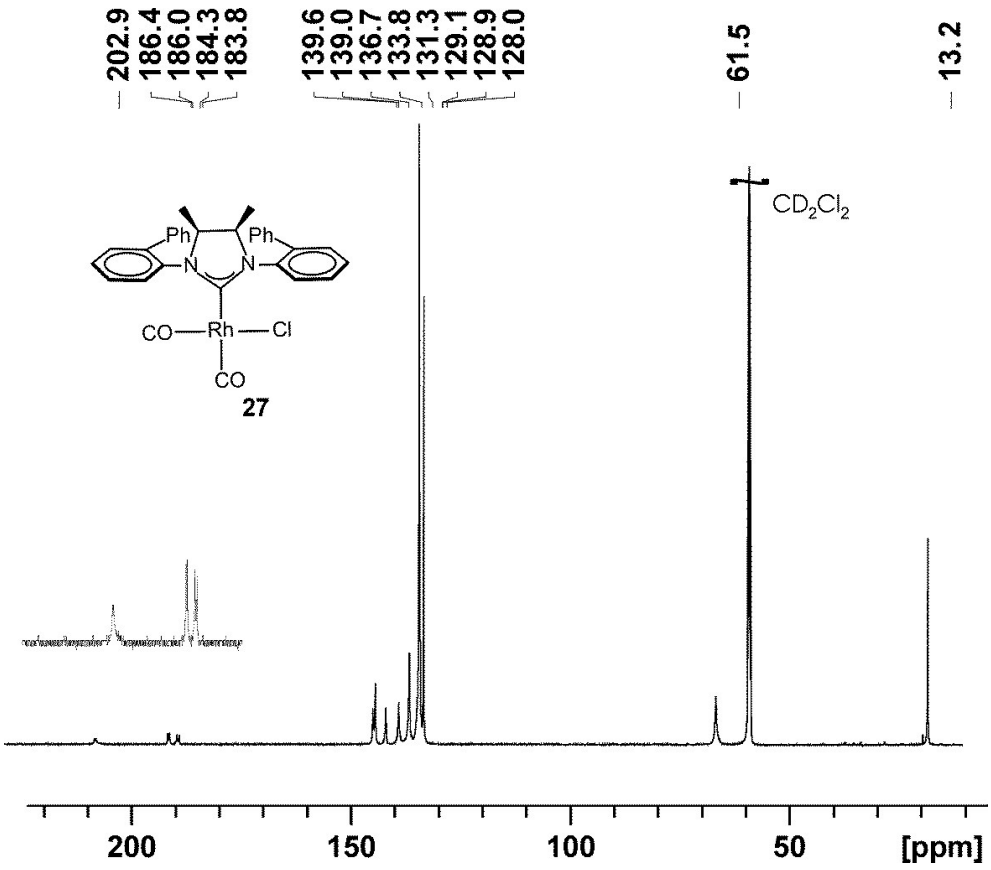


Figure S33. ^{13}C NMR (150 MHz, CD_2Cl_2) of **27**

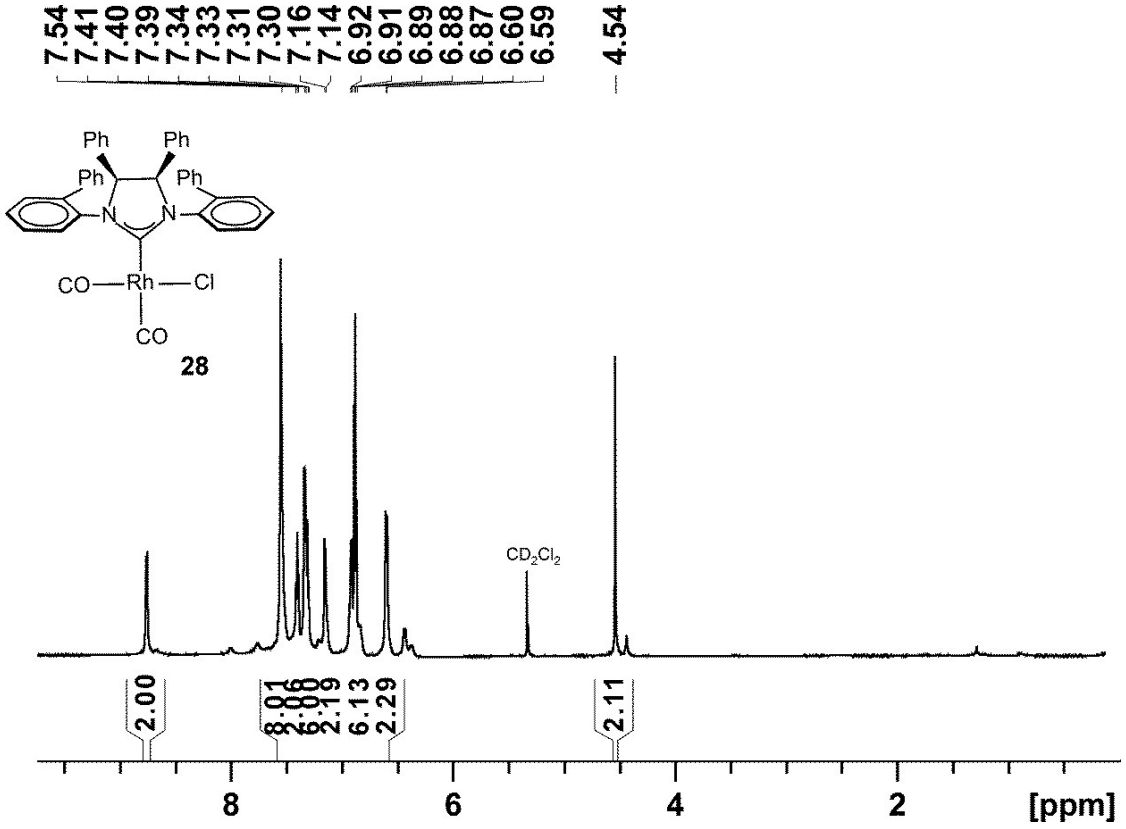


Figure S34. ^{1}H NMR (600 MHz, CD_2Cl_2) of **28**

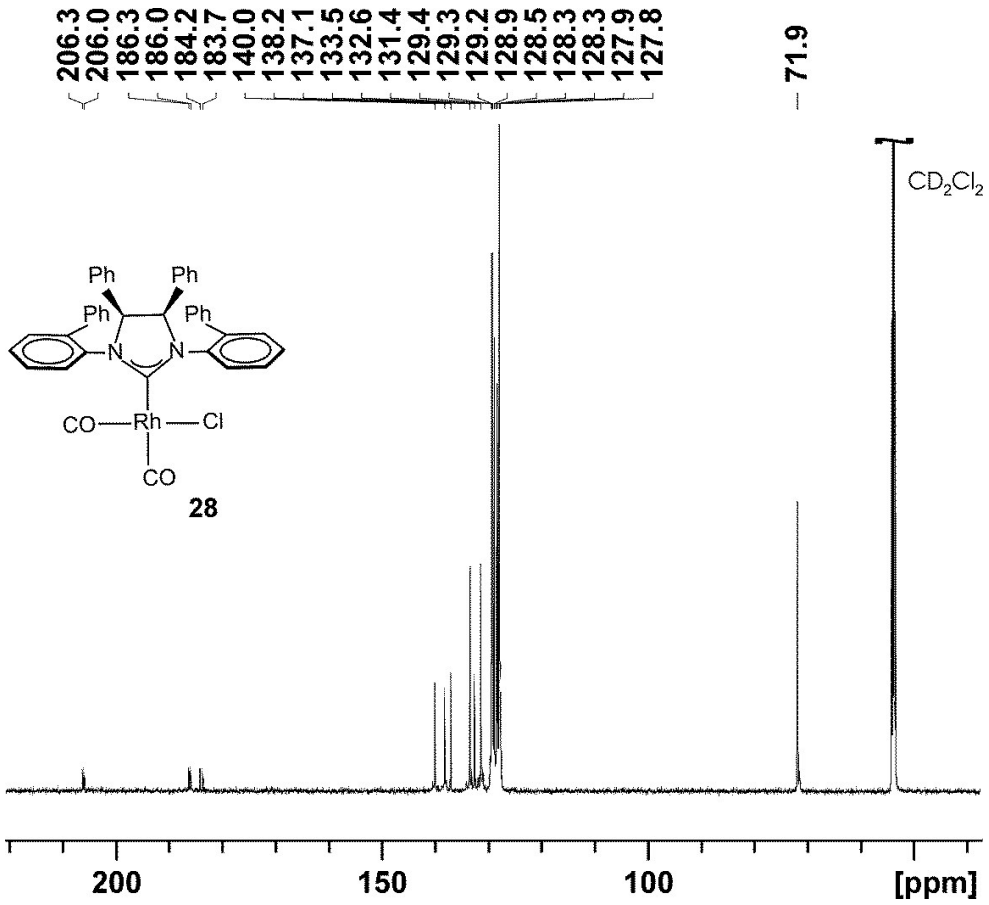
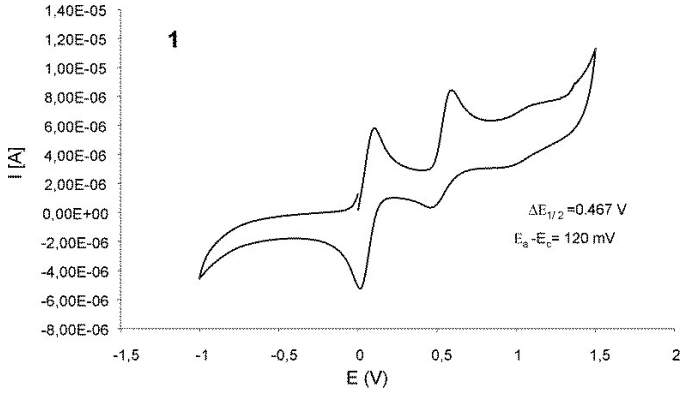
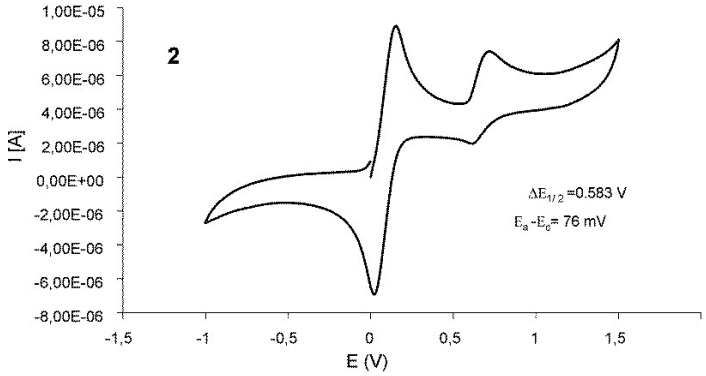
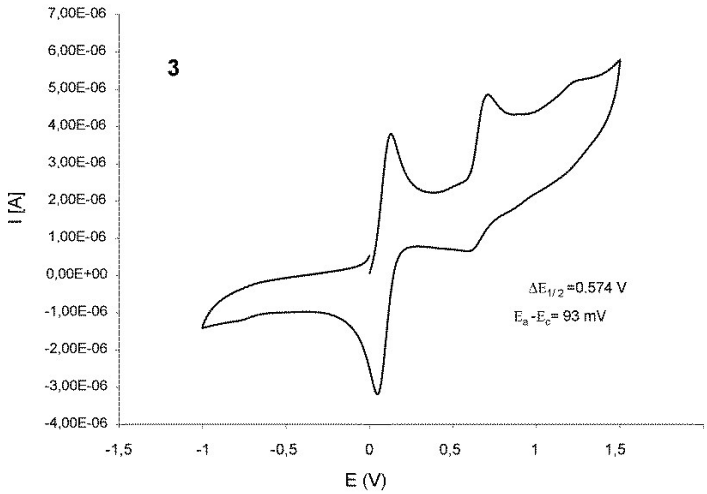


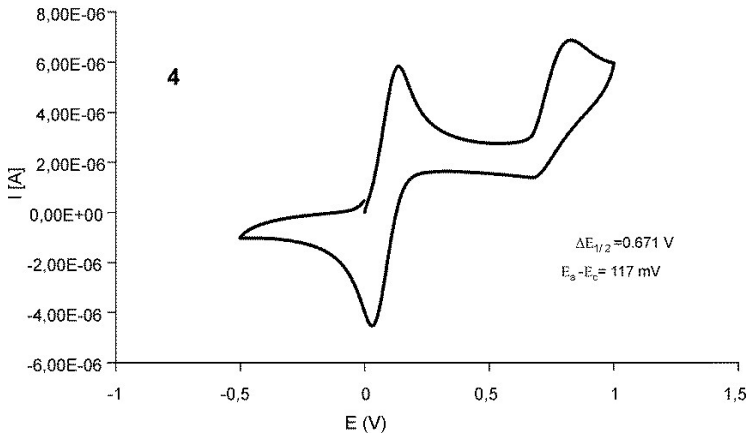
Figure S35. ^{13}C NMR (150 MHz, CD_2Cl_2) of **28**

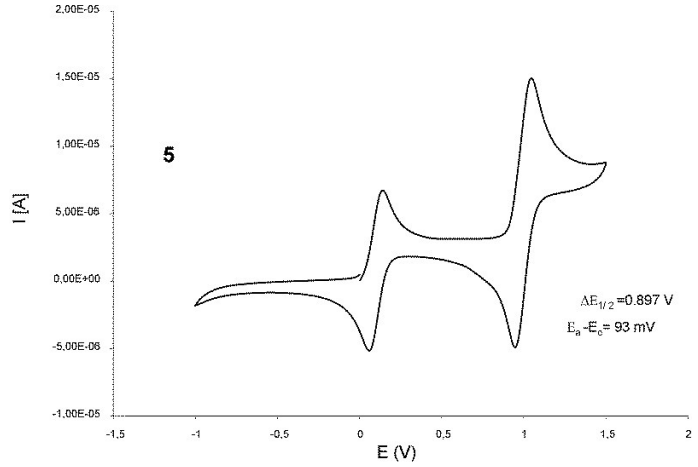
7. Cyclic Voltammograms of Ru-complexes 1-8

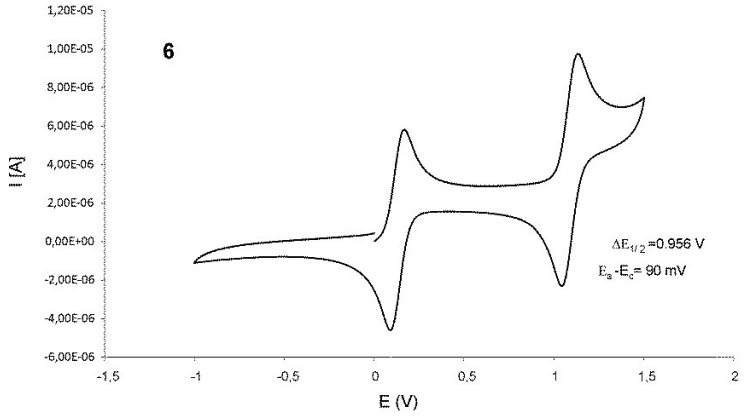


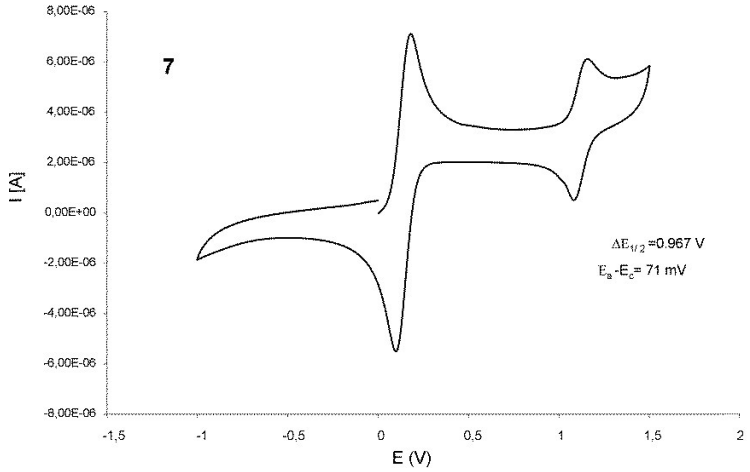


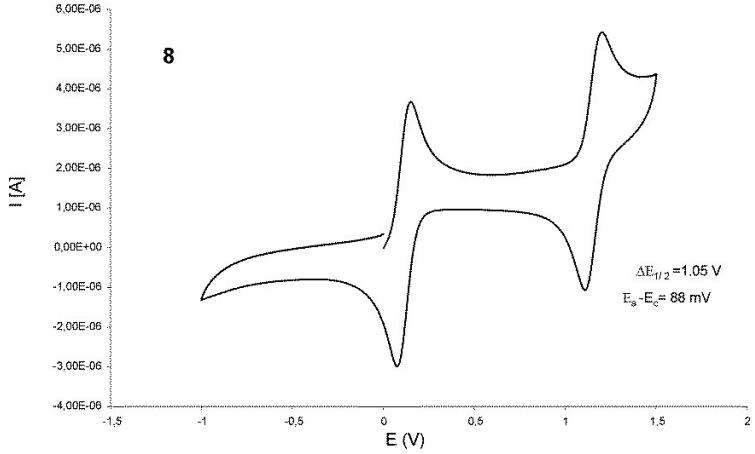





5
I [A]
E (V)
ΔE1/2 =0.897 V
Ea -Ec= 93 mV


6
I [A]
E (V)
ΔE1/2 =0.956 V
Ea -Ec= 90 mV


7
I [A]
E (V)
ΔE1/2 =0.967 V
Ea -Ec= 71 mV


8
I [A]
E (V)
ΔE1/2 =1.05 V
Ea -Ec= 88 mV

8. Crystal structure determinations

The crystal data of compounds **7** and **21-24** 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 package1[3] and corrected for Lorentz, polarization and absorption effects (SORTAV).[4] The structures were solved by direct methods using SIR97[5] 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.

In compounds **21, 22** and **24** ill-defined regions of residual eletron density were found, occupied probably by disordered solvent molecules of pentane, which can not be localized. For these reasons the program SQUEEZE was used to cancel out mathematically the effects of the disordered solvent, treated as a diffuse contribution to the overall scattering without specific atom positions. SQUEEZE is part of the PLATON [6] program system.

In structure of compound **23** the C7, C8, C9 and C10 atoms were found disordered and refined isotropically over two sites with occupancies 0.5.

All calculations were performed using SHELXL-2014/6[7] and PARST[8] implemented in WINGX[9] system of programs. The crystal data are given in Tables S4-S5. A selection of bond distances and angles is given in Tables S6-S7.

Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers CCDC 1483950-1483954 . 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]

Table S4 Crystallographic data.

[3] Otwinowski, Z.;Minor, W. *Methods in Enzymology*, C.W. Carter, R.M. Sweet Editors, Vol. 276, Part A, Academic Press, London, **1997**, 307-326.

[4] Blessing, R. H. *Acta Crystallogr. Sect A* **1995**, *51*, 33-38.

[5] 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.

[6] Spek, A. L. *Acta Crystallogr.* **2009**, D65, 148-155.

[7] Sheldrick, G. M. *Crystal Structure Refinement with SHELXL*, *Acta. Crystallogr*., **2015**, C71, 3-8.

[8] Nardelli, M. *J. Appl. Crystallogr*. **1995**, *28*, 659-659.

[9] Farrugia, L. J. *J. Appl. Crystallogr*. **1999**, *32*, 837-838.

Compound	**7**	**21**	**22**
Formula	$C_{39}H_{38}Cl_2N_2ORu$	$C_{27}H_{32}ClN_2Rh$	$C_{37}H_{38}ClN_2Rh$
M	722.68	522.90	649.05
Space group	*P2₁/n*	*P2₁/n*	*C2/c*
Crystal system	Monoclinic	Monoclinic	Monoclinic
a/Å	10.7017(1)	10.2032(2)	20.1677(6)
b/Å	23.3140(4)	19.7640(5)	15.6920(4)
c/Å	13.8832(2)	14.0720(3)	21.7767(6)
β/°	103.0940(9)	97.576(1)	100.467(2)
U/Å^3	3373.79(8)	2812.9(1)	6777.0(3)
Z	4	4	8
T/K	295	295	295
D_c/g cm^{-3}	1.423	1.235	1.272
F(000)	1488	1080	2688
μ(Mo-Kα)/mm^{-1}	0.657	0.716	0.609
Measured Reflections	45236	26544	20366
Unique Reflections	9744	8136	7372
R_{int}	0.0335	0.0320	0.0497
Obs. Refl.ns [I≥2σ(I)]	7855	6494	5050
θ_{min}- θ_{max}/°	3.01 – 30.03	1.79 – 30.00	3.13 – 27.00
hkl ranges	-14,14;-32,30;-19,19	-14,14;-25,27; -18,19	-25,24;-20,20; -27,27
R(F^2) (Obs.Refl.ns)	0.0299	0.0416	0.0408
wR(F^2) (All Refl.ns)	0.0696	0.1308	0.1126
No. Variables/Restraints	410/0	284/0	372/0
Goodness of fit	1.015	1.067	1.050
$\Delta\rho_{max}$; $\Delta\rho_{min}$ /e Å^{-3}	0.297; -0.405	0.671;-0.720	0.361;-0.449
CCDC Dep. N.	1483950	1483951	1483952

Table S5. Crystallographic data.

Compound	**23**	**24**
Formula	$C_{37}H_{38}ClN_2Rh$	$C_{47}H_{42}ClN_2Rh.1/2(CH_2Cl_2)$
M	649.05	815.65
Space group	*P2₁*	*P-1*
Crystal system	Monoclinic	Triclinic
a/Å	8.2473(2)	11.6821(3)
b/Å	18.8543(7)	16.0026(6)
c/Å	10.5818(3)	22.6928(9)
α/°	90	93.279(2)
β/°	111.131(2)	103.210(3)
γ/°	90	91.676(2)
U/Å^3	1534.80(8)	4119.4(3)
Z	2	4
T/K	295	295
D_c/g cm^{-3}	1.404	1.315
F(000)	672	1684
μ(Mo-Kα)/mm^{-1}	0.672	0.579
Measured Reflections	14176	44260
Unique Reflections	7586	16768
R_{int}	0.0512	0.0961
Obs. Refl.ns [I≥2σ(I)]	6598	10101
θ_{min}- θ_{max}/°	2.99 – 30.04	2.57 – 26.50
hkl ranges	-11,11;-26,24;-14,14	-14,14;-20,19; -27,28
R(F^2) (Obs.Refl.ns)	0.0392	0.0649
wR(F^2) (All Refl.ns)	0.1020	0.1803
No. Variables/Restraints	367/11	941/1
Goodness of fit	1.045	1.037
$\Delta\rho_{max}$; $\Delta\rho_{min}$ /e Å^{-3}	0.626; -0.767	0.946;-1.036
CCDC Dep. N.	1483953	1483954

Table S6. Selected bond distances and angles (Å and degrees) for compound **7**

Distances	**7**
Ru1-Cl1	2.3430(4)
Ru1-Cl2	2.3558(4)
Ru1-C1	1.963(2)
Ru1-C4	1.827(2)
Ru1-O1	2.289(1)
C1-N1	1.363(2)
C1-N2	1.346(2)
Angles	
Cl1-Ru1-Cl2	159.24(2)
Cl1-Ru1-C1	92.42(4)
Cl1-Ru1-C4	97.67(5)
Cl1-Ru1-O1	88.87(3)
Cl2-Ru1-C1	90.74(4)
Cl2-Ru1-C4	101.86(5)
Cl2-Ru1-O1	88.07(3)
C1-Ru1-C4	100.92(7)
C1-Ru1-O1	178.71(5)
C4-Ru1-O1	78.88(6)
Ru1-C1-N1	121.0(1)
Ru1-C1-N2	132.7(1)
N1-C1-N2	106.2(1)

Table S7. Selected bond distances and angles (Å and degrees) for compounds **21-24**.

Distances	**21**	**22**	**23**	**24**
Rh1-C1	2.003(2)	2.018(3)	2.021(3)	2.018(4)
				2.010(5)
Rh1-Cl1	2.4156(7)	2.4098(8)	2.4050(9)	2.417(1)
				2.415(1)
Rh1-$C_{4=5}$*	1.976(3)	1.983(3)	1.989(9)	1.980(5)
				1.995(5)
Rh1-$C_{8=9}$**	2.113(3)	2.103(3)	2.092(9)	2.105(5)
				2.104(5)
C1-N1	1.347(3)	1.333(3)	1.371(12)	1.355(5)
				1.352(6)
C1-N2	1.341(3)	1.347(3)	1.329(14)	1.352(5)
				1.370(6)
Angles				
C1-Rh1-Cl1	90.39(7)	88.99(7)	90.93(9)	90.6(1)
				90.4(1)
C1-Rh1- $C_{4=5}$	91.3(1)	92.6(1)	89.5(4)	92.6(3)
				92.9(3)
C1-Rh1- $C_{8=9}$	174.2(1)	178.3(1)	168.1(5)	177.2(3)
				179.1(3)
Cl1-Rh1- $C_{4=5}$	175.43(7)	177.09(7)	176.0(4)	176.0(2)
				176.5(2)
Cl1-Rh1- $C_{8=9}$	91.74(7)	91.73(7)	90.6(4)	89.8(2)
				90.1(2)
$C_{4=5}$-Rh1- $C_{8=9}$	87.0(1)	86.8(1)	85.7(5)	87.1(3)
				86.6(3)
Rh1-C1-N1	128.9(2)	124.9(2)	124.8(8)	124.4(3)
				126.3(3)
Rh1-C1-N2	123.5(2)	126.9(2)	127.5(8)	128.9(3)
				127.0(3)
N1-C1-N2	107.5(2)	108.0(2)	107.6(3)	106.7(4)
				106.7(4)

*$C_{4=5}$ = Centroid of C4=C5 bond
**$C_{8=9}$ = Centroid of C8=C9 bond

9. Computational details relative to calculations on Ruthenium catalysts 5-8

The DFT calculations were performed with the Gaussian09 set of programs,[10] using the BP86 functional of Becke and Perdew.[11] The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O, and Cl (SVP keyword in Gaussian).[12] For Ru we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/22111/411) scheme (standard SDD keywords in gaussian09).[13] The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations. Solvent effects including contributions of non electrostatic terms have been estimated in single-point calculations on the gas phase optimized structures, based on the polarizable continuous solvation model PCM using benzene as a solvent.[14] In conclusion, the energies reported correspond to the gas-phase free energy corrected by the solvation term.

10. Computational details relative to BDE analysis on Rh complexes

The DFT calculations were performed with the Gaussian09 set of programs,[1] using the B3LYP hybrid functional.[15] The electronic configuration of the molecular systems was described with the standard triple zeta basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O,

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[10] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; N. Kudin, K.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

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and Cl (TZVP keyword in Gaussian).[16] For Rh we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/22111/411) scheme (standard SDD keywords in gaussian09).[4] The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations.

[16] Schaefer, A., Huber, C. and Ahlrichs, R. *J. Chem. Phys.,* **1994,** *100,* 5829-35.

Cartesian coordinates of calculations relative to Ruthenium Hoveyda catalysts

```
21
substrate  E(gas)=-274.941110851  G(gas)=-274.787472  E(benzene)=-
274.941633779 A.U.
  C      3.039564     0.158158    -0.000001
  C      1.752529    -0.236111    -0.000001
  H      3.864460    -0.572485     0.000005
  H      1.546643    -1.322804     0.000000
  H      3.321844     1.225952     0.000003
  C      0.551967     0.690295    -0.000003
  H      0.612847     1.365297    -0.885079
  H      0.612848     1.365301     0.885071
  C     -0.848555     0.011739     0.000000
  C     -1.920836     1.123811    -0.000002
  C     -1.027514    -0.857257    -1.265149
  C     -1.027512    -0.857251     1.265153
  H     -2.944534     0.692813     0.000000
  H     -1.828898     1.773017     0.896966
  H     -1.828899     1.773012    -0.896972
  H     -2.035824    -1.322955    -1.285429
  H     -0.918705    -0.248299    -2.188115
  H     -0.282557    -1.678959    -1.317145
  H     -2.035822    -1.322948     1.285438
  H     -0.282555    -1.678953     1.317152
  H     -0.918701    -0.248288     2.188117
24
substrate-tetra E(gas)-314.226499705 G(gas)=-314.047838 E(benzene)=-
314.227026127 A.U.
  C      1.741554     1.374906    -0.000037
  C      1.582654     0.033093    -0.000006
  C      0.269829    -0.736964     0.000009
  C     -1.129818    -0.056014     0.000006
  C     -1.352570     0.793084    -1.272921
  C     -2.177193    -1.196672    -0.000016
  C     -1.352593     0.793054     1.272948
  H      2.752121     1.816555    -0.000047
  C      2.795935    -0.876148     0.000014
  H      0.900897     2.082677    -0.000055
  H      0.306980    -1.427338     0.877559
  H      0.306973    -1.427359    -0.877524
  H     -3.209424    -0.786939    -0.000027
  H     -2.071261    -1.843649    -0.897138
  H     -2.071285    -1.843662     0.897099
  H     -2.386246     1.200076     1.293325
  H     -1.218527     0.177061     2.187955
  H     -0.654173     1.649375     1.346157
  H     -2.386222     1.200108    -1.293306
  H     -0.654147     1.649406    -1.346097
  H     -1.218488     0.177112    -2.187939
  H      3.744406    -0.303392     0.000000
  H      2.795807    -1.545019     0.889629
  H      2.795806    -1.545057    -0.889573
69
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hov-me-me1 E(gas)-2324.67843485 G(gas)=-2324.199048 E(benzene)=-2324.68588245 A.U.

Ru	0.338824	-0.528083	0.103878
Cl	0.410313	-0.374356	2.469850
Cl	-0.183627	-1.595641	-1.935371
O	2.212826	-1.936586	0.252537
N	-1.249367	2.065799	-0.074072
N	-2.466865	0.219595	-0.100414
C	-1.168664	0.688364	-0.032245
C	-2.643348	2.530220	-0.347066
H	-2.763784	2.635317	-1.451052
C	-3.467153	1.298962	0.101474
H	-4.319139	1.147726	-0.593993
C	-3.003240	3.857342	0.315712
H	-2.852330	3.827699	1.412501
H	-4.066422	4.101152	0.112617
H	-2.386648	4.685501	-0.085593
C	-3.988728	1.322139	1.544983
H	-4.456544	0.348771	1.794756
H	-4.759053	2.108834	1.677451
H	-3.167205	1.501982	2.268403
C	-0.192877	3.005345	0.144180
C	0.216213	3.878682	-0.901834
C	1.219937	4.828851	-0.610730
H	1.548800	5.512348	-1.411155
C	1.819344	4.903813	0.657348
H	2.604760	5.651886	0.849856
C	1.420730	4.015635	1.671341
H	1.892249	4.054145	2.665801
C	0.410352	3.076163	1.417444
H	0.095370	2.359908	2.191559
C	-0.358452	3.769890	-2.295713
H	-0.470821	2.709201	-2.602668
H	0.294948	4.276505	-3.033210
H	-1.362982	4.241440	-2.376031
C	-2.867915	-1.153788	0.020593
C	-3.602683	-1.764171	-1.033204
C	-4.031533	-3.094081	-0.846448
H	-4.593491	-3.585596	-1.657734
C	-3.737666	-3.810765	0.326496
H	-4.083875	-4.851035	0.434552
C	-2.996766	-3.199523	1.349590
H	-2.755523	-3.748613	2.273361
C	-2.570492	-1.868655	1.199113
H	-1.994667	-1.370575	1.995006
C	-3.862141	-1.043701	-2.333573
H	-4.602477	-0.220440	-2.226198
H	-4.256668	-1.740377	-3.099055
H	-2.918923	-0.601118	-2.715972
C	1.695743	0.596470	-0.438901
H	1.541951	1.630629	-0.806932
C	3.072823	0.136599	-0.413563
C	4.170035	0.978183	-0.728559
H	3.963609	2.022583	-1.013101
C	5.485971	0.499443	-0.672832
H	6.329289	1.163229	-0.917929

```
  C      5.721809    -0.837342    -0.301310
  H      6.753017    -1.222182    -0.254680
  C      4.656861    -1.703906     0.012493
  H      4.868546    -2.743836     0.296168
  C      3.340166    -1.216389    -0.041701
  C      2.273920    -3.395770     0.429530
  H      3.145099    -3.593192     1.093195
  C      0.999246    -3.809410     1.154097
  H      0.108947    -3.632545     0.516329
  H      0.878896    -3.239637     2.095959
  H      1.048013    -4.892267     1.389545
  C      2.454669    -4.079610    -0.925855
  H      1.595428    -3.838781    -1.583955
  H      2.509472    -5.179028    -0.785164
  H      3.384267    -3.753054    -1.433487
83
hov-me-ph E(gas)-2707.88160392 G(gas)=-2707.305136 E(benzene)=-
2707.88899604 A.U.
  Ru     1.266944    -0.665787     0.151524
  Cl     0.400399    -1.417899    -1.908632
  Cl     2.173019    -0.999589     2.323075
  C     -0.475031    -0.078016     0.799892
  N     -1.552817    -0.939911     0.895499
  N     -0.929222     1.160487     1.205913
  C     -2.692975    -0.336827     1.637101
  H     -3.641914    -0.614656     1.135326
  C     -2.413255     1.167064     1.413539
  H     -2.887451     1.468649     0.451839
  C      1.936523     0.963029    -0.399166
  H      1.381758     1.920204    -0.326780
  C      3.236145     1.046042    -1.038821
  C      3.768703     2.264262    -1.532729
  H      3.172926     3.183149    -1.410603
  C      5.019511     2.301916    -2.162763
  H      5.422131     3.253414    -2.542521
  C      5.757137     1.112006    -2.307213
  H      6.740770     1.130974    -2.802982
  C      5.262168    -0.115408    -1.825686
  H      5.861575    -1.027248    -1.950876
  C      4.006643    -0.146821    -1.194493
  O      3.394879    -1.264413    -0.693456
  C      4.101103    -2.553815    -0.657806
  H      4.608544    -2.658262    -1.642550
  C      3.043642    -3.642126    -0.529161
  H      2.524150    -3.563985     0.447030
  H      3.533943    -4.635504    -0.583673
  H      2.289613    -3.565784    -1.336351
  C      5.118327    -2.559273     0.483915
  H      5.866544    -1.748329     0.379595
  H      5.662157    -3.526583     0.496319
  H      4.595514    -2.425220     1.452279
  C     -1.516168    -2.353787     0.683487
  C     -2.538228    -2.995272    -0.076168
  C     -2.504777    -4.405245    -0.173910
  H     -3.282957    -4.904323    -0.773054
  C     -1.489826    -5.167764     0.425175
```

H	-1.486896	-6.263483	0.313769
C	-0.483836	-4.522337	1.160548
H	0.313749	-5.103754	1.649478
C	-0.509921	-3.125543	1.302368
H	0.241812	-2.618599	1.929464
C	-3.621589	-2.251518	-0.786197
C	-3.317050	-1.218315	-1.705222
H	-2.260642	-0.963692	-1.890134
C	-4.347427	-0.558491	-2.395330
H	-4.095351	0.236481	-3.114954
C	-5.692701	-0.910833	-2.182071
H	-6.496152	-0.386825	-2.724140
C	-6.005015	-1.940287	-1.277302
H	-7.055028	-2.226379	-1.104391
C	-4.977711	-2.607063	-0.588221
H	-5.226170	-3.407741	0.127477
C	-0.143612	2.321465	1.483415
C	-0.386224	3.555400	0.809410
C	0.360574	4.688047	1.219286
H	0.193390	5.642853	0.696067
C	1.332317	4.609740	2.227374
H	1.905398	5.507633	2.507744
C	1.575695	3.380390	2.864131
H	2.340052	3.299046	3.652715
C	0.829690	2.249787	2.503334
H	1.005689	1.280359	2.993250
C	-1.350498	3.705979	-0.321240
C	-2.232007	4.814635	-0.356937
H	-2.242557	5.522315	0.487814
C	-3.099294	5.017038	-1.442749
H	-3.780198	5.883308	-1.443549
C	-3.098532	4.118066	-2.523273
H	-3.772802	4.278428	-3.379534
C	-2.228701	3.013070	-2.502654
H	-2.207499	2.308396	-3.349057
C	-1.367974	2.802399	-1.412620
H	-0.690569	1.934771	-1.419826
C	-2.720023	-0.817883	3.094284
H	-2.806646	-1.922691	3.126346
H	-3.592617	-0.397785	3.634093
H	-1.795586	-0.531967	3.636851
C	-2.891549	2.103402	2.519001
H	-2.381626	1.907164	3.482618
H	-3.983647	1.973856	2.664969
H	-2.717312	3.162332	2.247950

83

hov-ph-me E(gas)=-2707.87136391 G(gas)=-2707.295801 E(benzene)=-2707.87948579 A.U.

Ru	1.453913	-0.465406	0.064890
Cl	1.116941	0.057771	2.358988
Cl	1.637912	-1.915045	-1.786770
C	-0.329300	0.139046	-0.412157
N	-0.840405	1.399462	-0.645001
C	-2.323628	1.403034	-0.717278
H	-2.659207	2.047193	-1.554775
C	-2.593741	-0.089174	-1.104529

H	-2.532828	-0.142572	-2.215894
N	-1.386602	-0.745886	-0.540963
C	-2.985597	1.912205	0.559170
C	-4.167010	2.675635	0.455899
H	-4.573637	2.915168	-0.541023
C	-4.832125	3.134900	1.604844
H	-5.752283	3.732233	1.503453
C	-4.317232	2.839375	2.878700
H	-4.832148	3.202916	3.782313
C	-3.135279	2.086324	2.992253
H	-2.718208	1.857572	3.985986
C	-2.471514	1.624844	1.842415
H	-1.537891	1.048234	1.954811
C	-3.937969	-0.652965	-0.691018
C	-4.974825	-0.695425	-1.648623
H	-4.772412	-0.363040	-2.681074
C	-6.257491	-1.154194	-1.304729
H	-7.053511	-1.178385	-2.065908
C	-6.517781	-1.589288	0.005832
H	-7.519817	-1.957053	0.278453
C	-5.490618	-1.557880	0.965465
H	-5.685400	-1.900191	1.994088
C	-4.211529	-1.090366	0.622660
H	-3.417730	-1.067618	1.382389
C	-0.160858	2.663254	-0.595453
C	-0.054005	3.433538	-1.786600
C	0.577384	4.694029	-1.700292
H	0.675420	5.301198	-2.615503
C	1.093552	5.177410	-0.487367
H	1.583327	6.163696	-0.454135
C	0.989784	4.396910	0.676708
H	1.399822	4.759876	1.632061
C	0.358600	3.145300	0.623649
H	0.293789	2.510000	1.518443
C	-0.564751	2.923447	-3.114717
H	-0.413916	1.829396	-3.214342
H	-0.047312	3.424347	-3.956864
H	-1.652750	3.119104	-3.245498
C	-1.308970	-2.147761	-0.250198
C	-1.584992	-3.128541	-1.242460
C	-1.526547	-4.482885	-0.853850
H	-1.732129	-5.254064	-1.614447
C	-1.181560	-4.873408	0.450720
H	-1.138371	-5.942897	0.710920
C	-0.883723	-3.894058	1.410422
H	-0.607315	-4.177779	2.438077
C	-0.961065	-2.535844	1.061525
H	-0.752042	-1.756012	1.810221
C	-1.857863	-2.761936	-2.680026
H	-2.868742	-2.321440	-2.816588
H	-1.799045	-3.657325	-3.329506
H	-1.104381	-2.029990	-3.038843
C	2.437481	0.962100	-0.569576
H	2.015450	1.799646	-1.159126
C	3.869740	1.015573	-0.340226
C	4.665029	2.125024	-0.725764

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  H      4.171104     2.973934    -1.225448
  C      6.043015     2.147249    -0.472854
  H      6.649462     3.014541    -0.775940
  C      6.646834     1.050671     0.170402
  H      7.729757     1.058990     0.372572
  C      5.889907    -0.070412     0.562462
  H      6.387685    -0.914462     1.058913
  C      4.507514    -0.084491     0.310355
  O      3.647854    -1.095600     0.649932
  C      4.159943    -2.396904     1.107014
  H      4.948558    -2.174018     1.859750
  C      4.738232    -3.174675    -0.075232
  H      3.946265    -3.350832    -0.830817
  H      5.131614    -4.151092     0.275916
  H      5.568976    -2.628182    -0.564883
  C      3.005739    -3.111341     1.797726
  H      2.593286    -2.495812     2.620780
  H      3.368888    -4.073305     2.213600
  H      2.192553    -3.330630     1.075683
97
hov-ph-ph1 E(gas)=-3091,07472761 G(gas)=-3090.404963 E(benzene)=-
3091.08281085 A.U.
  Ru    -1.931001    -0.433942    -0.137279
  Cl    -1.909463    -1.220565     2.085576
  Cl    -2.107606    -0.668962    -2.500221
  C      0.001553    -0.197287    -0.195791
  N      0.871862    -1.251786     0.015272
  N      0.782055     0.917791    -0.424847
  C      2.279180    -0.904514    -0.299408
  H      2.948632    -1.312178     0.483231
  C      2.222581     0.648380    -0.129790
  H      2.390431     0.857509     0.950434
  C     -2.453015     1.307305     0.185292
  H     -1.749806     2.153430     0.318553
  C     -3.856453     1.635979     0.350804
  C     -4.302116     2.948757     0.651671
  H     -3.549190     3.747263     0.750624
  C     -5.664760     3.226335     0.821092
  H     -5.998631     4.248812     1.055018
  C     -6.604179     2.186526     0.690138
  H     -7.677774     2.395179     0.822602
  C     -6.199221     0.871658     0.388952
  H     -6.956033     0.081618     0.291501
  C     -4.830519     0.599008     0.221962
  O     -4.290528    -0.629136    -0.050437
  C     -5.153354    -1.783936    -0.338085
  H     -5.978984    -1.749631     0.406907
  C     -4.317985    -3.032553    -0.092524
  H     -3.486275    -3.091000    -0.823250
  H     -4.954986    -3.931891    -0.216435
  H     -3.886629    -3.028914     0.927290
  C     -5.699457    -1.685010    -1.762646
  H     -6.285931    -0.757624    -1.918689
  H     -6.364160    -2.549200    -1.969403
  H     -4.861119    -1.691079    -2.488156
  C      0.504793    -2.625020     0.193694
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C	1.108783	-3.406032	1.221527
C	0.779494	-4.779049	1.290936
H	1.232144	-5.382790	2.093501
C	-0.132612	-5.370729	0.403396
H	-0.375313	-6.440960	0.496473
C	-0.729979	-4.587111	-0.595061
H	-1.438232	-5.034197	-1.310285
C	-0.397961	-3.227650	-0.707087
H	-0.817795	-2.625297	-1.528474
C	2.050027	-2.845165	2.236209
C	1.685630	-1.737338	3.039087
H	0.690221	-1.283338	2.902435
C	2.568356	-1.253401	4.019210
H	2.268853	-0.395690	4.641846
C	3.822890	-1.859214	4.215413
H	4.510835	-1.473190	4.984622
C	4.190951	-2.964005	3.427820
H	5.170314	-3.447413	3.574187
C	3.310579	-3.453993	2.448396
H	3.604957	-4.313495	1.824478
C	0.339453	2.218782	-0.823553
C	0.587965	3.363384	-0.012074
C	0.225394	4.630609	-0.532397
H	0.402252	5.521600	0.090645
C	-0.393719	4.767720	-1.783069
H	-0.674998	5.767713	-2.149316
C	-0.664260	3.624044	-2.554334
H	-1.160320	3.712784	-3.533497
C	-0.284292	2.360699	-2.081503
H	-0.483561	1.455506	-2.674527
C	1.142717	3.293976	1.372659
C	2.180348	4.172367	1.769068
H	2.628876	4.845851	1.021662
C	2.654180	4.181281	3.091294
H	3.466260	4.869820	3.375261
C	2.094761	3.316513	4.048436
H	2.458660	3.329418	5.088217
C	1.065422	2.436946	3.668005
H	0.607117	1.764117	4.410219
C	0.596712	2.418179	2.343542
H	-0.215585	1.726371	2.070977
C	2.734459	-1.444091	-1.651123
C	3.237144	1.449056	-0.920103
C	4.071232	-1.869488	-1.799265
C	4.542444	-2.349085	-3.032768
C	3.675920	-2.417296	-4.137326
C	2.339456	-2.003111	-3.998107
C	1.869826	-1.519431	-2.764902
H	4.752870	-1.822496	-0.933843
H	5.589756	-2.677316	-3.129043
H	4.039774	-2.799654	-5.104451
H	1.650447	-2.059587	-4.855960
H	0.816395	-1.206314	-2.675939
C	4.366466	1.957413	-0.242489
C	5.371951	2.652609	-0.935839
C	5.252794	2.863091	-2.320048

C	4.126528	2.370541	-3.003102
C	3.128828	1.664955	-2.311525
H	4.453543	1.808847	0.846357
H	6.247533	3.038027	-0.389375
H	6.035111	3.413720	-2.866611
H	4.023541	2.533479	-4.087647
H	2.258227	1.279008	-2.860503

90

i-cm-me-me-a E(gas)=-2599.6003216 G(gas)=-2598.943884 E(benzene)=-2599.60819209 A.U.

Ru	-0.425826	0.341220	-0.114061
Cl	-0.365932	0.240152	-2.560652
Cl	-0.844673	0.286157	2.274168
N	-0.114651	-2.703455	-0.145245
N	-2.218159	-2.041603	-0.174848
C	-0.925913	-1.611816	-0.157296
C	-0.902111	-3.968623	-0.005154
H	-0.954250	-4.218649	1.080116
C	-2.312950	-3.502798	-0.456560
H	-3.084689	-3.952434	0.203293
C	-0.296314	-5.152106	-0.753991
H	-0.171072	-4.938864	-1.833583
H	-0.943774	-6.045822	-0.641339
H	0.700847	-5.405114	-0.342281
C	-2.679168	-3.769633	-1.921654
H	-3.660753	-3.311521	-2.156819
H	-2.761185	-4.858279	-2.116606
H	-1.925920	-3.337727	-2.611552
C	1.317963	-2.698294	-0.201064
C	2.080329	-3.091686	0.930754
C	3.483867	-3.146937	0.785525
H	4.093477	-3.443572	1.654682
C	4.114099	-2.811246	-0.422853
H	5.211669	-2.864442	-0.500471
C	3.343837	-2.393307	-1.521651
H	3.827122	-2.114391	-2.471297
C	1.946335	-2.339657	-1.410847
H	1.319238	-1.995450	-2.247982
C	1.426693	-3.408570	2.255602
H	0.627991	-2.675095	2.494115
H	2.170753	-3.388766	3.076054
H	0.962858	-4.420089	2.263270
C	-3.374103	-1.189586	-0.240214
C	-4.262271	-1.140104	0.869145
C	-5.427049	-0.355152	0.735114
H	-6.127911	-0.300639	1.584259
C	-5.702212	0.364087	-0.441039
H	-6.623072	0.964845	-0.511710
C	-4.799905	0.322722	-1.516443
H	-4.998988	0.891064	-2.438489
C	-3.634809	-0.456653	-1.416676
H	-2.900901	-0.490644	-2.237587
C	-3.945589	-1.852621	2.160577
H	-3.865694	-2.953373	2.029915
H	-4.727980	-1.662441	2.921150
H	-2.970622	-1.493336	2.557090

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  C      1.431352     0.727828    -0.198120
  H      1.781172     0.899612    -1.236650
  C      2.538741     0.769888     0.765700
  C      2.460538     0.261807     2.086254
  H      1.488607    -0.133011     2.418045
  C      3.563781     0.271940     2.948271
  H      3.471257    -0.130496     3.968815
  C      4.785190     0.801600     2.498575
  H      5.663905     0.817400     3.163973
  C      4.904001     1.331138     1.203473
  H      5.863030     1.759715     0.888325
  C      3.795143     1.331910     0.328045
  O      3.789772     1.873244    -0.920239
  C      4.954915     2.346845    -1.646245
  H      4.498727     2.576898    -2.632676
  C      5.505852     3.665154    -1.087936
  H      6.062980     3.541608    -0.138493
  H      4.680442     4.384431    -0.913963
  H      6.199699     4.115443    -1.827810
  C      6.004140     1.253950    -1.878579
  H      6.576149     0.993961    -0.966549
  H      6.728874     1.599709    -2.644364
  H      5.519019     0.332190    -2.257342
  C      0.256338     2.561301     0.040411
  C     -1.085427     2.401754    -0.419359
  H      1.016748     2.929322    -0.668251
  H     -1.232005     2.484864    -1.512023
  H      0.443014     2.777201     1.105533
  C     -2.292445     2.746932     0.433461
  H     -3.127533     2.057478     0.178567
  H     -2.055306     2.573768     1.503106
  C     -2.827348     4.211527     0.254880
  C     -4.054367     4.362134     1.181985
  C     -1.753717     5.240572     0.666651
  C     -3.263384     4.471253    -1.204002
  H     -4.488197     5.382371     1.106095
  H     -4.849376     3.633450     0.916483
  H     -3.780017     4.187286     2.243940
  H     -2.152939     6.275236     0.596841
  H     -1.419573     5.078236     1.713769
  H     -0.857756     5.184043     0.013548
  H     -3.720764     5.479060    -1.303457
  H     -2.407959     4.425478    -1.909606
  H     -4.015438     3.724634    -1.537038
90
i-cm-me-me-b E(gas)=-2599.59964521 G(gas)=-2598.943729 E(benzene)=-
2599.60751785
  Ru    -0.498780     0.327934     0.113655
  Cl    -0.516114     0.643491    -2.309128
  Cl    -0.894101    -0.076568     2.475562
  N     -0.168496    -2.659125    -0.453220
  N     -2.271966    -2.046067    -0.192860
  C     -0.985350    -1.598266    -0.214877
  C     -0.929703    -3.946240    -0.468001
  H     -0.877987    -4.385808     0.554979
  C     -2.381084    -3.443968    -0.700843
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H	-3.081976	-4.013436	-0.054451
C	-0.385957	-4.963641	-1.467287
H	-0.365048	-4.560728	-2.498806
H	-1.010879	-5.880205	-1.457355
H	0.648057	-5.258401	-1.198729
C	-2.888536	-3.474801	-2.147869
H	-3.888834	-3.000933	-2.207399
H	-2.989797	-4.517793	-2.510616
H	-2.207902	-2.923087	-2.827925
C	1.260524	-2.617871	-0.567043
C	2.075947	-3.156609	0.463554
C	3.473043	-3.151210	0.259690
H	4.124252	-3.556073	1.051482
C	4.045485	-2.621360	-0.907400
H	5.139802	-2.632488	-1.032982
C	3.222572	-2.063547	-1.900822
H	3.660167	-1.630380	-2.813904
C	1.830108	-2.063748	-1.730660
H	1.161206	-1.608260	-2.477519
C	1.483137	-3.681978	1.750272
H	0.665869	-3.023391	2.112124
H	2.254714	-3.741857	2.542797
H	1.060809	-4.704597	1.630322
C	-3.430348	-1.205676	-0.060659
C	-4.265680	-1.343015	1.082170
C	-5.429602	-0.547897	1.135642
H	-6.087582	-0.634418	2.015940
C	-5.756755	0.354747	0.108916
H	-6.675795	0.957788	0.183359
C	-4.908660	0.490952	-1.001811
H	-5.151876	1.198803	-1.809665
C	-3.744066	-0.291126	-1.087162
H	-3.052835	-0.190315	-1.939341
C	-3.890925	-2.255224	2.223563
H	-3.827402	-3.320809	1.914191
H	-4.632454	-2.189143	3.043630
H	-2.894359	-1.962226	2.621065
C	1.358134	0.730235	0.021036
H	1.661482	1.073738	-0.988808
C	2.508235	0.580636	0.921297
C	2.434894	-0.016534	2.205012
H	1.444211	-0.352973	2.549446
C	3.564055	-0.160372	3.019973
H	3.472731	-0.623620	4.014551
C	4.811100	0.291062	2.554604
H	5.712301	0.180343	3.179698
C	4.929532	0.895087	1.292796
H	5.913618	1.244776	0.958855
C	3.794141	1.059530	0.467607
O	3.801848	1.663706	-0.749687
C	4.949401	2.280604	-1.389339
H	4.483039	2.648284	-2.328087
C	5.465245	3.510413	-0.631260
H	5.994263	3.257624	0.308594
H	4.626209	4.191065	-0.382683
H	6.174358	4.067754	-1.277854

C	6.031276	1.271685	-1.794730
H	6.626176	0.895064	-0.939762
H	6.733455	1.755365	-2.505023
H	5.572557	0.402489	-2.306847
C	0.229552	2.473364	0.648671
C	-1.186328	2.377019	0.480671
H	0.800546	3.049307	-0.099367
H	-1.749263	2.196572	1.416364
H	0.646903	2.444125	1.667278
C	-1.942913	3.102391	-0.610591
H	-1.320539	3.154219	-1.527286
H	-2.842432	2.508335	-0.879596
C	-2.431376	4.545015	-0.232928
C	-3.210339	5.093703	-1.449618
C	-3.371023	4.510025	0.992937
C	-1.236261	5.476936	0.058963
H	-3.579560	6.123774	-1.255850
H	-2.569913	5.127384	-2.356515
H	-4.090509	4.457934	-1.684558
H	-3.789525	5.519098	1.196300
H	-4.223698	3.817424	0.827437
H	-2.843723	4.181058	1.912481
H	-1.585973	6.511913	0.262634
H	-0.658008	5.142524	0.945727
H	-0.539291	5.522150	-0.805326

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i-cm-me-me-c E(gas)=-2599.606365 G(gas)=-2598.952282 E(benzene)=-2599.61384575 A.U.

Ru	-0.422553	0.277944	-0.292425
Cl	-0.599328	-0.098257	-2.693583
Cl	-0.623340	0.535276	2.128512
N	0.019148	-2.725907	0.151632
N	-2.099604	-2.119495	0.201675
C	-0.825814	-1.670644	0.016305
C	-0.702931	-3.948541	0.622262
H	-0.641469	-3.968969	1.735908
C	-2.165589	-3.607996	0.228601
H	-2.856280	-3.927914	1.037083
C	-0.127236	-5.251971	0.077182
H	-0.114568	-5.272136	-1.030332
H	-0.726736	-6.112378	0.439333
H	0.913136	-5.395658	0.430793
C	-2.657944	-4.170103	-1.110883
H	-3.667090	-3.772413	-1.339468
H	-2.733379	-5.275958	-1.074088
H	-1.981746	-3.885385	-1.942508
C	1.451668	-2.683578	0.061139
C	2.244872	-2.593037	1.237233
C	3.647283	-2.638925	1.076496
H	4.282525	-2.570260	1.975088
C	4.244793	-2.759942	-0.188910
H	5.342515	-2.790585	-0.275683
C	3.443242	-2.829626	-1.339935
H	3.901800	-2.907225	-2.337547
C	2.046502	-2.792482	-1.210373
H	1.391750	-2.831862	-2.093840

C	1.624384	-2.428461	2.603887
H	0.882072	-1.598681	2.611863
H	2.400270	-2.206767	3.362977
H	1.098413	-3.350468	2.936691
C	-3.285512	-1.313633	0.107934
C	-4.069151	-1.089506	1.274517
C	-5.265159	-0.356705	1.122530
H	-5.885825	-0.170289	2.014318
C	-5.670077	0.150294	-0.124702
H	-6.611191	0.717447	-0.205076
C	-4.871053	-0.059814	-1.259965
H	-5.171828	0.340496	-2.240736
C	-3.680127	-0.796696	-1.143671
H	-3.029496	-0.963085	-2.016314
C	-3.614043	-1.562283	2.632686
H	-3.515564	-2.667819	2.688464
H	-4.328277	-1.251218	3.420017
H	-2.617563	-1.124303	2.862503
C	1.398471	0.784404	-0.067043
H	1.620535	1.034370	0.990886
C	2.598467	0.846425	-0.906447
C	2.632214	0.501125	-2.281855
H	1.688477	0.160229	-2.737217
C	3.804215	0.594272	-3.041304
H	3.792330	0.325401	-4.108897
C	4.992091	1.030912	-2.429039
H	5.924304	1.106730	-3.012538
C	5.008333	1.382617	-1.070057
H	5.947636	1.728692	-0.617294
C	3.827337	1.302085	-0.298415
O	3.767749	1.635297	1.018707
C	4.907172	2.187992	1.719836
H	5.821840	1.634036	1.405773
C	5.060612	3.678483	1.400518
H	4.160315	4.235189	1.733214
H	5.193754	3.854637	0.314303
H	5.942989	4.098114	1.926422
C	4.655310	1.919743	3.202447
H	3.724312	2.422140	3.536173
H	5.499171	2.303684	3.810883
H	4.548817	0.833606	3.393068
C	0.134703	2.537331	-0.562832
C	-1.258792	2.267259	-0.690589
H	0.730690	2.690024	-1.475672
H	-1.608417	2.130197	-1.731449
H	0.492677	3.043672	0.349488
C	-2.305075	2.740068	0.296637
H	-3.122489	1.986876	0.343075
H	-1.865771	2.783662	1.313799
C	-2.956775	4.124971	-0.047811
C	-4.004416	4.420909	1.048616
C	-1.894530	5.244722	-0.046557
C	-3.663581	4.082155	-1.420635
H	-4.503029	5.397843	0.870124
H	-4.790646	3.636950	1.073126
H	-3.534817	4.457277	2.054484

H	-2.364532	6.233721	-0.235869
H	-1.371022	5.303437	0.931873
H	-1.126304	5.086040	-0.832348
H	-4.195551	5.037413	-1.618806
H	-2.947936	3.923913	-2.254076
H	-4.413112	3.263247	-1.458706

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i-cm-me-me-d E(gas)=-2599.60520438 G(gas)=-2598.948638 E(benzene)=-2599.61287832 A.U.

Ru	-0.448255	0.357061	-0.055695
Cl	-0.800439	0.404892	-2.460335
Cl	-0.500448	0.139163	2.380600
N	0.051478	-2.655531	-0.167536
N	-2.069876	-2.158509	0.161170
C	-0.832633	-1.629211	-0.055758
C	-0.581022	-3.964098	0.183737
H	-0.416109	-4.136312	1.273611
C	-2.083040	-3.638438	-0.028294
H	-2.686572	-4.102891	0.779837
C	-0.014278	-5.149867	-0.590824
H	-0.107580	-5.014678	-1.686267
H	-0.545055	-6.080566	-0.302914
H	1.059973	-5.289185	-0.356744
C	-2.673011	-4.028341	-1.389311
H	-3.715939	-3.662256	-1.472430
H	-2.693727	-5.130784	-1.508493
H	-2.088828	-3.591284	-2.224696
C	1.460448	-2.540340	-0.415869
C	2.389997	-2.619412	0.656010
C	3.762452	-2.573961	0.326545
H	4.501901	-2.631975	1.142294
C	4.202195	-2.452257	-1.001805
H	5.281113	-2.419452	-1.220963
C	3.266529	-2.360387	-2.045184
H	3.600079	-2.247655	-3.088019
C	1.896027	-2.403912	-1.747761
H	1.138733	-2.316703	-2.541180
C	1.935929	-2.721797	2.092088
H	1.168625	-1.950538	2.327254
H	2.789578	-2.585861	2.784967
H	1.490193	-3.715910	2.316897
C	-3.296559	-1.414929	0.242801
C	-4.017411	-1.387386	1.469486
C	-5.258661	-0.716254	1.477910
H	-5.830887	-0.678444	2.419441
C	-5.771642	-0.092359	0.327476
H	-6.746667	0.418782	0.371117
C	-5.037655	-0.115877	-0.869434
H	-5.423445	0.378233	-1.774726
C	-3.799688	-0.778787	-0.910827
H	-3.193825	-0.790549	-1.830169
C	-3.458335	-2.007327	2.725945
H	-3.321391	-3.106383	2.630836
H	-4.130607	-1.829177	3.588046
H	-2.462547	-1.565403	2.951312
C	1.385187	0.824940	0.141464

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  H      1.678341     0.891180     1.209104
  C      2.530370     1.035619    -0.750646
  C      2.450717     1.039115    -2.166679
  H      1.464210     0.840044    -2.615891
  C      3.567185     1.292714    -2.971843
  H      3.466224     1.299122    -4.068165
  C      4.814181     1.533889    -2.369077
  H      5.704058     1.731120    -2.989084
  C      4.944331     1.529128    -0.971308
  H      5.928810     1.722460    -0.523598
  C      3.819630     1.286235    -0.150851
  O      3.874069     1.267559     1.208447
  C      5.077566     1.621848     1.929778
  H      5.949520     1.147693     1.422485
  C      5.255688     3.143158     1.965199
  H      4.399284     3.616340     2.488541
  H      5.318856     3.574557     0.946034
  H      6.185716     3.411219     2.507870
  C      4.924049     1.009096     3.320439
  H      4.036043     1.430142     3.834884
  H      5.821539     1.222073     3.935868
  H      4.795022    -0.089223     3.253457
  C      0.120326     2.613475    -0.037984
  C     -1.230283     2.365937     0.347033
  H      0.348216     2.907784    -1.075658
  H     -1.427811     2.374994     1.434598
  H      0.825456     2.972124     0.730335
  C     -2.417240     2.711004    -0.531561
  H     -2.138554     2.601152    -1.599739
  H     -3.232173     1.979168    -0.339712
  C     -3.013282     4.144088    -0.297703
  C     -4.218726     4.294648    -1.253117
  C     -3.500375     4.313663     1.158121
  C     -1.969575     5.231529    -0.627525
  H     -4.689068     5.295685    -1.145982
  H     -3.909753     4.176127    -2.313438
  H     -4.996609     3.530650    -1.041229
  H     -4.003392     5.295427     1.291639
  H     -4.228170     3.520908     1.433899
  H     -2.663166     4.269940     1.885327
  H     -2.410355     6.245807    -0.519661
  H     -1.090975     5.176530     0.048815
  H     -1.600106     5.133284    -1.670684
104
i-cm-me-ph-a E(gas)=-2982.80179087 G(gas)=-2982.049835 E(benzene)=-
2982.80957599 A.U.
  Ru    -0.376841     1.066931     0.038112
  Cl     0.668741     0.566150    -2.100507
  Cl    -1.056940     1.798982     2.272258
  C      0.996335    -0.164691     0.888888
  N      2.317748     0.161091     1.015632
  N      0.829936    -1.434240     1.354257
  C      3.052895    -0.824131     1.861928
  H      4.040526    -1.030438     1.403652
  C      2.142746    -2.068582     1.712065
  H      2.484831    -2.649458     0.826109
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C	-2.142352	0.365351	-0.135234
H	-2.776034	0.641210	0.731224
C	-2.826133	-0.567109	-1.041959
C	-2.212159	-1.163530	-2.171732
H	-1.168095	-0.885120	-2.384703
C	-2.897881	-2.054705	-3.004597
H	-2.390069	-2.501570	-3.872789
C	-4.235584	-2.374222	-2.715346
H	-4.790317	-3.079831	-3.355136
C	-4.887922	-1.799546	-1.613130
H	-5.933974	-2.063440	-1.417194
C	-4.209157	-0.888848	-0.771852
O	-4.763733	-0.260991	0.298860
C	-6.154552	-0.341398	0.707344
H	-6.148199	0.346596	1.579521
C	-7.114272	0.253950	-0.329934
H	-6.763297	1.255477	-0.650439
H	-8.118240	0.375065	0.126925
H	-7.228973	-0.376757	-1.232928
C	-6.550564	-1.726030	1.235562
H	-6.682170	-2.482637	0.437658
H	-7.511745	-1.646406	1.784468
H	-5.782798	-2.099377	1.942070
C	2.881946	1.441082	0.716826
C	4.119264	1.541480	0.014703
C	4.671505	2.830731	-0.165250
H	5.618484	2.918625	-0.721010
C	4.028421	3.986913	0.303829
H	4.485126	4.975307	0.137895
C	2.804194	3.871055	0.979448
H	2.294644	4.765943	1.369918
C	2.239746	2.602720	1.195489
H	1.306264	2.494615	1.775394
C	4.850464	0.365366	-0.544215
C	4.211363	-0.554567	-1.410638
H	3.149264	-0.404938	-1.668561
C	4.934350	-1.627719	-1.957891
H	4.426565	-2.332114	-2.635138
C	6.296587	-1.804698	-1.654535
H	6.855878	-2.649884	-2.086674
C	6.940908	-0.893492	-0.799881
H	8.007648	-1.021717	-0.555214
C	6.224155	0.183481	-0.252069
H	6.729440	0.890188	0.426221
C	-0.405831	-2.145363	1.500767
C	-0.630095	-3.379839	0.824021
C	-1.812312	-4.094016	1.139508
H	-2.008023	-5.040567	0.611721
C	-2.748390	-3.607626	2.062631
H	-3.658283	-4.190598	2.276697
C	-2.524600	-2.373565	2.695947
H	-3.252121	-1.971056	3.418113
C	-1.353706	-1.652901	2.421481
H	-1.159303	-0.683909	2.908313
C	0.295570	-3.949571	-0.198992
C	0.630517	-5.325937	-0.165660

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  H      0.256877    -5.952527     0.660400
  C      1.440229    -5.898635    -1.160362
  H      1.692495    -6.970068    -1.109531
  C      1.925272    -5.107462    -2.216325
  H      2.552062    -5.556287    -3.003467
  C      1.602892    -3.739061    -2.258941
  H      1.962795    -3.107891    -3.087172
  C      0.803712    -3.160267    -1.259350
  H      0.561742    -2.087624    -1.319927
  C      3.245787    -0.281490     3.283658
  H      3.822054     0.665182     3.251184
  H      3.817105    -0.999483     3.905839
  H      2.275189    -0.073368     3.778952
  C      2.068584    -3.000010     2.918134
  H      1.660679    -2.491709     3.813866
  H      3.082600    -3.380530     3.157890
  H      1.428209    -3.876513     2.699269
  C     -2.006133     2.227628    -1.126852
  C     -0.862891     3.030655    -0.800824
  H     -2.963587     2.493721    -0.646931
  H     -2.073010     1.791599    -2.136011
  H     -0.090556     3.071928    -1.592357
  C     -0.955269     4.247058     0.095686
  C     -1.303275     5.590556    -0.636597
  H     -1.699536     4.064798     0.897931
  H      0.017913     4.394545     0.608628
  C     -1.319095     6.701513     0.437558
  C     -0.238071     5.934499    -1.701368
  C     -2.693200     5.517059    -1.303382
  H     -1.567095     7.686976    -0.011981
  H     -2.070537     6.489323     1.227587
  H     -0.329958     6.796868     0.934447
  H     -0.436707     6.932173    -2.148287
  H      0.780655     5.960275    -1.259034
  H     -0.225376     5.197931    -2.531517
  H     -2.960298     6.492821    -1.762828
  H     -2.724217     4.752618    -2.107498
  H     -3.484061     5.267294    -0.563705
104
i-cm-me-ph-b E(gas)=-2982.80239411 G(gas)=-2982.04948 E(benzene)=-
2982.81011803 A.U.
  Ru     0.252355     1.108628    -0.325219
  Cl    -0.668542     0.667679     1.877443
  Cl     0.818690     1.673417    -2.644322
  C     -0.861021    -0.455919    -0.976023
  N     -2.214387    -0.375980    -1.149827
  N     -0.475139    -1.731519    -1.257909
  C     -2.759873    -1.580509    -1.841302
  H     -3.705577    -1.882995    -1.348564
  C     -1.654592    -2.621053    -1.525011
  H     -1.912306    -3.128821    -0.568500
  C      2.107480     0.728308    -0.093350
  H      2.678974     0.920440    -1.023203
  C      2.961876     0.146146     0.949416
  C      2.482614    -0.353776     2.186612
  H      1.401579    -0.272161     2.378380
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C	3.337320	-0.916506	3.140940
H	2.930672	-1.298015	4.089931
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H	5.402272	-1.439571	3.607448
C	5.236691	-0.500956	1.664582
H	6.316135	-0.568112	1.484510
C	4.384961	0.079265	0.697679
O	4.802112	0.609281	-0.482428
C	6.181357	0.752395	-0.913603
H	6.033310	1.250685	-1.895262
C	6.981562	1.718520	-0.031923
H	6.418735	2.661924	0.116824
H	7.937538	1.968403	-0.536935
H	7.226457	1.301266	0.964465
C	6.872518	-0.588362	-1.193790
H	7.177122	-1.129976	-0.276917
H	7.787470	-0.407813	-1.795274
H	6.203128	-1.249265	-1.779660
C	-2.980886	0.828793	-1.048056
C	-4.221209	0.842442	-0.344313
C	-4.969651	2.042326	-0.354040
H	-5.921297	2.066874	0.200193
C	-4.513882	3.198216	-1.008379
H	-5.120074	4.117515	-0.984153
C	-3.286525	3.170203	-1.687996
H	-2.917784	4.060968	-2.220468
C	-2.531368	1.985632	-1.719921
H	-1.592959	1.937889	-2.299169
C	-4.762462	-0.335532	0.397034
C	-3.993000	-1.006503	1.378416
H	-2.968943	-0.657639	1.595228
C	-4.543139	-2.086545	2.088881
H	-3.935762	-2.595043	2.853926
C	-5.858737	-2.516546	1.837214
H	-6.281624	-3.365528	2.397840
C	-6.631874	-1.853123	0.868691
H	-7.663610	-2.180768	0.662769
C	-6.088688	-0.770420	0.157108
H	-6.693638	-0.259264	-0.609435
C	0.867059	-2.229279	-1.308677
C	1.283822	-3.311824	-0.480848
C	2.580675	-3.839767	-0.695067
H	2.921160	-4.665684	-0.051036
C	3.445116	-3.311500	-1.664061
H	4.448908	-3.745590	-1.796507
C	3.028169	-2.222937	-2.448822
H	3.695401	-1.789242	-3.210073
C	1.741326	-1.693064	-2.277176
H	1.394081	-0.842235	-2.885274
C	0.444003	-3.901474	0.603366
C	0.329128	-5.307990	0.728107
H	0.809948	-5.957358	-0.021493
C	-0.397001	-5.883798	1.783800
H	-0.478382	-6.980263	1.856898
C	-1.015095	-5.063386	2.743529
H	-1.576971	-5.512527	3.578102

C	-0.908415	-3.665497	2.630171
H	-1.374031	-3.009099	3.382640
C	-0.194009	-3.085455	1.568884
H	-0.122100	-1.987834	1.505814
C	-3.020745	-1.285127	-3.323707
H	-3.752583	-0.457933	-3.420603
H	-3.448786	-2.171204	-3.834231
H	-2.092499	-0.982920	-3.850611
C	-1.398012	-3.678324	-2.594718
H	-1.063040	-3.231615	-3.551433
H	-2.326986	-4.255706	-2.779229
H	-0.622856	-4.394759	-2.259988
C	1.684618	2.770094	0.457110
C	0.414791	3.269640	0.028901
H	2.564580	2.985548	-0.171457
H	1.874366	2.663280	1.537718
H	0.393725	3.684468	-0.995766
C	-0.596617	3.853710	0.997408
C	-0.460033	5.397466	1.242894
H	-1.621855	3.665837	0.610843
H	-0.531390	3.325140	1.969933
C	-1.586312	5.800143	2.221472
C	0.905185	5.735552	1.878199
C	-0.627917	6.189873	-0.072356
H	-1.549302	6.887867	2.445586
H	-2.587345	5.574475	1.796490
H	-1.499352	5.251448	3.183120
H	0.974786	6.820721	2.106809
H	1.056564	5.181538	2.829305
H	1.748645	5.484366	1.201386
H	-0.612767	7.283647	0.122447
H	0.184403	5.971972	-0.796628
H	-1.594032	5.950033	-0.565648

104

i-cm-me-ph-c E(gas)=-2982.8024814 G(gas)=-2982.049295 E(benzene)=-2982.80981827 A.U.

Ru	-0.109335	1.213106	-0.424653
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Cl	0.111262	1.975168	-2.738383
C	-0.721634	-0.627194	-1.019500
N	-2.045724	-0.968286	-1.078696
N	0.009337	-1.739953	-1.301377
C	-2.246823	-2.315115	-1.686970
H	-3.023236	-2.859822	-1.113202
C	-0.861656	-2.957438	-1.422999
H	-0.886433	-3.447658	-0.423700
C	1.690619	1.266690	0.196896
H	1.748678	0.989811	1.269767
C	3.020694	1.484315	-0.375209
C	3.257739	2.038299	-1.660492
H	2.377135	2.260973	-2.284814
C	4.549488	2.300700	-2.127771
H	4.697304	2.744747	-3.124298
C	5.653505	1.984703	-1.315513
H	6.679144	2.176512	-1.671043
C	5.469582	1.415763	-0.046279

H	6.348339	1.167471	0.560785
C	4.168151	1.162289	0.445519
O	3.893973	0.606420	1.652139
C	4.850173	0.369073	2.720699
H	4.169700	0.012742	3.522757
C	5.815777	-0.782100	2.411896
H	5.258030	-1.648738	2.004583
H	6.310503	-1.105367	3.351212
H	6.612011	-0.510141	1.691444
C	5.512894	1.655855	3.224838
H	6.240811	2.083640	2.507846
H	6.055491	1.441760	4.168815
H	4.746221	2.426847	3.441564
C	-3.131694	-0.051276	-0.923168
C	-4.264306	-0.388782	-0.123691
C	-5.336604	0.532632	-0.082043
H	-6.208150	0.288266	0.545734
C	-5.298969	1.752535	-0.776584
H	-6.150186	2.448311	-0.710339
C	-4.173025	2.073569	-1.550212
H	-4.128537	3.018014	-2.114925
C	-3.102799	1.167673	-1.634249
H	-2.239994	1.387378	-2.285941
C	-4.374356	-1.653649	0.663416
C	-3.364796	-2.045367	1.576141
H	-2.474552	-1.406494	1.707127
C	-3.513189	-3.221520	2.330177
H	-2.721934	-3.510302	3.040085
C	-4.660567	-4.023769	2.191905
H	-4.768463	-4.945394	2.786013
C	-5.671248	-3.639164	1.293703
H	-6.574819	-4.258923	1.176698
C	-5.529685	-2.463160	0.538026
H	-6.318395	-2.170711	-0.174261
C	1.423769	-1.798719	-1.514103
C	2.255365	-2.646120	-0.725863
C	3.616873	-2.759201	-1.101194
H	4.274272	-3.402155	-0.494665
C	4.148014	-2.051297	-2.188679
H	5.214380	-2.155852	-2.443490
C	3.317998	-1.199788	-2.936848
H	3.721956	-0.627717	-3.785977
C	1.961143	-1.084350	-2.604899
H	1.293983	-0.424963	-3.181649
C	1.772908	-3.405997	0.465409
C	2.122277	-4.770097	0.625506
H	2.700017	-5.276091	-0.165186
C	1.730357	-5.488323	1.767340
H	2.007122	-6.550374	1.866294
C	0.986354	-4.854081	2.777820
H	0.682492	-5.413829	3.676981
C	0.634598	-3.500213	2.630615
H	0.062428	-2.983201	3.417624
C	1.017053	-2.779996	1.486562
H	0.730388	-1.718311	1.406144
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  C     -0.377833    -3.965048    -2.460766
  H     -0.256113    -3.508336    -3.462630
  H     -1.106449    -4.797951    -2.537970
  H      0.594683    -4.401742    -2.162167
  C      0.712134     3.264850     0.351380
  C     -0.683492     3.288290     0.080806
  H      1.410981     3.669278    -0.396191
  H      1.044050     3.295548     1.403027
  H     -0.948333     3.642027    -0.933903
  C     -1.742616     3.478966     1.145494
  C     -2.139159     4.972094     1.422166
  H     -2.662462     2.934272     0.840702
  H     -1.407545     3.010090     2.092655
  C     -3.247349     4.953872     2.498657
  C     -0.931052     5.772129     1.954006
  C     -2.685498     5.651508     0.147175
  H     -3.574886     5.985116     2.751915
  H     -4.138150     4.390805     2.147824
  H     -2.892581     4.470178     3.433432
  H     -1.229193     6.811797     2.209038
  H     -0.511570     5.308489     2.872610
  H     -0.115566     5.836160     1.203319
  H     -3.037944     6.681229     0.370751
  H     -1.912970     5.732128    -0.645800
  H     -3.544460     5.085436    -0.271883
104
i-cm-me-ph-d E(gas)=-2982.8007061 G(gas)=-2982.047233 E(benzene)=-
2982.80818773 A.U.
  Ru    -0.051523     1.193910     0.116160
  Cl     0.671132     0.328547    -2.046517
  Cl    -0.366224     2.160393     2.334942
  C      0.944264    -0.371483     0.930573
  N      2.310022    -0.452384     0.950531
  N      0.449395    -1.541807     1.420081
  C      2.784815    -1.627326     1.736934
  H      3.630610    -2.103905     1.202677
  C      1.539983    -2.545361     1.658615
  H      1.622440    -3.171519     0.741809
  C     -1.830417     0.748451    -0.409453
  H     -1.842672     0.214168    -1.381621
  C     -3.172936     0.826677     0.176309
  C     -3.479591     1.526308     1.371694
  H     -2.640888     1.999862     1.907320
  C     -4.785254     1.615481     1.865088
  H     -4.989019     2.173913     2.791770
  C     -5.828878     0.978687     1.169983
  H     -6.863125     1.030748     1.547791
  C     -5.572348     0.267204    -0.011876
  H     -6.404589    -0.223555    -0.530409
  C     -4.259241     0.184951    -0.530888
  O     -3.918918    -0.469190    -1.670649
  C     -4.841771    -1.064906    -2.621802
  H     -4.130933    -1.407486    -3.403265
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C	-5.540966	-2.316465	-2.076163
H	-4.804256	-2.981759	-1.583451
H	-5.996034	-2.876481	-2.919253
H	-6.346982	-2.091330	-1.350499
C	-5.770396	-0.034068	-3.273627
H	-6.548697	0.351290	-2.586146
H	-6.285205	-0.500697	-4.138772
H	-5.184945	0.828380	-3.651082
C	3.198766	0.602458	0.578337
C	4.354414	0.336917	-0.215216
C	5.235097	1.412286	-0.474709
H	6.120397	1.219750	-1.101273
C	4.987781	2.709653	0.000770
H	5.692556	3.523525	-0.231220
C	3.838785	2.957083	0.766852
H	3.636743	3.964192	1.164090
C	2.956911	1.904866	1.065259
H	2.085004	2.076398	1.720205
C	4.671363	-1.002693	-0.795288
C	3.725699	-1.703032	-1.582985
H	2.734497	-1.252530	-1.762294
C	4.061657	-2.941729	-2.154312
H	3.317305	-3.472157	-2.768967
C	5.336844	-3.501710	-1.954896
H	5.592552	-4.474328	-2.405048
C	6.284674	-2.810301	-1.180432
H	7.286687	-3.238953	-1.017568
C	5.955080	-1.570333	-0.607559
H	6.696585	-1.035984	0.008520
C	-0.921711	-1.844923	1.702774
C	-1.581792	-2.932901	1.061040
C	-2.883992	-3.265476	1.508920
H	-3.408599	-4.099325	1.015982
C	-3.526100	-2.542263	2.524030
H	-4.544401	-2.821548	2.837138
C	-2.869921	-1.454798	3.124665
H	-3.364540	-0.868564	3.914183
C	-1.570099	-1.117851	2.722241
H	-1.039086	-0.269529	3.181397
C	-0.980823	-3.727921	-0.050996
C	-1.035962	-5.143648	-0.020608
H	-1.470235	-5.648343	0.857805
C	-0.532408	-5.910387	-1.084466
H	-0.578904	-7.010267	-1.035092
C	0.029304	-5.275930	-2.206393
H	0.418702	-5.875246	-3.045014
C	0.088911	-3.871303	-2.248589
H	0.514726	-3.355732	-3.124264
C	-0.405063	-3.100750	-1.182721
H	-0.348060	-2.002151	-1.250919
C	3.235359	-1.199123	3.139666
H	4.059494	-0.461305	3.063080
H	3.616375	-2.067710	3.714052
H	2.408839	-0.729777	3.711773
C	1.293988	-3.452434	2.860246
H	1.127874	-2.876532	3.791881

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  H      2.167327    -4.120319     3.007662
  H      0.408540    -4.095566     2.692340
  C     -1.313884     2.730926    -1.116995
  C      0.024264     3.165505    -0.871388
  H     -2.131303     3.221870    -0.564918
  H     -1.561863     2.345724    -2.119873
  H      0.750515     2.952185    -1.677379
  C      0.318178     4.383928    -0.018806
  C      0.344990     5.744092    -0.801734
  H     -0.421878     4.454370     0.804559
  H      1.309367     4.261920     0.465079
  C      0.701200     6.847487     0.220270
  C      1.415771     5.724549    -1.914889
  C     -1.035142     6.056599    -1.416988
  H      0.729203     7.846004    -0.266327
  H     -0.042668     6.891692     1.043928
  H      1.697456     6.667361     0.677702
  H      1.497246     6.721306    -2.399136
  H      2.416331     5.464907    -1.507889
  H      1.176454     4.989776    -2.711514
  H     -1.028185     7.050909    -1.912761
  H     -1.324726     5.307088    -2.182901
  H     -1.829436     6.074155    -0.640169
104
i-cm-ph-me-a E(gas)=-2982.79301855 G(gas)=-2982.042101 E(benzene)=-
2982.80137637 A.U.
  Ru     0.870911     0.828388     0.298008
  Cl     0.928883     1.061181     2.710075
  Cl     0.481665     0.897048    -2.119639
  C     -1.024939     0.171769     0.479929
  N     -2.067510     1.012062     0.725047
  N     -1.502124    -1.103946     0.423816
  C     -3.381070     0.325826     0.604180
  H     -4.046616     0.636796     1.434830
  C     -2.931532    -1.155986     0.858049
  H     -2.946396    -1.300775     1.961920
  C      2.192172    -0.491526    -0.069737
  H      2.380953    -0.607394    -1.156164
  C      2.909172    -1.496893     0.727863
  C      2.670497    -1.724868     2.105943
  H      1.928012    -1.081130     2.602658
  C      3.359429    -2.710199     2.823541
  H      3.154626    -2.858698     3.894969
  C      4.310223    -3.504735     2.161043
  H      4.858467    -4.289670     2.707354
  C      4.581957    -3.310357     0.797350
  H      5.333581    -3.941942     0.309242
  C      3.903936    -2.308675     0.066884
  O      4.123316    -2.020905    -1.243869
  C      5.136858    -2.624420    -2.090060
  H      4.968300    -2.065709    -3.035317
  C      6.563533    -2.307851    -1.625436
  H      6.674648    -1.221820    -1.432721
  H      7.280309    -2.587179    -2.425178
  H      6.855001    -2.852637    -0.706223
  C      4.870781    -4.104070    -2.395872
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H	5.107669	-4.781411	-1.551930
H	5.494921	-4.415352	-3.259088
H	3.808115	-4.253250	-2.672911
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C	-2.257881	3.051766	2.102272
C	-2.200802	4.459207	2.167622
H	-2.416734	4.951632	3.129968
C	-1.859885	5.238816	1.049036
H	-1.828036	6.336588	1.136407
C	-1.553134	4.616294	-0.170755
H	-1.281782	5.216055	-1.053570
C	-1.608299	3.215509	-0.270592
H	-1.363043	2.705152	-1.213874
C	-2.552580	2.230585	3.333325
C	-0.718503	-2.280720	0.170938
C	-0.472124	-3.222201	1.204315
C	0.258538	-4.382650	0.868067
H	0.466247	-5.121891	1.658744
C	0.745032	-4.600121	-0.429806
H	1.314124	-5.516092	-0.654338
C	0.519275	-3.640066	-1.430494
H	0.906957	-3.789211	-2.450361
C	-0.213999	-2.483694	-1.129511
H	-0.382065	-1.703451	-1.888079
C	-0.929422	-2.989344	2.625104
C	-4.092129	0.624659	-0.710325
C	-3.779398	-2.247572	0.240262
C	3.120263	1.394483	0.250720
C	2.242398	2.528295	0.212197
H	3.727183	1.190652	-0.647897
H	3.566557	1.105882	1.215581
H	2.028219	2.974382	1.202092
C	2.177269	3.475450	-0.965612
C	3.199533	4.665367	-0.923117
H	2.315851	2.908055	-1.908747
H	1.158576	3.915117	-1.015829
C	2.942370	5.528651	-2.178674
C	2.989643	5.532070	0.338384
C	4.654001	4.149716	-0.957286
H	3.642144	6.390864	-2.221891
H	3.075100	4.936307	-3.108923
H	1.907707	5.933005	-2.184144
H	3.648680	6.426535	0.316254
H	1.940046	5.888165	0.413434
H	3.222822	4.974358	1.269210
H	5.370972	4.997933	-0.993173
H	4.899374	3.547233	-0.057840
H	4.837799	3.517509	-1.852555
C	-5.493583	0.782780	-0.708267
C	-6.192725	1.032375	-1.901108
C	-5.493076	1.133300	-3.115725
C	-4.094730	0.984284	-3.126693
C	-3.395097	0.731988	-1.934192
H	-6.047082	0.711236	0.243102
H	-7.287317	1.155404	-1.879388
H	-6.036357	1.335578	-4.052646

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  H     -3.536000     1.070839    -4.072245
  H     -2.295973     0.632022    -1.966636
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  C     -5.543035    -3.925433     0.528562
  C     -5.470069    -4.247107    -0.837276
  C     -4.552254    -3.572764    -1.662158
  C     -3.715108    -2.578914    -1.130486
  H     -4.752673    -2.693408     2.135750
  H     -6.254607    -4.450535     1.185425
  H     -6.124833    -5.026365    -1.258826
  H     -4.486446    -3.821777    -2.733114
  H     -3.003485    -2.057430    -1.785963
  H     -2.670856     2.880385     4.222404
  H     -3.483754     1.631471     3.234880
  H     -1.714583     1.525259     3.523229
  H     -0.377534    -3.645391     3.326611
  H     -0.759659    -1.936728     2.934423
  H     -2.011651    -3.211644     2.754360
104
i-cm-ph-me-b E(gas)=-2982.79334347 G(gas)=-2982.042914 E(benzene)=-
2982.80168912 A.U.
  Ru    -0.939383     0.740536    -0.005862
  Cl    -1.169137     1.104936    -2.390664
  Cl    -0.406391     0.611896     2.384400
  C      0.978478     0.240373    -0.358251
  N      1.953072     1.181360    -0.494654
  N      1.539352    -0.989402    -0.534919
  C      3.311095     0.581424    -0.549258
  H      3.907854     1.074566    -1.343130
  C      2.945273    -0.866420    -1.030661
  H      2.910206    -0.826711    -2.142545
  C     -2.137888    -0.703359     0.295492
  H     -2.234286    -0.953408     1.371954
  C     -2.909046    -1.626646    -0.546731
  C     -2.706924    -1.791394    -1.939563
  H     -1.960438    -1.143192    -2.422182
  C     -3.434439    -2.727242    -2.685211
  H     -3.253574    -2.833171    -3.765920
  C     -4.394269    -3.525801    -2.041249
  H     -4.975718    -4.267487    -2.612987
  C     -4.637719    -3.386415    -0.665149
  H     -5.407928    -4.008796    -0.194231
  C     -3.914986    -2.440760     0.094893
  O     -4.115150    -2.186270     1.416709
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  C     -4.535208    -4.413508     2.454327
  H     -4.766489    -5.029668     1.563481
  H     -5.059460    -4.865654     3.321560
  H     -3.445110    -4.475831     2.644702
  C      1.756674     2.605086    -0.411827
  C      1.903323     3.393577    -1.586989
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C	1.332357	4.595347	0.931633
H	1.106549	5.052964	1.907426
C	1.462456	3.199979	0.831837
H	1.319726	2.556375	1.712075
C	2.128799	2.761359	-2.938178
C	0.858167	-2.246401	-0.411149
C	0.655873	-3.076278	-1.544661
C	0.042207	-4.330596	-1.333211
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C	-0.378438	-4.743412	-0.060003
H	-0.855886	-5.727921	0.066639
C	-0.204490	-3.890318	1.043052
H	-0.542702	-4.194248	2.046170
C	0.416080	-2.645250	0.867155
H	0.547887	-1.950289	1.711464
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C	4.078238	0.700533	0.762376
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C	-3.198422	1.207832	0.319678
C	-2.338739	2.316279	0.585085
H	-3.711023	0.723477	1.167104
H	-3.705063	1.140241	-0.657120
H	-2.108229	2.501448	1.650442
C	-2.262386	3.528431	-0.324326
C	-3.248036	4.692746	0.044405
H	-1.231045	3.943546	-0.291381
H	-2.443162	3.215614	-1.372916
C	-3.002212	5.832162	-0.970078
C	-4.714322	4.225439	-0.067120
C	-2.979036	5.221199	1.470708
H	-3.675331	6.693799	-0.771833
H	-1.955135	6.198201	-0.915849
H	-3.184860	5.490128	-2.010865
H	-5.411385	5.065923	0.138964
H	-4.939821	3.842806	-1.085459
H	-4.944717	3.416653	0.657586
H	-3.621602	6.100439	1.691581
H	-3.190028	4.455594	2.246114
H	-1.920985	5.538196	1.588651
C	5.474675	0.895378	0.718368
C	6.228951	0.973931	1.900764
C	5.590539	0.865399	3.148182
C	4.197907	0.678124	3.202054
C	3.442723	0.594859	2.019220
H	5.979802	0.986580	-0.257880
H	7.318426	1.128555	1.846725
H	6.177109	0.934172	4.078295
H	3.687010	0.600521	4.175069
H	2.348836	0.460633	2.087389
C	4.821604	-2.444562	-1.596863
C	5.757230	-3.441200	-1.271776
C	5.769340	-3.995797	0.019235

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  H      6.473571    -3.789787    -2.032633
  H      6.495846    -4.782754     0.277201
  H      4.847232    -3.975890     1.992039
  H      3.202853    -2.194969     1.415060
  H      2.127249     3.527561    -3.737983
  H      3.098407     2.220873    -2.999512
  H      1.318928     2.029405    -3.150560
  H      0.535632    -3.264753    -3.699103
  H      0.742373    -1.578930    -3.118140
  H      2.131193    -2.717950    -3.114397
104
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E(benzene)=-2982.80718462 A.U.
  Ru    -0.991584     0.719589     0.207391
  Cl    -0.291381     0.844123     2.544104
  Cl    -1.398658     0.868801    -2.193837
  N      1.501528    -0.927340    -0.470522
  N      1.811994     1.257041    -0.586817
  C      0.905850     0.283470    -0.286422
  C      2.810274    -0.766974    -1.176310
  H      2.600722    -0.751698    -2.270403
  C      3.177354     0.705196    -0.780132
  H      3.663584     1.193727    -1.648593
  C      3.850564    -1.835784    -0.921639
  C      4.074489     0.889892     0.438857
  C      0.884766    -2.206172    -0.251046
  C      0.427429    -2.988730    -1.344827
  C     -0.099471    -4.265785    -1.051762
  H     -0.457165    -4.890418    -1.887002
  C     -0.187932    -4.747927     0.264033
  H     -0.603722    -5.749982     0.454665
  C      0.240659    -3.945386     1.333902
  H      0.154908    -4.301922     2.371585
  C      0.777557    -2.676669     1.072056
  H      1.106547    -2.021049     1.892263
  C      0.459937    -2.472714    -2.763506
  H      0.035740    -1.445929    -2.824763
  H     -0.130923    -3.129131    -3.432467
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  C      1.556728     2.673210    -0.575251
  C      1.536589     3.384315    -1.808222
  C      1.348608     4.781274    -1.749724
  H      1.326139     5.349669    -2.693975
  C      1.175804     5.455451    -0.528421
  H      1.034576     6.548071    -0.521824
  C      1.175600     4.733759     0.675549
  H      1.033991     5.247655     1.639059
  C      1.370894     3.342512     0.651485
  H      1.365281     2.757804     1.582402
  C      1.653774     2.674168    -3.134097
  H      2.637234     2.172222    -3.262800
  H      1.534022     3.385754    -3.974317
  H      0.862035     1.896810    -3.213795
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C	-2.193896	-0.754825	0.187109
H	-2.602223	-0.926021	-0.830101
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C	-2.323204	-1.788092	2.516541
H	-1.663034	-0.987437	2.887764
C	-2.813540	-2.770660	3.383831
H	-2.548354	-2.745884	4.452097
C	-3.643249	-3.787479	2.878153
H	-4.035150	-4.570786	3.547504
C	-3.988032	-3.818437	1.518160
H	-4.641331	-4.621400	1.149797
C	-3.504876	-2.824920	0.636312
O	-3.796591	-2.795305	-0.690559
C	-4.725643	-3.728957	-1.291237
H	-4.532676	-4.743113	-0.871380
C	-6.169929	-3.307673	-1.002992
H	-6.370947	-2.307503	-1.439433
H	-6.373786	-3.256964	0.085404
H	-6.880622	-4.032199	-1.451549
C	-4.395163	-3.743650	-2.782411
H	-4.531976	-2.734332	-3.221696
H	-5.059403	-4.453022	-3.316527
H	-3.344066	-4.052133	-2.947719
C	-3.249835	1.145807	0.678205
C	-2.428854	2.309487	0.685340
H	-3.551071	0.700407	1.638527
H	-2.067371	2.617971	1.684534
H	-3.932252	0.983984	-0.173327
C	-2.519768	3.409055	-0.351624
H	-1.510501	3.853581	-0.496223
H	-2.810144	2.973581	-1.329264
C	-3.502179	4.577574	0.010464
C	-3.422839	5.609878	-1.136605
C	-4.951861	4.059836	0.123760
C	-3.091876	5.261308	1.333536
H	-4.107308	6.465285	-0.950508
H	-2.393653	6.013878	-1.242017
H	-3.705388	5.153668	-2.109088
H	-5.653460	4.897723	0.325104
H	-5.278861	3.566505	-0.816600
H	-5.065073	3.326248	0.949485
H	-3.734262	6.145321	1.534952
H	-3.189001	4.578455	2.203193
H	-2.038179	5.610699	1.294230
C	5.456309	1.098106	0.247038
C	6.322583	1.236915	1.344262
C	5.813570	1.173757	2.653012
C	4.436327	0.973911	2.854122
C	3.569303	0.833334	1.756645
H	5.860919	1.151524	-0.777564
H	7.398685	1.401861	1.175312
H	6.488909	1.288687	3.515893
H	4.026024	0.932598	3.875748
H	2.489981	0.690959	1.937171
C	4.583845	-2.339179	-2.018111
C	5.594605	-3.297599	-1.833089

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  C      5.879150    -3.774807    -0.542565
  C      5.149592    -3.286372     0.556057
  C      4.145636    -2.322707     0.370419
  H      4.356782    -1.973589    -3.033877
  H      6.155817    -3.677195    -2.701711
  H      6.666352    -4.530833    -0.392594
  H      5.364450    -3.658283     1.570348
  H      3.584916    -1.944930     1.236723
104
i-cm-ph-me-d E(gas)=-2982.79080103 G(gas)=-2982.041302 E(benzene)=-
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  Ru    -0.894648     0.892712    -0.121126
  Cl    -1.121712     0.878703    -2.551884
  Cl    -0.295669     1.144715     2.230347
  C      0.945920     0.132056    -0.427228
  N      2.016341     0.912524    -0.750153
  N      1.352528    -1.168773    -0.424500
  C      3.285551     0.140535    -0.771418
  H      3.891422     0.438770    -1.650933
  C      2.718678    -1.297496    -1.021375
  H      2.594104    -1.397406    -2.123868
  C     -2.292066    -0.398597    -0.096795
  H     -2.661197    -0.617209    -1.119627
  C     -2.957597    -1.230310     0.910365
  C     -2.710408    -1.141475     2.304702
  H     -1.946381    -0.419871     2.636330
  C     -3.404003    -1.924793     3.232710
  H     -3.193017    -1.823945     4.308560
  C     -4.367035    -2.842610     2.776211
  H     -4.918359    -3.474133     3.492026
  C     -4.638612    -2.972336     1.405696
  H     -5.387903    -3.702359     1.077000
  C     -3.954708    -2.175583     0.458590
  O     -4.153661    -2.235833    -0.883679
  C     -5.258693    -2.901195    -1.551479
  H     -5.083718    -2.578602    -2.599833
  C     -5.141888    -4.430985    -1.530980
  H     -4.102203    -4.737724    -1.761422
  H     -5.806181    -4.859014    -2.310140
  H     -5.431053    -4.884370    -0.562250
  C     -6.626164    -2.353654    -1.128149
  H     -6.909656    -2.641192    -0.096584
  H     -7.405900    -2.743964    -1.814412
  H     -6.637688    -1.247090    -1.194499
  C      2.021514     2.344466    -0.899857
  C      2.186970     2.902470    -2.199141
  C      2.278717     4.306675    -2.297223
  H      2.403727     4.757991    -3.295181
  C      2.206816     5.134635    -1.164109
  H      2.288189     6.227391    -1.278619
  C      2.026040     4.567170     0.106791
  H      1.962388     5.204383     1.002570
  C      1.934832     3.171239     0.238386
  H      1.780053     2.709480     1.223881
  C      2.215964     2.037981    -3.435038
  C      0.526238    -2.313063    -0.154837
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C	-0.945587	-4.620691	0.466348
H	-1.517034	-5.533176	0.699145
C	-0.483813	-3.792233	1.501815
H	-0.697143	-4.037417	2.553324
C	0.253012	-2.641305	1.187204
H	0.617981	-1.969156	1.978326
C	0.247630	-2.743315	-2.665781
C	4.133348	0.342935	0.479678
C	3.553203	-2.468070	-0.547462
C	-3.085780	1.650535	0.191106
C	-2.191580	2.671989	-0.234025
H	-3.349220	1.566907	1.257963
H	-3.837159	1.277932	-0.524686
H	-2.207066	2.905961	-1.314280
C	-1.736914	3.795859	0.675462
C	-2.646039	5.074961	0.648857
H	-1.658362	3.422907	1.717108
H	-0.714466	4.110642	0.374137
C	-1.995996	6.111178	1.593181
C	-2.726567	5.670140	-0.774227
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H	-1.911043	5.716377	2.627886
H	-0.974534	6.381059	1.250583
H	-3.290926	6.627337	-0.767878
H	-1.714250	5.877354	-1.182015
H	-3.241836	4.988063	-1.482036
H	-4.692086	5.667726	1.191367
H	-4.582168	4.020674	0.498522
H	-4.040327	4.322745	2.182483
C	5.538709	0.328315	0.360759
C	6.358912	0.475252	1.491773
C	5.780002	0.646255	2.761083
C	4.379854	0.669558	2.888674
C	3.558706	0.518907	1.757662
H	5.998424	0.199409	-0.633417
H	7.454784	0.463397	1.379201
H	6.419846	0.769098	3.649545
H	3.916435	0.812297	3.877968
H	2.462134	0.552179	1.878843
C	4.270399	-3.217857	-1.504831
C	5.095208	-4.286820	-1.115793
C	5.205164	-4.627940	0.242679
C	4.489191	-3.892958	1.204444
C	3.672180	-2.819973	0.814682
H	4.178718	-2.959139	-2.573283
H	5.646949	-4.859320	-1.878287
H	5.845080	-5.469572	0.552380
H	4.567763	-4.156334	2.271089
H	3.122078	-2.248989	1.575674
H	2.314383	2.657574	-4.347843
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H	1.273204	1.451079	-3.503681

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  H     -0.411596    -3.342759    -3.324252
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118
i-cm-ph-ph-a E(gas)=-3365.99529433 G(gas)=-3365.149926 E(benzene)=-
3366.00357323 A.U.
  Ru    -1.270386     1.021962    -0.151393
  Cl    -0.739961     1.071991    -2.519594
  Cl    -1.492686     1.302041     2.276672
  C      0.601467     0.299190     0.164322
  N      1.729472     1.064411     0.065345
  N      0.979770    -0.981244     0.441274
  C      2.940213     0.343160     0.543979
  H      3.781611     0.523633    -0.152385
  C      2.468031    -1.138737     0.365913
  H      2.718998    -1.437087    -0.675885
  C     -2.698387    -0.236402    -0.015076
  H     -3.137080    -0.248240     1.002690
  C     -3.247234    -1.304317    -0.861537
  C     -2.781890    -1.592721    -2.168877
  H     -1.984187    -0.951294    -2.574711
  C     -3.317413    -2.635902    -2.932570
  H     -2.931020    -2.835158    -3.943635
  C     -4.344633    -3.427484    -2.390659
  H     -4.772101    -4.259690    -2.973409
  C     -4.844536    -3.171053    -1.104301
  H     -5.649676    -3.800838    -0.707867
  C     -4.320919    -2.111670    -0.329528
  O     -4.757797    -1.771672     0.912484
  C     -5.912481    -2.332638     1.591694
  H     -5.916909    -1.719955     2.518306
  C     -7.229784    -2.054251     0.857495
  H     -7.300032    -0.983097     0.580636
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  C     -5.713119    -3.791425     2.023026
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  H     -6.479944    -4.055728     2.780410
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  H      3.408131     4.888413    -1.957342
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  C      0.938419     4.707873     0.405483
  H      0.270831     5.346072     1.005348
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H	-0.742581	-1.158226	2.421192
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C	2.392971	-4.652983	-2.921304
H	2.999158	-5.554746	-3.104874
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C	0.859674	-2.348256	-2.424494
H	0.259408	-1.440334	-2.253154
C	3.365464	0.784251	1.939753
C	3.072942	-2.162554	1.303725
C	-3.433485	1.597460	-0.730040
C	-2.579111	2.733517	-0.526063
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H	-3.606792	1.246720	-1.759795
H	-2.099970	3.118467	-1.446351
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C	-3.797459	4.928420	0.159884
H	-3.238330	3.246399	1.463021
H	-1.873057	4.207409	0.869818
C	-3.892300	5.873669	1.378769
C	-3.237972	5.714220	-1.046986
C	-5.209349	4.403309	-0.178169
H	-4.568970	6.729580	1.168546
H	-4.284504	5.342006	2.271622
H	-2.896962	6.288209	1.646530
H	-3.870717	6.600720	-1.266878
H	-2.206646	6.077380	-0.850297
H	-3.206267	5.095706	-1.968003
H	-5.899277	5.246640	-0.395755
H	-5.202949	3.742893	-1.070384
H	-5.640453	3.828336	0.669526
C	4.741029	0.825082	2.249710
C	5.179792	1.204146	3.529306
C	4.243453	1.557356	4.516343
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C	2.430617	1.142845	2.935807
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  C      3.311710    -3.212272     3.498117
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  H      4.395363    -2.931514    -0.242503
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  H      4.831191    -4.764955     3.670473
  H      2.994920    -3.293358     4.550000
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118
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  N     -1.728607     0.947515    -0.246260
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  C     -2.431663    -1.283210    -0.097863
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  H      3.018455    -0.468417    -1.329328
  C      3.414793    -1.088126     0.679767
  C      3.037938    -1.235333     2.038146
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  C      3.736006    -2.073567     2.914567
  H      3.411342    -2.170564     3.961690
  C      4.848384    -2.789938     2.441161
  H      5.408003    -3.458356     3.115696
  C      5.270019    -2.662006     1.108123
  H      6.151150    -3.220930     0.771670
  C      4.576751    -1.813318     0.216419
  O      4.933568    -1.586697    -1.075985
  C      6.056249    -2.194487    -1.769249
  H      5.942811    -1.736999    -2.775157
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  H      7.663109    -2.189586    -0.237935
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H	-3.106593	0.409351	4.436984
C	-4.969237	1.322488	3.778780
H	-5.567703	0.879565	4.590906
C	-5.577523	2.160865	2.828336
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C	0.741680	-4.428240	0.244771
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C	-1.920842	-3.203527	4.432202
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C	-0.629750	-2.083257	2.687563
H	-0.072059	-1.194251	2.351294
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C	-3.087922	-2.456399	-0.796058
C	3.465887	1.761513	-0.120033
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H	3.831196	1.692615	0.917765
H	2.450972	3.027886	-1.529101
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C	3.094333	5.201010	0.345805
H	1.143530	4.229730	0.350207
H	2.269179	3.556498	1.547352
C	2.593183	6.231761	1.382590
C	4.575571	4.876368	0.633586
C	2.962492	5.805591	-1.069340
H	3.184251	7.171031	1.327386
H	1.526942	6.490048	1.209539
H	2.678385	5.836296	2.416849
H	5.195948	5.796949	0.586158
H	4.702748	4.436394	1.645794
H	4.991692	4.157577	-0.103187
H	3.539315	6.751980	-1.147230
H	3.345542	5.119988	-1.853520

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  H      1.903033     6.037124    -1.309988
  C     -4.900946     0.320993    -2.091123
  C     -5.452432     0.459429    -3.375805
  C     -4.608535     0.611565    -4.489432
  C     -3.214216     0.624624    -4.308001
  C     -2.662191     0.481373    -3.023514
  H     -5.566662     0.210129    -1.219095
  H     -6.546509     0.455700    -3.505651
  H     -5.037343     0.727462    -5.497712
  H     -2.544301     0.751860    -5.173286
  H     -1.565416     0.503894    -2.905807
  C     -4.072047    -3.190495    -0.099828
  C     -4.755963    -4.248178    -0.722901
  C     -4.451783    -4.596067    -2.049936
  C     -3.464291    -3.878509    -2.748202
  C     -2.789979    -2.814043    -2.128772
  H     -4.299406    -2.930648     0.946998
  H     -5.523522    -4.807954    -0.164941
  H     -4.981143    -5.429237    -2.539395
  H     -3.217049    -4.147170    -3.787440
  H     -2.023133    -2.257527    -2.686170
118
i-cm-ph-ph-c E(gas)=-3365.99567538 G(gas)=-3365.147868 E(benzene)=-
3366.00353022 A.U.
  Ru     1.232417     1.131365    -0.429795
  Cl     1.092874     1.284859     2.000200
  Cl     1.100870     1.200218    -2.876908
  C     -0.577435     0.223674    -0.336268
  N     -1.729258     0.933732    -0.132651
  N     -0.896877    -1.100496    -0.361118
  C     -2.942889     0.086697    -0.271980
  H     -3.662528     0.329495     0.533551
  C     -2.328787    -1.322259     0.026146
  H     -2.355197    -1.461802     1.129313
  C      2.713484    -0.030533    -0.135699
  H      2.912225    -0.144883     0.949766
  C      3.586352    -0.890712    -0.937036
  C      3.700399    -0.819510    -2.349657
  H      3.041119    -0.108704    -2.873864
  C      4.603611    -1.615301    -3.061463
  H      4.676647    -1.525698    -4.156287
  C      5.408618    -2.534192    -2.363890
  H      6.120097    -3.176312    -2.908440
  C      5.317166    -2.653306    -0.969065
  H      5.949928    -3.385979    -0.454355
  C      4.422824    -1.839893    -0.235223
  O      4.266963    -1.880529     1.111256
  C      5.070530    -2.652682     2.044167
  H      4.632949    -2.318554     3.008542
  C      4.820075    -4.162048     1.938541
  H      3.731898    -4.365842     1.890009
  H      5.221887    -4.662666     2.843807
  H      5.301163    -4.629562     1.056778
  C      6.546235    -2.237501     2.047673
  H      7.097608    -2.569102     1.146106
  H      7.047998    -2.682554     2.931674
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H	6.637635	-1.135293	2.124192
C	-1.821544	2.362042	-0.080885
C	-2.583976	3.004388	0.938982
C	-2.707510	4.411660	0.880459
H	-3.284234	4.916065	1.671844
C	-2.088024	5.172849	-0.123531
H	-2.201303	6.268346	-0.130960
C	-1.328224	4.526876	-1.110363
H	-0.846104	5.102027	-1.916226
C	-1.209575	3.127430	-1.095491
H	-0.667454	2.610520	-1.904451
C	-3.250137	2.273630	2.058091
C	-2.524550	1.392854	2.896355
H	-1.446317	1.240184	2.716333
C	-3.168788	0.744569	3.963808
H	-2.590984	0.066036	4.610742
C	-4.536378	0.959812	4.213916
H	-5.034678	0.445956	5.051574
C	-5.262641	1.838643	3.391406
H	-6.334058	2.015543	3.578546
C	-4.623952	2.491903	2.323991
H	-5.198158	3.169957	1.671972
C	-0.012719	-2.190230	-0.652609
C	0.179475	-3.254813	0.273032
C	0.932508	-4.372256	-0.163796
H	1.092153	-5.201259	0.543884
C	1.502371	-4.429899	-1.443418
H	2.087461	-5.312927	-1.744917
C	1.336070	-3.350469	-2.326867
H	1.792023	-3.370518	-3.328345
C	0.575220	-2.241620	-1.933099
H	0.426136	-1.388556	-2.613728
C	-0.331560	-3.248806	1.675789
C	-1.003441	-4.384759	2.191134
H	-1.216211	-5.233558	1.521903
C	-1.416286	-4.432010	3.532842
H	-1.942826	-5.323039	3.911360
C	-1.158736	-3.346458	4.389120
H	-1.474174	-3.385490	5.444216
C	-0.495267	-2.212407	3.887117
H	-0.273491	-1.358214	4.546936
C	-0.088237	-2.156215	2.543125
H	0.436896	-1.255746	2.182072
C	-3.635606	0.276311	-1.616959
C	-3.019000	-2.508690	-0.613293
C	3.385270	2.044155	-0.475039
C	2.355971	3.027581	-0.527579
H	3.887199	1.743167	-1.407001
H	3.980907	1.961418	0.450060
H	2.077624	3.347528	-1.549910
C	2.115648	4.040008	0.572019
C	2.909737	5.384638	0.415374
H	1.032650	4.287520	0.608096
H	2.359738	3.584996	1.553141
C	2.520629	6.281852	1.611927
C	4.432070	5.133287	0.448168

C	2.534388	6.106747	-0.897600
H	3.049705	7.257959	1.566366
H	1.429051	6.486237	1.622358
H	2.780287	5.799102	2.577821
H	4.989321	6.093536	0.402734
H	4.735471	4.613429	1.382175
H	4.767407	4.514238	-0.410246
H	3.038972	7.094663	-0.960259
H	2.834926	5.526885	-1.795233
H	1.439670	6.284414	-0.958317
C	-5.041134	0.173762	-1.680274
C	-5.717877	0.307721	-2.903977
C	-4.994736	0.556789	-4.083347
C	-3.594327	0.670015	-4.029084
C	-2.916782	0.530463	-2.805591
H	-5.612539	-0.015542	-0.756506
H	-6.816109	0.225167	-2.934508
H	-5.523145	0.669923	-5.043505
H	-3.018927	0.872752	-4.946404
H	-1.818528	0.629339	-2.785534
C	-3.869414	-3.303326	0.185514
C	-4.581423	-4.380022	-0.369988
C	-4.440656	-4.685265	-1.734425
C	-3.588302	-3.905995	-2.536778
C	-2.886322	-2.823130	-1.983470
H	-3.967594	-3.076600	1.259819
H	-5.242575	-4.986962	0.268990
H	-4.992078	-5.532559	-2.172586
H	-3.469577	-4.140665	-3.606435
H	-2.227224	-2.218846	-2.623006

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i-cm-ph-ph-d E(gas)=-3365.99377465 G(gas)=-3365.148163 E(benzene)=-3366.00166254 A.U.

Ru	1.311221	1.042673	0.040488
Cl	0.938344	0.908459	2.442324
Cl	1.363187	1.490965	-2.369763
C	-0.576122	0.348924	-0.188202
N	-1.673578	1.118763	0.082840
N	-1.007095	-0.901328	-0.516670
C	-2.938112	0.453325	-0.325973
H	-3.708395	0.602628	0.454727
C	-2.482714	-1.043022	-0.284991
H	-2.621476	-1.394335	0.761538
C	2.628151	-0.323042	0.252326
H	2.630341	-0.724946	1.285883
C	3.532310	-1.079920	-0.621865
C	3.816241	-0.728459	-1.966060
H	3.278344	0.136470	-2.386336
C	4.728622	-1.449235	-2.743690
H	4.931608	-1.145296	-3.782194
C	5.376164	-2.566620	-2.186278
H	6.094497	-3.149925	-2.785277
C	5.118954	-2.957423	-0.863599
H	5.636803	-3.833917	-0.456134
C	4.209584	-2.227965	-0.062573
O	3.907274	-2.521182	1.227848

C	4.512016	-3.568872	2.032207
H	3.993083	-3.402971	3.000020
C	4.135105	-4.977445	1.558089
H	3.044234	-5.038410	1.373184
H	4.390230	-5.710388	2.351270
H	4.661464	-5.286014	0.633712
C	6.008640	-3.343740	2.278288
H	6.635834	-3.540826	1.386841
H	6.351537	-4.021843	3.086961
H	6.192815	-2.301431	2.608088
C	-1.639947	2.497184	0.462626
C	-2.460044	2.979820	1.524555
C	-2.436118	4.366504	1.796732
H	-3.057141	4.744774	2.624151
C	-1.617318	5.251962	1.078534
H	-1.618212	6.325039	1.326101
C	-0.800405	4.757480	0.051192
H	-0.164022	5.439174	-0.534329
C	-0.823853	3.388696	-0.263660
H	-0.240033	3.003641	-1.116959
C	-3.320421	2.099824	2.370771
C	-2.778307	0.982488	3.051292
H	-1.702957	0.759093	2.947014
C	-3.598720	0.187972	3.869784
H	-3.162766	-0.676679	4.394577
C	-4.963768	0.491142	4.025924
H	-5.601424	-0.137464	4.667997
C	-5.508550	1.603835	3.361435
H	-6.576082	1.851011	3.477703
C	-4.692841	2.402770	2.542464
H	-5.124563	3.266208	2.010846
C	-0.201906	-2.006740	-0.949861
C	-0.174217	-3.228433	-0.218780
C	0.503987	-4.325766	-0.804361
H	0.534914	-5.276298	-0.248339
C	1.163560	-4.218377	-2.036819
H	1.690141	-5.090418	-2.455531
C	1.162747	-2.991481	-2.720698
H	1.691834	-2.883966	-3.679908
C	0.471795	-1.897013	-2.183283
H	0.450448	-0.929519	-2.708975
C	-0.779059	-3.406889	1.134546
C	-1.580748	-4.541167	1.413335
H	-1.821169	-5.243892	0.599681
C	-2.084798	-4.769453	2.704428
H	-2.711235	-5.655448	2.896953
C	-1.790702	-3.871988	3.746527
H	-2.177048	-4.055532	4.762034
C	-0.998300	-2.740702	3.481061
H	-0.747655	-2.031834	4.286591
C	-0.500490	-2.502828	2.188520
H	0.122918	-1.610266	2.015611
C	-3.475714	0.988463	-1.648731
C	-3.216253	-1.998244	-1.202244
C	3.500103	1.577362	0.642965
C	2.648489	2.721841	0.499088

H	4.292933	1.431515	-0.107768
H	3.720189	1.226791	1.664931
H	2.181932	3.084322	1.434231
C	2.906965	3.769155	-0.565418
C	3.885303	4.920810	-0.142007
H	3.296975	3.283881	-1.483636
H	1.946028	4.241478	-0.856752
C	3.976668	5.897935	-1.335773
C	3.349449	5.678856	1.092882
C	5.293675	4.368280	0.163690
H	4.664499	6.740926	-1.110414
H	4.353636	5.386729	-2.246950
H	2.982840	6.329406	-1.581212
H	3.997264	6.549391	1.331721
H	2.321620	6.062442	0.917921
H	3.317367	5.034163	1.995658
H	5.995822	5.194871	0.404796
H	5.287163	3.676551	1.031887
H	5.710225	3.818128	-0.707271
C	-4.872154	1.052657	-1.838565
C	-5.412946	1.510131	-3.051621
C	-4.559758	1.918535	-4.091382
C	-3.166630	1.865605	-3.908562
C	-2.624869	1.404529	-2.696202
H	-5.544772	0.738721	-1.023198
H	-6.506066	1.553710	-3.182296
H	-4.980534	2.284423	-5.041667
H	-2.489348	2.189895	-4.714682
H	-1.528693	1.377559	-2.574063
C	-4.198527	-2.845068	-0.644835
C	-4.950755	-3.709758	-1.458002
C	-4.718540	-3.749225	-2.843365
C	-3.735693	-2.916387	-3.407299
C	-2.993377	-2.043498	-2.595747
H	-4.370378	-2.828070	0.443925
H	-5.715330	-4.360678	-1.004672
H	-5.300420	-4.431215	-3.483866
H	-3.545402	-2.943042	-4.491948
H	-2.232780	-1.392662	-3.050071

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i-tet-cm-me-me-a E(gas)=-2638.87390527 G(gas)=-2638.191532 E(benzene)=-2638.88120784 A.U.

Ru	0.377556	-0.283287	-0.146057
Cl	0.235031	0.043996	-2.585312
Cl	0.755084	-0.147876	2.264175
N	0.148721	2.768349	-0.066407
N	2.229219	2.057904	-0.238526
C	0.929598	1.662672	-0.168503
C	0.972951	4.010470	0.070334
H	1.079338	4.227804	1.158093
C	2.351941	3.528136	-0.457900
H	3.160374	3.927144	0.190631
C	0.360627	5.227307	-0.617412
H	0.183642	5.048135	-1.695941
H	1.030739	6.104596	-0.508342
H	-0.611978	5.487287	-0.154573

C	2.672325	3.848936	-1.922824
H	3.631395	3.374604	-2.212517
H	2.779842	4.942221	-2.074511
H	1.883161	3.467644	-2.602051
C	-1.285683	2.796329	-0.031893
C	-1.966915	3.184854	1.152402
C	-3.375046	3.274898	1.093857
H	-3.923146	3.569305	2.003871
C	-4.086436	2.973800	-0.077942
H	-5.185328	3.049896	-0.085719
C	-3.394665	2.557744	-1.228375
H	-3.941953	2.305116	-2.150206
C	-1.994657	2.473289	-1.205936
H	-1.424651	2.129381	-2.083500
C	-1.228457	3.453076	2.443259
H	-0.445526	2.685336	2.620125
H	-1.925795	3.440506	3.304025
H	-0.730402	4.448266	2.445822
C	3.358880	1.180330	-0.382675
C	4.274029	1.046503	0.697689
C	5.412209	0.238251	0.489916
H	6.134085	0.120609	1.314699
C	5.636204	-0.421933	-0.730712
H	6.537323	-1.042682	-0.859239
C	4.708151	-0.296382	-1.777735
H	4.868094	-0.818879	-2.733941
C	3.568415	0.506469	-1.603799
H	2.811186	0.603109	-2.397791
C	4.012198	1.700945	2.031535
H	3.979799	2.809543	1.959211
H	4.799378	1.437165	2.764666
H	3.028671	1.365625	2.428968
C	-1.464673	-0.756210	-0.221930
H	-1.797321	-0.934899	-1.265051
C	-2.599037	-0.785070	0.717052
C	-2.557143	-0.256959	2.030179
H	-1.597204	0.149792	2.381383
C	-3.684452	-0.256484	2.861694
H	-3.620460	0.162919	3.877598
C	-4.892676	-0.793744	2.387469
H	-5.789045	-0.801407	3.028962
C	-4.974234	-1.342946	1.097417
H	-5.921492	-1.782467	0.761893
C	-3.841161	-1.354553	0.254492
O	-3.799050	-1.924312	-0.982555
C	-4.951712	-2.322625	-1.770668
H	-4.463795	-2.558263	-2.740612
C	-5.595803	-3.620919	-1.266804
H	-6.200812	-3.485112	-0.348612
H	-4.816382	-4.381298	-1.058555
H	-6.266581	-4.027188	-2.052150
C	-5.932057	-1.172700	-2.024994
H	-6.516685	-0.890517	-1.127511
H	-6.650115	-1.472374	-2.816034
H	-5.386717	-0.275208	-2.379308
C	-0.313904	-2.456712	0.143451

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  C      1.010420    -2.406717    -0.433918
  H     -1.095951    -2.949807    -0.461032
  C      1.156648    -2.880883    -1.868792
  H     -0.425070    -2.571013     1.233874
  C      2.226577    -2.590906     0.480148
  H      3.075843    -1.999052     0.070803
  H      1.981456    -2.147301     1.464659
  C      2.766052    -4.049270     0.747274
  C      3.721622    -3.933463     1.960089
  C      1.620093    -5.016265     1.107437
  C      3.579010    -4.614828    -0.439899
  H      4.177556    -4.917718     2.201274
  H      4.547258    -3.219880     1.752736
  H      3.186044    -3.573290     2.863380
  H      2.022612    -6.017705     1.372086
  H      1.038164    -4.648247     1.978778
  H      0.913009    -5.156011     0.262947
  H      4.059091    -5.576251    -0.155751
  H      2.955034    -4.811680    -1.333166
  H      4.385834    -3.913247    -0.741073
  H      1.167680    -3.993903    -1.889357
  H      0.324759    -2.530162    -2.507274
  H      2.102042    -2.525749    -2.323752
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i-tet-cm-me-me-b E(gas)=-2638.87312923 G(gas)=-2638.190551 E(benzene)=-
2638.88045199 A.U.
  Ru    -0.444277     0.278373     0.227041
  Cl    -0.452532     0.610865    -2.214979
  Cl    -0.758024    -0.456339     2.534818
  N     -0.784446    -2.656231    -0.579635
  N     -2.698189    -1.595013    -0.307852
  C     -1.345257    -1.460121    -0.273351
  C     -1.820678    -3.726751    -0.723643
  H     -1.906661    -4.250157     0.256572
  C     -3.109877    -2.884228    -0.933540
  H     -3.944510    -3.324392    -0.347890
  C     -1.489691    -4.753862    -1.802771
  H     -1.343162    -4.280602    -2.793377
  H     -2.307684    -5.498913    -1.883395
  H     -0.560066    -5.300931    -1.548337
  C     -3.559830    -2.679059    -2.385103
  H     -4.424525    -1.986121    -2.418999
  H     -3.881440    -3.637997    -2.839668
  H     -2.747829    -2.242780    -3.001798
  C      0.619735    -2.937043    -0.682038
  C      1.261536    -3.740895     0.297474
  C      2.622871    -4.055230     0.091056
  H      3.141617    -4.673531     0.841904
  C      3.329216    -3.580756    -1.025251
  H      4.391550    -3.843120    -1.152297
  C      2.684126    -2.756948    -1.963530
  H      3.232092    -2.364792    -2.834823
  C      1.328355    -2.438718    -1.793271
  H      0.799648    -1.775485    -2.496003
  C      0.537803    -4.215797     1.536053
  H     -0.087543    -3.405735     1.967892
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H	1.259603	-4.544153	2.309684
H	-0.128888	-5.082014	1.327489
C	-3.640208	-0.535747	-0.069707
C	-4.462764	-0.587739	1.089328
C	-5.422390	0.433706	1.252466
H	-6.066842	0.414675	2.146636
C	-5.562156	1.472377	0.315765
H	-6.323091	2.253189	0.474597
C	-4.727086	1.517167	-0.812565
H	-4.822800	2.331227	-1.548133
C	-3.765336	0.511067	-1.006820
H	-3.084455	0.531222	-1.872737
C	-4.279613	-1.661417	2.132830
H	-4.460843	-2.680347	1.728059
H	-4.973123	-1.511415	2.983324
H	-3.235722	-1.636922	2.515834
C	1.450047	0.453286	0.128842
H	1.773019	0.847171	-0.856816
C	2.605679	0.035717	0.942393
C	2.515465	-0.800684	2.081144
H	1.509534	-1.109166	2.403558
C	3.653659	-1.214709	2.785143
H	3.550634	-1.867179	3.665912
C	4.922600	-0.791798	2.355945
H	5.828783	-1.109720	2.897054
C	5.056294	0.053180	1.242237
H	6.055842	0.392242	0.944650
C	3.914058	0.483789	0.532053
O	3.932379	1.358046	-0.513313
C	5.112924	1.771193	-1.251405
H	4.644229	2.345642	-2.078863
C	5.993401	2.753410	-0.467440
H	6.587606	2.270626	0.333306
H	5.370743	3.546280	-0.006400
H	6.705853	3.242145	-1.164027
C	5.864779	0.596603	-1.886785
H	6.421453	-0.015789	-1.150717
H	6.596658	0.985846	-2.624501
H	5.156891	-0.065996	-2.423761
C	0.647179	2.132222	1.025574
C	-0.695305	2.465945	0.597481
H	1.468453	2.646629	0.497984
C	-1.787666	2.593480	1.651576
H	0.833791	1.927576	2.093267
C	-0.850172	3.337706	-0.648304
H	-0.064557	3.037480	-1.370012
H	-1.810854	3.086125	-1.146384
C	-0.792208	4.906886	-0.504857
C	-0.566461	5.459693	-1.933456
C	-2.118246	5.502274	0.023167
C	0.374333	5.365274	0.394566
H	-0.551014	6.570944	-1.933262
H	0.396591	5.104438	-2.356960
H	-1.374349	5.132727	-2.622093
H	-2.090772	6.612248	-0.026697
H	-2.981332	5.160449	-0.586795

H	-2.322931	5.227596	1.076367
H	0.429051	6.474764	0.426995
H	0.262343	5.007441	1.439481
H	1.350820	4.997440	0.013521
H	-1.758207	3.613147	2.097184
H	-2.792992	2.467092	1.199112
H	-1.668243	1.859017	2.468678

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i-tet-cm-me-me-c E(gas)=-2638.8795928 G(gas)=-2638.196823 E(benzene)=-2638.88657631 A.U.

Ru	0.373267	-0.271053	-0.228393
Cl	0.538706	0.382423	-2.600995
Cl	0.534046	-0.428245	2.206145
N	0.017195	2.730200	0.170156
N	2.135511	2.120108	0.159627
C	0.857186	1.675395	0.027247
C	0.756717	3.966135	0.576773
H	0.731793	4.022363	1.690097
C	2.205490	3.610184	0.146337
H	2.922516	3.946561	0.924649
C	0.164244	5.250744	0.005746
H	0.114848	5.230358	-1.100687
H	0.776166	6.122240	0.316895
H	-0.864129	5.408030	0.387460
C	2.656391	4.133774	-1.222809
H	3.662302	3.737279	-1.466761
H	2.723815	5.240686	-1.221618
H	1.959709	3.816491	-2.025299
C	-1.415116	2.705134	0.061990
C	-2.220066	2.751531	1.231594
C	-3.619395	2.817285	1.053051
H	-4.263369	2.854898	1.947382
C	-4.202718	2.824328	-0.224705
H	-5.298474	2.874323	-0.326694
C	-3.389014	2.752636	-1.367598
H	-3.836431	2.735269	-2.373214
C	-1.994693	2.696130	-1.221851
H	-1.331268	2.617036	-2.096555
C	-1.612549	2.702132	2.613358
H	-0.851803	1.893771	2.683185
H	-2.391072	2.512748	3.378516
H	-1.115880	3.659655	2.886827
C	3.323212	1.316921	0.061152
C	4.106182	1.091065	1.227207
C	5.310795	0.372582	1.071069
H	5.932653	0.185453	1.961844
C	5.725088	-0.114061	-0.180934
H	6.673609	-0.668157	-0.265413
C	4.927392	0.100521	-1.316738
H	5.237322	-0.285243	-2.300596
C	3.726096	0.819181	-1.195425
H	3.067991	0.985332	-2.062829
C	3.647360	1.556717	2.587086
H	3.530503	2.660579	2.639483
H	4.370379	1.260079	3.371965
H	2.658128	1.106607	2.825549

C	-1.445505	-0.827734	-0.038863
H	-1.735585	-0.929436	1.026261
C	-2.617532	-0.941219	-0.926361
C	-2.575924	-0.753420	-2.328961
H	-1.606733	-0.470159	-2.770048
C	-3.717242	-0.888653	-3.130028
H	-3.648302	-0.735714	-4.218208
C	-4.946579	-1.214229	-2.531712
H	-5.854986	-1.322408	-3.146708
C	-5.034259	-1.411604	-1.144270
H	-6.004826	-1.673125	-0.700409
C	-3.885111	-1.284300	-0.331584
O	-3.893461	-1.471227	1.017493
C	-5.087753	-1.880108	1.723242
H	-5.960400	-1.335579	1.294042
C	-5.297286	-3.391804	1.589163
H	-4.440832	-3.938155	2.035663
H	-5.388088	-3.700386	0.528387
H	-6.222120	-3.703225	2.117446
C	-4.892616	-1.431323	3.170471
H	-4.003171	-1.923938	3.614252
H	-5.780976	-1.695660	3.779465
H	-4.742323	-0.334915	3.223487
C	-0.255912	-2.483454	-0.129823
C	1.071281	-2.311382	-0.703467
H	-1.001568	-2.954646	-0.791383
C	1.218755	-2.652519	-2.177490
H	-0.318019	-2.767229	0.933562
C	2.298568	-2.537783	0.186619
H	3.122442	-1.882156	-0.174365
H	2.046384	-2.190402	1.207976
C	2.891600	-3.992782	0.325696
C	3.872245	-3.938334	1.522783
C	1.785354	-5.022388	0.633618
C	3.691908	-4.437923	-0.919622
H	4.363600	-4.922802	1.678645
H	4.669993	-3.184443	1.352090
H	3.348172	-3.664343	2.462442
H	2.224041	-6.029318	0.802619
H	1.217995	-4.746604	1.547712
H	1.059030	-5.112861	-0.201336
H	4.213743	-5.398628	-0.718948
H	3.052044	-4.593664	-1.809996
H	4.464911	-3.686379	-1.186469
H	1.246484	-3.758790	-2.297416
H	0.375277	-2.262695	-2.776547
H	2.153165	-2.240033	-2.604835

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i-tet-cm-me-me-d E(gas)=-3022.0736683 G(gas)=-3021.295213 E(benzene)=-3022.08061767 A.U.

Ru	-0.439302	0.315454	0.026320
Cl	-0.801065	0.389936	-2.395029
Cl	-0.343437	-0.222301	2.417109
N	0.123217	-2.663587	-0.333558
N	-2.001274	-2.253161	0.081136
C	-0.781707	-1.677686	-0.105166

C	-0.475297	-4.017464	-0.118452
H	-0.278284	-4.307058	0.940207
C	-1.989004	-3.705952	-0.257264
H	-2.559756	-4.263529	0.514996
C	0.095506	-5.093947	-1.036523
H	-0.026608	-4.835423	-2.106689
H	-0.409376	-6.063312	-0.846147
H	1.177613	-5.234931	-0.843537
C	-2.609967	-3.967447	-1.635159
H	-3.662594	-3.620450	-1.651647
H	-2.610767	-5.051847	-1.867315
H	-2.059289	-3.431684	-2.435089
C	1.525007	-2.493506	-0.595124
C	2.480612	-2.723718	0.431417
C	3.844297	-2.617339	0.080816
H	4.603231	-2.789112	0.862079
C	4.251159	-2.294274	-1.224252
H	5.324250	-2.219194	-1.461090
C	3.289710	-2.055931	-2.219726
H	3.596922	-1.783394	-3.240807
C	1.926837	-2.156398	-1.901844
H	1.149219	-1.952818	-2.653437
C	2.063619	-3.042886	1.847069
H	1.271100	-2.343811	2.195719
H	2.926240	-2.963940	2.537816
H	1.667769	-4.078582	1.940458
C	-3.240353	-1.555976	0.286605
C	-3.902974	-1.668514	1.540563
C	-5.160479	-1.041408	1.668860
H	-5.688375	-1.111078	2.634185
C	-5.744637	-0.329279	0.607039
H	-6.730653	0.143339	0.742350
C	-5.067654	-0.215751	-0.617845
H	-5.511072	0.347216	-1.453950
C	-3.813836	-0.829931	-0.777326
H	-3.251171	-0.738584	-1.719644
C	-3.270363	-2.392810	2.702744
H	-3.145857	-3.479648	2.504290
H	-3.888892	-2.291719	3.616076
H	-2.260770	-1.971268	2.904386
C	1.362080	0.912550	0.204889
H	1.671353	0.939763	1.269796
C	2.498463	1.172570	-0.692549
C	2.391137	1.311119	-2.098952
H	1.394031	1.169157	-2.546249
C	3.498364	1.609914	-2.902130
H	3.375885	1.720606	-3.990713
C	4.763174	1.760359	-2.307481
H	5.646224	1.990257	-2.925940
C	4.919312	1.621472	-0.919388
H	5.917707	1.744270	-0.477724
C	3.803892	1.333268	-0.100675
O	3.883556	1.182840	1.249918
C	5.109421	1.439228	1.974163
H	5.958207	0.990177	1.408191
C	5.331012	2.945938	2.142496

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  H      4.499750     3.391539     2.727132
  H      5.383303     3.465612     1.164813
  H      6.279815     3.139259     2.684298
  C      4.966710     0.707305     3.307391
  H      4.102659     1.104111     3.878765
  H      5.882887     0.839072     3.918076
  H      4.803487    -0.376290     3.144935
  C      0.084906     2.561682     0.020599
  C     -1.255491     2.367660     0.515734
  H      0.234157     2.818848    -1.040114
  C     -1.506233     2.657579     1.984065
  H      0.802305     3.028786     0.718360
  C     -2.434826     2.585127    -0.435628
  H     -2.128904     2.241011    -1.443081
  H     -3.272517     1.925258    -0.119832
  C     -3.023198     4.040282    -0.597925
  C     -3.929297     3.993920    -1.852908
  C     -3.900481     4.471185     0.599629
  C     -1.904610     5.076751    -0.828149
  H     -4.408623     4.980035    -2.033175
  H     -3.350926     3.722202    -2.760692
  H     -4.739178     3.243066    -1.732926
  H     -4.414758     5.430878     0.375950
  H     -4.683319     3.713290     0.814865
  H     -3.315312     4.622212     1.527383
  H     -2.336463     6.083209    -1.016359
  H     -1.232184     5.162636     0.051242
  H     -1.279638     4.810863    -1.706843
  H     -1.600792     3.757492     2.127429
  H     -2.444692     2.189758     2.341609
  H     -0.682445     2.292353     2.624059
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i-tet-cm-me-ph-a E(gas)=-3022.06629793 G(gas)=-3021.289849 E(benzene)=-
3022.07420716 A.U.
  Ru    -0.576639     0.791697    -0.016334
  Cl     0.514236     0.208519    -2.117314
  Cl    -1.309621     1.336978     2.276665
  C      1.122085     0.084550     0.862077
  N      2.256846     0.832283     0.992259
  N      1.384169    -1.169658     1.321730
  C      3.281439     0.146962     1.834300
  H      4.277324     0.272722     1.363508
  C      2.828536    -1.329938     1.702419
  H      3.354259    -1.782511     0.832494
  C     -2.125082    -0.314368    -0.119248
  H     -2.816395    -0.127583     0.728249
  C     -2.567199    -1.471112    -0.920263
  C     -1.716415    -2.232148    -1.756112
  H     -0.676184    -1.895929    -1.862756
  C     -2.173811    -3.368434    -2.435967
  H     -1.484063    -3.944580    -3.071366
  C     -3.514811    -3.762339    -2.296556
  H     -3.891570    -4.652020    -2.826991
  C     -4.398761    -3.023682    -1.492618
  H     -5.447882    -3.335732    -1.422395
  C     -3.945106    -1.877485    -0.804339
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O	-4.733552	-1.053831	-0.055279
C	-6.063357	-1.377350	0.433259
H	-6.241971	-0.522590	1.120198
C	-7.133895	-1.301871	-0.663411
H	-7.011673	-0.374499	-1.258341
H	-8.139121	-1.274511	-0.193836
H	-7.113860	-2.163930	-1.359115
C	-6.095052	-2.653891	1.280109
H	-5.968889	-3.577186	0.681597
H	-7.070262	-2.721194	1.805031
H	-5.294520	-2.626225	2.046154
C	2.373145	2.229167	0.691395
C	3.481211	2.716827	-0.063013
C	3.591143	4.115596	-0.243037
H	4.434868	4.498862	-0.838454
C	2.643394	5.009196	0.280433
H	2.757815	6.091659	0.111687
C	1.557522	4.512100	1.017518
H	0.813539	5.198227	1.452075
C	1.431052	3.129584	1.232702
H	0.609606	2.729696	1.851095
C	4.524760	1.834048	-0.664072
C	4.177889	0.763022	-1.522208
H	3.114810	0.563900	-1.741257
C	5.183555	-0.018882	-2.115124
H	4.900288	-0.841972	-2.789444
C	6.541889	0.244765	-1.861861
H	7.323878	-0.375134	-2.328875
C	6.895499	1.307010	-1.011818
H	7.956217	1.522687	-0.805391
C	5.895091	2.096887	-0.421185
H	6.174550	2.924282	0.251285
C	0.438853	-2.237183	1.479625
C	0.649470	-3.515225	0.884500
C	-0.278480	-4.542017	1.192321
H	-0.139282	-5.527694	0.721571
C	-1.379616	-4.323985	2.030702
H	-2.084514	-5.145455	2.234618
C	-1.577871	-3.053340	2.595709
H	-2.435369	-2.860602	3.259669
C	-0.666566	-2.022148	2.329473
H	-0.803410	-1.020947	2.769772
C	1.773566	-3.845583	-0.042301
C	2.508115	-5.042730	0.148571
H	2.285857	-5.677997	1.021293
C	3.519534	-5.424317	-0.747698
H	4.081279	-6.356135	-0.573334
C	3.810734	-4.621260	-1.864044
H	4.595512	-4.923174	-2.575945
C	3.090965	-3.429673	-2.063358
H	3.297711	-2.798255	-2.942122
C	2.089295	-3.035411	-1.160034
H	1.540061	-2.096217	-1.341488
C	3.300878	0.735711	3.250516
H	3.545318	1.816257	3.207246
H	4.075087	0.242393	3.872026

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  H      2.317530     0.628429     3.752754
  C      3.045060    -2.212395     2.928573
  H      2.473931    -1.853011     3.807011
  H      4.122948    -2.230499     3.189749
  H      2.736777    -3.255424     2.721364
  C     -2.420449     1.354260    -1.269114
  C     -1.721058     2.546956    -0.841292
  H     -3.463494     1.251787    -0.923134
  H     -2.219751     0.956399    -2.277930
  C     -0.800720     3.243202    -1.836146
  C     -2.409272     3.439835     0.189304
  C     -3.422912     4.540792    -0.307958
  H     -2.948242     2.780973     0.898609
  H     -1.638824     3.955496     0.801274
  C     -4.244271     4.961947     0.935622
  C     -2.706992     5.802328    -0.844277
  C     -4.391756     3.999267    -1.379584
  H     -4.961652     5.771808     0.681850
  H     -4.823784     4.108173     1.345983
  H     -3.583619     5.336851     1.745997
  H     -3.446071     6.603970    -1.059767
  H     -1.989046     6.202557    -0.096969
  H     -2.145636     5.614196    -1.780229
  H     -5.137974     4.775024    -1.655273
  H     -3.865532     3.699927    -2.310301
  H     -4.954113     3.115794    -1.009487
  H     -1.403703     3.903621    -2.499218
  H     -0.065618     3.890514    -1.315942
  H     -0.255544     2.525471    -2.475733
107
i-tet-cm-me-ph-b E(gas)=-3022.0673856 G(gas)=-3021.289645 E(benzene)=-
3022.07532761 A.U.
  Ru    -0.446798     0.942746     0.362566
  Cl     0.389224     0.410864    -1.863095
  Cl    -0.969065     1.277457     2.751768
  C      0.926314    -0.418942     1.009344
  N      2.240286    -0.106176     1.210951
  N      0.770866    -1.755137     1.219237
  C      2.984164    -1.226051     1.860662
  H      3.973708    -1.333761     1.371952
  C      2.085432    -2.431593     1.483130
  H      2.445550    -2.848369     0.516576
  C     -2.270251     0.432349     0.168716
  H     -2.861741     0.687184     1.071957
  C     -3.072964    -0.342910    -0.792890
  C     -2.527582    -1.182701    -1.792961
  H     -1.434405    -1.206175    -1.896667
  C     -3.340697    -1.954829    -2.632675
  H     -2.884597    -2.605634    -3.394099
  C     -4.736529    -1.890986    -2.490056
  H     -5.390985    -2.489758    -3.144277
  C     -5.320813    -1.056802    -1.522561
  H     -6.413903    -1.005853    -1.448858
  C     -4.508451    -0.275310    -0.672591
  O     -4.972501     0.612948     0.252197
  C     -6.345112     0.706488     0.719318
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H	-6.228342	1.436291	1.548775
C	-7.281932	1.347598	-0.313112
H	-6.820238	2.261451	-0.738266
H	-8.228109	1.644654	0.185035
H	-7.543094	0.671219	-1.150610
C	-6.860210	-0.599275	1.334146
H	-7.062627	-1.386590	0.581857
H	-7.807243	-0.399371	1.876735
H	-6.126572	-0.997285	2.063468
C	2.805885	1.210997	1.163379
C	4.018446	1.450912	0.450221
C	4.587325	2.743562	0.533771
H	5.514637	2.941210	-0.026857
C	3.986653	3.774024	1.273863
H	4.456333	4.769712	1.309809
C	2.789610	3.523317	1.962423
H	2.310281	4.314192	2.560675
C	2.209506	2.244756	1.916606
H	1.292370	2.024002	2.488485
C	4.716874	0.415014	-0.367153
C	4.039431	-0.306298	-1.379529
H	2.968643	-0.112791	-1.562626
C	4.735981	-1.239275	-2.165898
H	4.199446	-1.785426	-2.957262
C	6.107019	-1.474268	-1.957335
H	6.644190	-2.209849	-2.577215
C	6.788387	-0.761408	-0.955634
H	7.862271	-0.937204	-0.782305
C	6.099374	0.177641	-0.170321
H	6.633836	0.729084	0.620305
C	-0.468794	-2.476087	1.227519
C	-0.674929	-3.620694	0.403066
C	-1.891339	-4.331518	0.561032
H	-2.069724	-5.205671	-0.084439
C	-2.877303	-3.927734	1.470835
H	-3.815250	-4.499325	1.552763
C	-2.661358	-2.788975	2.264296
H	-3.421250	-2.456034	2.988777
C	-1.458986	-2.077766	2.150456
H	-1.270381	-1.186821	2.771376
C	0.296515	-4.121320	-0.616285
C	0.612006	-5.502477	-0.661513
H	0.190319	-6.176052	0.102175
C	1.459047	-6.021625	-1.654082
H	1.694943	-7.097954	-1.663140
C	2.000490	-5.170402	-2.632938
H	2.656455	-5.575358	-3.420071
C	1.696182	-3.798017	-2.598449
H	2.100505	-3.122435	-3.369069
C	0.861723	-3.271276	-1.597898
H	0.639604	-2.190757	-1.597591
C	3.172528	-0.953211	3.358443
H	3.748329	-0.017016	3.503418
H	3.741536	-1.773427	3.840672
H	2.199198	-0.838893	3.877968
C	2.002062	-3.556066	2.510978

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  H      1.571340    -3.212232     3.471852
  H      3.016128    -3.962881     2.702335
  H      1.377537    -4.388279     2.132562
  C     -1.984032     2.317590    -0.667101
  C     -0.924976     3.102982    -0.078290
  H     -3.004272     2.493565    -0.282014
  H     -1.923682     2.054677    -1.735396
  C     -1.286222     3.966674     1.117361
  C      0.204369     3.619343    -0.977004
  C      0.013691     4.998480    -1.719761
  H      1.135004     3.698303    -0.372638
  H      0.401324     2.856150    -1.753884
  C      1.111667     5.045799    -2.810659
  C     -1.368154     5.088106    -2.398622
  C      0.223061     6.215255    -0.789844
  H      1.076310     6.007025    -3.367129
  H      2.124239     4.951052    -2.364014
  H      0.990795     4.220815    -3.543676
  H     -1.454264     6.026296    -2.987919
  H     -1.534172     4.239091    -3.094749
  H     -2.195793     5.085425    -1.658412
  H      0.220312     7.157171    -1.379951
  H     -0.566723     6.309954    -0.019470
  H      1.200218     6.152617    -0.265389
  H     -1.816470     4.878682     0.761881
  H     -1.944884     3.435922     1.828846
  H     -0.386946     4.300364     1.672100
107
i-tet-cm-me-ph-c E(gas)=-3022.07269777 G(gas)=-3021.297127 E(benzene)=-
3022.08021712 A.U.
  Ru     0.024038    -1.185649    -0.364733
  Cl     0.563105    -0.341543     1.867602
  Cl    -0.232121    -1.741717    -2.751606
  C      0.705254     0.616538    -1.015133
  N      2.034137     0.894431    -1.165603
  N      0.004297     1.758788    -1.253602
  C      2.257099     2.225043    -1.801687
  H      3.087858     2.740344    -1.278729
  C      0.918935     2.932578    -1.470046
  H      1.026936     3.452761    -0.492286
  C     -1.786203    -1.267253     0.239075
  H     -1.885924    -0.844921     1.258675
  C     -3.103770    -1.526728    -0.362539
  C     -3.298774    -2.204530    -1.591287
  H     -2.399815    -2.493448    -2.157348
  C     -4.575971    -2.473673    -2.096291
  H     -4.691522    -3.006382    -3.052824
  C     -5.704927    -2.048728    -1.373415
  H     -6.719062    -2.244840    -1.758225
  C     -5.559381    -1.366970    -0.155636
  H     -6.456343    -1.040926     0.384150
  C     -4.273765    -1.102811     0.370862
  O     -4.033926    -0.456985     1.541200
  C     -5.032394    -0.044189     2.511292
  H     -4.378330     0.370687     3.307343
  C     -5.912229     1.108635     2.012424
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H	-5.283726	1.893541	1.546578
H	-6.444272	1.560825	2.875003
H	-6.676848	0.794076	1.275167
C	-5.795874	-1.225052	3.123038
H	-6.519598	-1.689574	2.424781
H	-6.362900	-0.872808	4.009526
H	-5.088641	-2.008887	3.461470
C	3.103167	-0.051145	-1.046129
C	4.263241	0.259671	-0.274726
C	5.322615	-0.677846	-0.275367
H	6.214601	-0.455385	0.331367
C	5.250459	-1.883576	-0.991047
H	6.093977	-2.591207	-0.960383
C	4.101359	-2.174505	-1.742068
H	4.031838	-3.107284	-2.323597
C	3.038653	-1.256459	-1.777778
H	2.148954	-1.453052	-2.399381
C	4.425876	1.519466	0.511645
C	3.456296	1.941588	1.453571
H	2.549902	1.333537	1.615451
C	3.663465	3.112514	2.202340
H	2.902603	3.424491	2.934831
C	4.829148	3.880361	2.029442
H	4.982062	4.797882	2.619955
C	5.799748	3.466704	1.100598
H	6.717145	4.059538	0.955231
C	5.599956	2.295837	0.350659
H	6.357408	1.981315	-0.385650
C	-1.419428	1.896106	-1.357046
C	-2.127831	2.854820	-0.574708
C	-3.502099	3.048893	-0.860472
H	-4.058558	3.786165	-0.259979
C	-4.167863	2.308484	-1.847546
H	-5.239838	2.479554	-2.033981
C	-3.461382	1.341551	-2.581762
H	-3.968802	0.737918	-3.349878
C	-2.093219	1.149117	-2.345232
H	-1.520723	0.402928	-2.919203
C	-1.516427	3.653307	0.529115
C	-1.733051	5.052070	0.596824
H	-2.299482	5.550212	-0.207009
C	-1.226308	5.811507	1.664311
H	-1.400253	6.899295	1.692414
C	-0.501219	5.184357	2.692748
H	-0.109607	5.776381	3.535503
C	-0.282871	3.795922	2.637564
H	0.269348	3.287201	3.444082
C	-0.777434	3.033770	1.565670
H	-0.596270	1.945591	1.550078
C	2.600785	2.065980	-3.288529
H	3.521251	1.458374	-3.401290
H	2.791842	3.052495	-3.757016
H	1.786475	1.558317	-3.844933
C	0.413162	3.926037	-2.511652
H	0.206072	3.440489	-3.485456
H	1.171868	4.720382	-2.666027

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  H     -0.516927     4.418102    -2.168516
  C     -0.835204    -3.023021     0.757857
  C      0.447066    -3.329168     0.154131
  H     -1.700059    -3.588138     0.374136
  H     -0.844577    -2.812335     1.839833
  C      0.439060    -4.298094    -1.017520
  C      1.697087    -3.348548     1.040585
  C      2.076799    -4.679450     1.798108
  H      2.577525    -3.061102     0.425405
  H      1.583052    -2.556389     1.805005
  C      3.112341    -4.271085     2.874700
  C      0.852476    -5.304332     2.498522
  C      2.745604    -5.725846     0.877156
  H      3.467788    -5.159284     3.440156
  H      3.998999    -3.785610     2.414395
  H      2.677886    -3.553366     3.601749
  H      1.153412    -6.196002     3.089465
  H      0.376545    -4.585910     3.198804
  H      0.079109    -5.633845     1.772799
  H      3.132538    -6.576858     1.478443
  H      2.050896    -6.147749     0.124857
  H      3.606425    -5.284144     0.331554
  H      0.329598    -5.336113    -0.631522
  H     -0.390998    -4.101939    -1.719408
  H      1.384962    -4.254667    -1.592143
107
i-tet-cm-me-ph-d E(gas)=-3022.06418335 G(gas)=-3021.288438 E(benzene)=-
3022.07214213 A.U.
  Ru    -0.389301     1.040216    -0.027687
  Cl     0.545499     0.149985    -2.108923
  Cl    -0.946095     1.815603     2.243952
  C      1.044844    -0.084697     0.871590
  N      2.343609     0.326820     0.966183
  N      0.964897    -1.353039     1.358022
  C      3.162063    -0.596836     1.803471
  H      4.144083    -0.753309     1.313723
  C      2.322652    -1.896268     1.706547
  H      2.679668    -2.482681     0.830819
  C     -2.008786     0.159179    -0.529206
  H     -1.875803    -0.435617    -1.454567
  C     -3.305290    -0.132316     0.105016
  C     -3.840064     0.589044     1.201365
  H     -3.212316     1.375381     1.648199
  C     -5.103909     0.304362     1.731172
  H     -5.490808     0.887186     2.581303
  C     -5.866239    -0.736972     1.172542
  H     -6.859973    -0.981491     1.582023
  C     -5.373089    -1.482844     0.091336
  H     -5.982361    -2.296382    -0.320136
  C     -4.104123    -1.193741    -0.461435
  O     -3.545161    -1.862017    -1.503961
  C     -4.219445    -2.815127    -2.367886
  H     -3.425112    -2.998569    -3.122186
  C     -4.497042    -4.156677    -1.678017
  H     -3.600220    -4.491059    -1.119489
  H     -4.727356    -4.922301    -2.447745
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H	-5.352338	-4.123416	-0.974428
C	-5.417394	-2.208300	-3.107372
H	-6.289952	-2.025038	-2.450061
H	-5.740851	-2.902186	-3.910704
H	-5.133120	-1.247724	-3.582327
C	2.827202	1.627113	0.612260
C	4.012201	1.773893	-0.169148
C	4.483488	3.086037	-0.407365
H	5.387432	3.209676	-1.024541
C	3.815439	4.218772	0.084535
H	4.209091	5.224683	-0.130802
C	2.650364	4.056490	0.849381
H	2.122032	4.931226	1.260231
C	2.167077	2.765730	1.122250
H	1.281364	2.623414	1.764607
C	4.780630	0.624193	-0.733903
C	4.156024	-0.365401	-1.531218
H	3.074369	-0.294504	-1.739065
C	4.916225	-1.412885	-2.078336
H	4.417752	-2.172293	-2.701020
C	6.300705	-1.495074	-1.843505
H	6.888572	-2.321280	-2.274497
C	6.930381	-0.513802	-1.058127
H	8.014285	-0.567445	-0.867014
C	6.176781	0.537764	-0.510691
H	6.671473	1.299092	0.114231
C	-0.224762	-2.122755	1.582724
C	-0.379037	-3.424225	1.020669
C	-1.503145	-4.185368	1.426855
H	-1.633736	-5.191061	0.996429
C	-2.458767	-3.680529	2.319971
H	-3.326202	-4.297424	2.603299
C	-2.307813	-2.382676	2.835333
H	-3.055427	-1.962225	3.525392
C	-1.189775	-1.616500	2.477658
H	-1.051946	-0.599201	2.877554
C	0.559507	-4.024128	0.026263
C	1.027096	-5.350366	0.200682
H	0.745155	-5.907456	1.109146
C	1.853002	-5.957998	-0.759523
H	2.210970	-6.987843	-0.599429
C	2.219408	-5.254323	-1.920266
H	2.859989	-5.731923	-2.678999
C	1.759677	-3.937901	-2.104627
H	2.025667	-3.377841	-3.015576
C	0.943051	-3.321507	-1.141528
H	0.593339	-2.289539	-1.315552
C	3.372088	-0.014535	3.207198
H	3.893676	0.961408	3.136850
H	4.002840	-0.686357	3.823557
H	2.408612	0.151153	3.731465
C	2.331086	-2.791115	2.942366
H	1.910432	-2.280449	3.830733
H	3.371769	-3.099795	3.170903
H	1.743489	-3.712220	2.765208
C	-1.989419	2.023689	-1.380526

C	-0.994732	2.992069	-0.955418
H	-3.014186	2.192824	-1.016790
H	-1.904839	1.643111	-2.412787
C	0.086106	3.406599	-1.944576
C	-1.439276	4.064031	0.042803
C	-2.147763	5.368671	-0.491490
H	-2.123748	3.588078	0.771429
H	-0.560938	4.390670	0.639188
C	-2.801618	6.034667	0.744373
C	-1.147969	6.382222	-1.095075
C	-3.247857	5.048556	-1.524274
H	-3.292685	6.992067	0.467081
H	-3.570596	5.375938	1.199911
H	-2.045313	6.257103	1.526919
H	-1.662000	7.340308	-1.325079
H	-0.326153	6.606308	-0.382105
H	-0.687014	6.023690	-2.035971
H	-3.769517	5.977952	-1.838756
H	-2.836122	4.573237	-2.439410
H	-4.015926	4.365375	-1.103185
H	-0.325928	4.168145	-2.643999
H	0.946844	3.872435	-1.423463
H	0.451971	2.554034	-2.544622

107

i-tet-cm-ph-me-a E(gas)=-3405.26783922 G(gas)=-3404.395026 E(benzene)=-3405.27595889 A.U.

Ru	0.846608	0.656332	0.459927
Cl	0.749177	0.444110	2.885521
Cl	0.442809	0.836378	-1.973023
C	-1.115195	0.174236	0.504027
N	-2.078032	1.115138	0.696641
N	-1.709681	-1.046162	0.417689
C	-3.448503	0.566223	0.527415
H	-4.101391	0.931235	1.346260
C	-3.161982	-0.959796	0.767149
H	-3.256653	-1.129674	1.862900
C	2.158811	-0.652304	0.023712
H	2.394909	-0.654777	-1.060541
C	2.814498	-1.775653	0.716801
C	2.406946	-2.278796	1.975487
H	1.587136	-1.755825	2.489196
C	3.024364	-3.392634	2.559089
H	2.682108	-3.763540	3.537449
C	4.078715	-4.029707	1.884583
H	4.575093	-4.907688	2.329265
C	4.527000	-3.551808	0.642013
H	5.369623	-4.052904	0.149917
C	3.915474	-2.425439	0.049539
O	4.319130	-1.840733	-1.114259
C	5.228992	-2.425627	-2.083507
H	5.142312	-1.691899	-2.913275
C	6.690339	-2.402395	-1.616416
H	6.946412	-1.406929	-1.201194
H	7.355994	-2.590759	-2.484246
H	6.918962	-3.166416	-0.847624
C	4.744292	-3.776050	-2.621671

H	4.827877	-4.596420	-1.882257
H	5.350662	-4.056326	-3.507705
H	3.685320	-3.704518	-2.941081
C	-1.841752	2.524191	0.873493
C	-2.090379	3.115218	2.143772
C	-1.913929	4.510552	2.257299
H	-2.099320	4.987712	3.233583
C	-1.497696	5.294519	1.167769
H	-1.373514	6.382118	1.292411
C	-1.233068	4.688618	-0.070750
H	-0.898535	5.291288	-0.929527
C	-1.406252	3.302181	-0.218447
H	-1.191626	2.803452	-1.174912
C	-2.471715	2.283066	3.343423
C	-1.038356	-2.293354	0.172760
C	-0.998190	-3.303398	1.169674
C	-0.386483	-4.530135	0.829636
H	-0.344611	-5.325373	1.591806
C	0.188723	-4.746822	-0.431429
H	0.662424	-5.714892	-0.658870
C	0.174219	-3.719223	-1.389558
H	0.635122	-3.868511	-2.378663
C	-0.444498	-2.497129	-1.089252
H	-0.454037	-1.668422	-1.815123
C	-1.540203	-3.080480	2.561797
C	-4.094571	0.953599	-0.797279
C	-4.075955	-1.944990	0.069260
C	3.099995	1.081282	0.647917
C	2.363721	2.300941	0.395316
H	3.848361	0.792434	-0.109666
H	3.360740	0.822494	1.687818
C	2.041409	3.212826	1.571955
C	2.537288	2.976864	-0.963076
C	3.725451	3.992128	-1.170761
H	2.639604	2.179100	-1.724963
H	1.595465	3.505437	-1.223172
C	3.890219	4.154535	-2.701705
C	3.417669	5.388978	-0.582221
C	5.049356	3.461976	-0.582447
H	4.684561	4.894060	-2.940577
H	4.163741	3.191675	-3.182704
H	2.947407	4.506216	-3.172037
H	4.216662	6.110527	-0.858657
H	2.457555	5.785951	-0.975214
H	3.349119	5.383698	0.523141
H	5.881604	4.166357	-0.797306
H	4.997189	3.335418	0.519314
H	5.324816	2.480330	-1.023333
C	-5.478286	1.225598	-0.827014
C	-6.121888	1.554438	-2.031699
C	-5.382883	1.622588	-3.225238
C	-4.001440	1.360741	-3.203470
C	-3.357313	1.026965	-1.999534
H	-6.061468	1.180224	0.108113
H	-7.203055	1.766162	-2.035743
H	-5.882196	1.886976	-4.171141

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  H     -3.412249     1.420190    -4.132546
  H     -2.269181     0.836980    -2.003441
  C     -5.123838    -2.535123     0.808656
  C     -6.031611    -3.416746     0.197866
  C     -5.894599    -3.729197    -1.165183
  C     -4.849671    -3.153066    -1.909109
  C     -3.948431    -2.265420    -1.299598
  H     -5.229696    -2.299146     1.881206
  H     -6.843368    -3.866214     0.791643
  H     -6.599199    -4.425374    -1.647453
  H     -4.733425    -3.396234    -2.977102
  H     -3.135488    -1.821745    -1.891607
  H     -2.561727     2.914343     4.249028
  H     -3.442161     1.758612     3.207050
  H     -1.695002     1.508732     3.529012
  H     -1.145647    -3.843619     3.261331
  H     -1.252782    -2.079325     2.947156
  H     -2.649450    -3.154561     2.591962
  H      2.897432     3.900380     1.754644
  H      1.158180     3.848341     1.354548
  H      1.853059     2.644951     2.501171
107
i-tet-cm-ph-me-b E(gas)=-3405.26909708 G(gas)=-3404.395777 E(benzene)=-
3405.27705418 A.U.
  Ru    -0.922824     0.648939     0.011723
  Cl    -1.112450     0.921693    -2.403187
  Cl    -0.233848     0.371899     2.365792
  C      1.023915     0.236997    -0.337989
  N      1.966842     1.213385    -0.419432
  N      1.618279    -0.962842    -0.578411
  C      3.344537     0.664564    -0.524849
  H      3.904490     1.210217    -1.311610
  C      3.023771    -0.777756    -1.056507
  H      2.996147    -0.704440    -2.166640
  C     -2.147580    -0.774742     0.323674
  H     -2.247142    -0.997675     1.405910
  C     -2.889163    -1.749835    -0.493079
  C     -2.674791    -1.957109    -1.877110
  H     -1.941427    -1.308375    -2.377951
  C     -3.373220    -2.937772    -2.593329
  H     -3.182339    -3.076551    -3.668598
  C     -4.314247    -3.739642    -1.927032
  H     -4.871790    -4.516675    -2.475108
  C     -4.570353    -3.556980    -0.558022
  H     -5.328467    -4.180870    -0.069258
  C     -3.878429    -2.564733     0.170204
  O     -4.101276    -2.260240     1.479598
  C     -4.896347    -3.042602     2.409567
  H     -4.689896    -2.501513     3.357680
  C     -6.403599    -2.927117     2.147082
  H     -6.689117    -1.866113     1.999511
  H     -6.959305    -3.309317     3.028435
  H     -6.742360    -3.502241     1.263018
  C     -4.380098    -4.474866     2.586990
  H     -4.584764    -5.125775     1.714654
  H     -4.869954    -4.932629     3.471200
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H	-3.286510	-4.470246	2.767414
C	1.726295	2.625706	-0.276158
C	1.812910	3.461516	-1.424293
C	1.647409	4.849791	-1.232791
H	1.709975	5.514403	-2.109969
C	1.395672	5.395350	0.037656
H	1.276541	6.484745	0.151299
C	1.288830	4.551147	1.154627
H	1.082386	4.966662	2.153310
C	1.456950	3.165221	0.998290
H	1.364050	2.484210	1.856569
C	2.022960	2.888364	-2.804112
C	0.971758	-2.245141	-0.535744
C	0.794270	-3.005481	-1.720949
C	0.219913	-4.289185	-1.590683
H	0.070952	-4.893685	-2.500320
C	-0.187991	-4.795289	-0.347471
H	-0.637380	-5.798999	-0.285237
C	-0.039620	-4.009921	0.808207
H	-0.369469	-4.387509	1.788808
C	0.544662	-2.738671	0.713692
H	0.657142	-2.094528	1.600112
C	1.154864	-2.461661	-3.083014
C	4.137313	0.766395	0.772537
C	4.001703	-1.875259	-0.693370
C	-3.187658	1.040248	0.176276
C	-2.435304	2.195500	0.603098
H	-3.839661	0.566921	0.931656
H	-3.557139	0.988796	-0.860863
C	-2.488453	2.554170	2.077308
C	-2.233420	3.354228	-0.379487
C	-3.310142	4.506353	-0.427248
H	-1.249115	3.832059	-0.174236
H	-2.168074	2.930781	-1.400336
C	-3.019883	5.304469	-1.722240
C	-4.740465	3.934031	-0.505598
C	-3.200110	5.485910	0.763656
H	-3.719681	6.161529	-1.824964
H	-1.985863	5.710000	-1.718711
H	-3.126266	4.665162	-2.623661
H	-5.484172	4.753148	-0.609977
H	-4.859876	3.260375	-1.380438
H	-5.008389	3.356781	0.404372
H	-3.865637	6.361570	0.603159
H	-3.491860	5.027046	1.728367
H	-2.162909	5.868122	0.871282
C	5.521057	1.032345	0.706686
C	6.297418	1.101236	1.875454
C	5.693683	0.911408	3.130402
C	4.313608	0.652133	3.205698
C	3.536768	0.577766	2.036493
H	5.998519	1.188729	-0.275219
H	7.376368	1.312744	1.805340
H	6.297359	0.972397	4.050093
H	3.830009	0.509448	4.185344
H	2.452635	0.383106	2.118071

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  C      4.947972    -2.284694    -1.657614
  C      5.908735    -3.264974    -1.356692
  C      5.927163    -3.859697    -0.083751
  C      4.984058    -3.464912     0.881733
  C      4.030723    -2.478478     0.582732
  H      4.930519    -1.827837    -2.661759
  H      6.639819    -3.569426    -2.122435
  H      6.673552    -4.633907     0.155374
  H      4.989537    -3.929120     1.880623
  H      3.299706    -2.177841     1.346562
  H      1.991534     3.685641    -3.572270
  H      3.001453     2.370340    -2.903380
  H      1.225558     2.146919    -3.032001
  H      0.664983    -3.052562    -3.881963
  H      0.830153    -1.404504    -3.188230
  H      2.250018    -2.506550    -3.271938
  H     -3.455612     3.059850     2.295474
  H     -2.407732     1.660897     2.723962
  H     -1.674092     3.250035     2.359926
107
i-tet-cm-ph-me-c E(gas)=-3405.26770069 G(gas)=-3404.394605 E(benzene)=-
3405.27522401 A.U.
  Ru    -0.971391     0.684318     0.147061
  Cl    -0.078500     0.640534     2.446936
  Cl    -1.324183     0.739544    -2.274459
  N      1.496943    -0.972807    -0.553657
  N      1.883830     1.203227    -0.540295
  C      0.942792     0.246526    -0.317879
  C      2.843876    -0.830842    -1.188165
  H      2.693450    -0.793662    -2.290393
  C      3.237411     0.623184    -0.745195
  H      3.734549     1.127251    -1.598804
  C      3.843182    -1.929397    -0.895051
  C      4.140884     0.756841     0.474862
  C      0.843272    -2.240824    -0.381571
  C      0.533160    -3.054050    -1.503707
  C     -0.028947    -4.324432    -1.248806
  H     -0.267987    -4.973860    -2.107382
  C     -0.302027    -4.766654     0.055468
  H     -0.742115    -5.763600     0.216686
  C     -0.028347    -3.928080     1.148782
  H     -0.262989    -4.249609     2.175093
  C      0.547778    -2.668846     0.928165
  H      0.755167    -1.984100     1.765049
  C      0.746188    -2.577127    -2.920645
  H      0.381300    -1.534598    -3.043911
  H      0.197101    -3.220055    -3.636601
  H      1.818604    -2.607798    -3.213777
  C      1.675363     2.626447    -0.477956
  C      1.658298     3.376521    -1.687357
  C      1.529284     4.777719    -1.581363
  H      1.512328     5.376923    -2.506469
  C      1.412715     5.417916    -0.335593
  H      1.318264     6.514693    -0.290991
  C      1.408093     4.657962     0.845041
  H      1.306438     5.146816     1.826503
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C	1.542384	3.261386	0.773328
H	1.522598	2.643158	1.682050
C	1.724399	2.704372	-3.036667
H	2.673511	2.145514	-3.185724
H	1.647331	3.448833	-3.853084
H	0.887967	1.977892	-3.140065
C	-2.264728	-0.718628	0.194351
H	-2.593635	-0.996501	-0.827032
C	-2.784878	-1.660025	1.198344
C	-2.545790	-1.561862	2.591439
H	-1.891937	-0.745594	2.936402
C	-3.078979	-2.481086	3.503444
H	-2.872025	-2.373690	4.579449
C	-3.872056	-3.541751	3.031392
H	-4.296133	-4.276705	3.735000
C	-4.139267	-3.676711	1.660044
H	-4.767456	-4.510177	1.316697
C	-3.612829	-2.746628	0.734780
O	-3.837398	-2.811606	-0.604983
C	-4.674704	-3.835434	-1.191452
H	-4.469704	-4.801152	-0.674194
C	-6.154254	-3.466095	-1.045946
H	-6.365416	-2.514110	-1.575514
H	-6.444123	-3.341125	0.016655
H	-6.795581	-4.257980	-1.485259
C	-4.229296	-3.954874	-2.647699
H	-4.377024	-2.993073	-3.180458
H	-4.817167	-4.738686	-3.167236
H	-3.155260	-4.220182	-2.705660
C	-3.233920	1.119679	0.299761
C	-2.429367	2.263328	0.685880
H	-3.880767	0.693538	1.083884
C	-2.473114	2.670755	2.150146
H	-3.648411	1.102316	-0.721719
C	-2.200637	3.383738	-0.335774
H	-1.204978	3.844034	-0.146726
H	-2.144570	2.920455	-1.340376
C	-3.245553	4.562711	-0.425616
C	-2.936121	5.304135	-1.749352
C	-4.692297	4.030379	-0.480141
C	-3.102903	5.580787	0.728677
H	-3.608957	6.178762	-1.879686
H	-1.889439	5.675463	-1.763228
H	-3.067117	4.636566	-2.626771
H	-5.410933	4.867181	-0.615338
H	-4.833817	3.328160	-1.328861
H	-4.976736	3.497488	0.451711
H	-3.750106	6.465272	0.543417
H	-3.395658	5.162574	1.711180
H	-2.056349	5.942633	0.813788
C	5.519451	0.985469	0.282984
C	6.392349	1.082654	1.379492
C	5.892569	0.958184	2.687346
C	4.518553	0.736656	2.888035
C	3.645023	0.635683	1.791527
H	5.916270	1.089795	-0.740827

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  H      4.115868     0.646263     3.909588
  H      2.567113     0.476550     1.971206
  C      4.672764    -2.384313    -1.942874
  C      5.652466    -3.365338    -1.714578
  C      5.806963    -3.914988    -0.430727
  C      4.980872    -3.474307     0.618513
  C      4.008884    -2.486881     0.391171
  H      4.547943    -1.962310    -2.954541
  H      6.291240    -3.706061    -2.544902
  H      6.568455    -4.689832    -0.247789
  H      5.094036    -3.902445     1.627049
  H      3.371164    -2.148310     1.219910
  H     -3.429968     3.201177     2.353969
  H     -2.412632     1.799316     2.827687
  H     -1.643525     3.356603     2.410897
107
i-tet-cm-ph-me-d E(gas)=-3405.26712354 G(gas)=-3404.394482 E(benzene)=-
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  Ru    -0.924452     0.796818    -0.177244
  Cl    -0.973088     0.461537    -2.611666
  Cl    -0.336172     1.101293     2.179640
  C      0.975430     0.147654    -0.436297
  N      2.002540     0.984666    -0.752500
  N      1.452258    -1.127073    -0.414834
  C      3.313469     0.284786    -0.761607
  H      3.905283     0.607861    -1.641722
  C      2.828536    -1.184040    -1.000683
  H      2.714560    -1.298748    -2.102256
  C     -2.315955    -0.504126    -0.103163
  H     -2.683900    -0.750892    -1.119721
  C     -2.928409    -1.370222     0.914125
  C     -2.680278    -1.263771     2.305861
  H     -1.953518    -0.502944     2.633035
  C     -3.318819    -2.087648     3.239582
  H     -3.107478    -1.972572     4.313960
  C     -4.224233    -3.064489     2.789709
  H     -4.732787    -3.727010     3.509129
  C     -4.494323    -3.212781     1.420511
  H     -5.204079    -3.983834     1.097718
  C     -3.866660    -2.375923     0.469216
  O     -4.080378    -2.433265    -0.871146
  C     -4.999579    -3.325377    -1.553357
  H     -4.831726    -3.018390    -2.607546
  C     -4.598061    -4.802240    -1.449974
  H     -3.511724    -4.916420    -1.637339
  H     -5.143350    -5.382956    -2.222579
  H     -4.829406    -5.255163    -0.466207
  C     -6.468260    -3.028777    -1.225162
  H     -6.759029    -3.333523    -0.200581
  H     -7.121034    -3.575059    -1.937216
  H     -6.676833    -1.945553    -1.335616
  C      1.928106     2.412055    -0.922795
  C      2.069204     2.961391    -2.228827
  C      2.077687     4.367416    -2.346050
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H	2.180177	4.811560	-3.349811
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C	1.804079	4.644402	0.053676
H	1.701323	5.288867	0.940551
C	1.790125	3.247732	0.203986
H	1.655759	2.792134	1.195333
C	2.174815	2.082710	-3.450827
C	0.706789	-2.309087	-0.082714
C	0.346359	-3.245845	-1.087671
C	-0.294977	-4.431726	-0.667046
H	-0.577097	-5.174489	-1.431837
C	-0.587509	-4.679958	0.683680
H	-1.087612	-5.617432	0.974129
C	-0.256057	-3.723530	1.657042
H	-0.502493	-3.892840	2.716177
C	0.393105	-2.541973	1.270861
H	0.654272	-1.770419	2.011076
C	0.596547	-2.983944	-2.552805
C	4.141831	0.545960	0.491240
C	3.728441	-2.298024	-0.512017
C	-3.114775	1.431780	0.233591
C	-2.386099	2.523429	-0.353149
H	-3.236126	1.392709	1.327515
H	-3.963774	1.029404	-0.346225
C	-2.730632	2.926212	-1.774715
C	-1.861497	3.633783	0.560943
C	-2.818103	4.836596	0.920444
H	-1.546947	3.173561	1.517991
H	-0.944743	4.068617	0.106545
C	-2.158565	5.558633	2.121206
C	-2.952245	5.863051	-0.227942
C	-4.214991	4.340179	1.345578
H	-2.758034	6.441340	2.431305
H	-2.063210	4.883644	2.997466
H	-1.139910	5.917832	1.861767
H	-3.502955	6.762947	0.122227
H	-1.954943	6.197865	-0.584198
H	-3.503554	5.462906	-1.101007
H	-4.851363	5.192177	1.667911
H	-4.744082	3.825310	0.516173
H	-4.151348	3.630617	2.197524
C	5.546110	0.614132	0.378626
C	6.350576	0.816148	1.512411
C	5.756268	0.959651	2.778036
C	4.356648	0.899861	2.899296
C	3.551496	0.694421	1.765420
H	6.017587	0.506140	-0.612528
H	7.445790	0.868176	1.404943
H	6.383395	1.124945	3.668672
H	3.881016	1.019780	3.885808
H	2.454367	0.662968	1.880632
C	4.514940	-2.991978	-1.457177
C	5.404688	-4.002279	-1.054859
C	5.511067	-4.340697	0.304632
C	4.726409	-3.661818	1.253900

C	3.844309	-2.646390	0.851310
H	4.427309	-2.734974	-2.526404
H	6.010436	-4.531251	-1.807748
H	6.201889	-5.136992	0.624645
H	4.801605	-3.924124	2.321028
H	3.238953	-2.120156	1.602742
H	2.139439	2.690285	-4.376311
H	3.125409	1.505473	-3.473192
H	1.334254	1.354909	-3.471425
H	-0.001582	-3.674108	-3.180323
H	0.315429	-1.941605	-2.818971
H	1.663238	-3.141226	-2.826318
H	-3.637444	3.571470	-1.764483
H	-1.908706	3.504694	-2.241188
H	-2.931650	2.049455	-2.416807

Cartesian coordinates relative to BDE analysis on Rh complexes

6
rh-co-relax SCF Done: -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

43
nhc-me-me SCF Done: -847.008850537 A.U.

C	-3.288802	-0.251722	-0.981337
C	-2.400900	0.365577	-0.086173
C	-2.810323	1.471291	0.658092
C	-4.101302	1.968484	0.542696
C	-4.999143	1.349495	-0.319509
C	-4.587802	0.255755	-1.070928
N	-1.061537	-0.104095	0.077824
C	-0.735247	-1.453496	0.635712
C	0.781669	-1.301046	0.890943
N	1.092140	-0.137877	0.000891
C	0.008753	0.608120	-0.318541
C	2.421226	0.358160	-0.148170
C	1.200933	-1.013813	2.332088
C	-1.597225	-1.851804	1.824758
C	-2.865523	-1.397748	-1.863194
H	1.299512	-2.193756	0.542928
H	-0.874583	-2.194906	-0.157397
H	-5.281694	-0.207173	-1.763663
H	-6.010997	1.723385	-0.417695
H	-4.403175	2.830762	1.124345
H	-2.094795	1.939096	1.321470
C	3.423975	-0.426458	-0.742272
C	4.709341	0.114637	-0.840340
C	5.002093	1.395437	-0.391289
C	3.992764	2.172936	0.166820
C	2.713202	1.651789	0.289708
C	3.147720	-1.794166	-1.312718
H	5.489269	-0.479698	-1.303370

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  H      6.006871     1.787847    -0.489539
  H      4.200545     3.179128     0.509758
  H      1.911644     2.241863     0.712767
  H      0.976965    -1.862327     2.981467
  H      2.275716    -0.833234     2.377770
  H      0.695911    -0.130672     2.726708
  H     -2.644481    -1.924359     1.528987
  H     -1.291722    -2.828798     2.205435
  H     -1.528841    -1.127795     2.636641
  H     -3.560460    -1.515850    -2.694992
  H     -1.868441    -1.229845    -2.273747
  H     -2.843623    -2.348160    -1.321395
  H      3.892697    -2.047868    -2.067624
  H      3.184760    -2.576890    -0.548551
  H      2.162246    -1.835509    -1.779385
57
nhc-ph-me SCF Done: -1230.59154485 A.U.
  C     -2.092506     1.544058    -0.546400
  C     -1.668241     1.155796     0.725519
  C     -2.156911     1.853699     1.832557
  C     -3.035512     2.920520     1.677550
  C     -3.449418     3.298552     0.405173
  C     -2.976976     2.604447    -0.704279
  C     -0.688188     0.030759     0.953867
  C      0.830079     0.364684     0.791900
  N      1.328736    -0.948554     0.284289
  C      0.369469    -1.733080    -0.253086
  N     -0.809887    -1.158226     0.052863
  C      2.720671    -1.221923     0.110887
  C      1.194406     1.528394    -0.110476
  C      1.232077     1.411879    -1.500602
  C      1.547323     2.507602    -2.295862
  C      1.833780     3.738345    -1.713290
  C      1.806300     3.864445    -0.328873
  C      1.492629     2.765128     0.463051
  C     -2.053935    -1.729158    -0.362749
  C     -2.257543    -1.916146    -1.730548
  C     -3.435544    -2.471058    -2.208194
  C     -4.433802    -2.835641    -1.312063
  C     -4.224531    -2.666114     0.050013
  C     -3.037244    -2.128934     0.555841
  C     -2.836560    -2.050620     2.047174
  H      1.234551     0.573706     1.779081
  H     -0.820078    -0.311690     1.983064
  H     -4.990605    -2.980101     0.750005
  H     -5.363087    -3.262810    -1.668551
  H     -3.573780    -2.610977    -3.273229
  H     -1.467787    -1.628571    -2.411668
  H     -1.846264     1.558529     2.829257
  H     -3.400878     3.449473     2.549477
  H     -4.138811     4.124369     0.278727
  H     -3.299462     2.888319    -1.698632
  H     -1.737058     1.012146    -1.417403
  H      1.476910     2.871822     1.542252
  H      2.034718     4.815936     0.135889
  H      2.083270     4.590415    -2.333756
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  H      1.575127     2.398684    -3.373417
  H      1.021570     0.456786    -1.964119
  C      3.613066    -1.171615     1.194664
  C      4.962262    -1.442466     0.946488
  C      5.423195    -1.781489    -0.317754
  C      4.522041    -1.865495    -1.373609
  C      3.182271    -1.582757    -1.156682
  C      3.168775    -0.894662     2.608580
  H      5.658644    -1.409664     1.777020
  H      6.473961    -1.992937    -0.473546
  H      4.860248    -2.144108    -2.364078
  H      2.465963    -1.654379    -1.963015
  H     -3.582205    -2.657774     2.560861
  H     -1.849346    -2.419300     2.333047
  H     -2.934581    -1.027898     2.420132
  H      3.886243    -1.310826     3.316583
  H      3.097281     0.177121     2.817798
  H      2.194923    -1.341704     2.815384
57
nhc-me-ph
  C      3.319184    -0.485587    -0.487336
  C      2.394057    -1.504129    -0.189557
  C      2.806087    -2.837164    -0.178882
  C      4.104138    -3.184548    -0.525108
  C      5.013720    -2.190990    -0.863245
  C      4.622159    -0.858710    -0.829962
  N      1.034237    -1.213613     0.156715
  C      0.656778    -0.396029     1.355003
  C     -0.840946    -0.728799     1.488743
  N     -1.148144    -1.201533     0.106502
  C     -0.043228    -1.582917    -0.562048
  C     -2.500516    -1.415344    -0.317411
  C     -1.218779    -1.803844     2.512986
  C      1.523043    -0.664364     2.576045
  C      2.992722     0.974444    -0.421565
  H     -1.408162     0.179421     1.689177
  H      0.760996     0.653749     1.070332
  H      5.331839    -0.079193    -1.078310
  H      6.027482    -2.450591    -1.142108
  H      4.401915    -4.225811    -0.525978
  H      2.099394    -3.603532     0.106652
  C     -3.374744    -0.331116    -0.501542
  C     -4.682813    -0.600483    -0.923799
  C     -5.121502    -1.899230    -1.146640
  C     -4.257812    -2.966167    -0.925474
  C     -2.956174    -2.722017    -0.503662
  C     -2.975083     1.084207    -0.233723
  H     -5.356038     0.233210    -1.086374
  H     -6.136743    -2.075813    -1.487114
  H     -4.595319    -3.984670    -1.073978
  H     -2.284669    -3.546342    -0.311327
  H     -1.021200    -1.458744     3.529619
  H     -2.283898    -2.023474     2.437742
  H     -0.666199    -2.730555     2.343459
  H      2.560853    -0.408535     2.368096
  H      1.191406    -0.038801     3.407999
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  H      1.482388    -1.708070     2.885796
  C      3.630096     1.780963     0.535572
  C      3.388597     3.153422     0.575948
  C      2.513496     3.739859    -0.350425
  C      1.881050     2.945162    -1.308568
  C      2.118259     1.571059    -1.349614
  H      4.323474     1.331136     1.249432
  H      3.888155     3.762926     1.325508
  H      2.328599     4.809559    -0.325626
  H      1.202648     3.391890    -2.038861
  H      1.601910     0.965712    -2.089999
  C     -2.141446     1.787006    -1.113414
  C     -1.831738     3.120976    -0.864219
  C     -2.342816     3.766952     0.257684
  C     -3.170454     3.072137     1.139187
  C     -3.490019     1.740305     0.890268
  H     -1.733585     1.287162    -1.981616
  H     -1.193008     3.658548    -1.557958
  H     -2.101620     4.806726     0.442750
  H     -3.572549     3.566076     2.016584
  H     -4.142616     1.203709     1.572137
71
nhc-ph-ph SCF Done: -1614.18539511 A.U.
  C     -1.796451    -2.478533    -0.791529
  C     -1.476212    -1.183009    -1.201896
  C     -1.886425    -0.765911    -2.469976
  C     -2.583660    -1.622486    -3.315531
  C     -2.895082    -2.910906    -2.896224
  C     -2.502091    -3.333315    -1.629854
  C     -0.687398    -0.222387    -0.346161
  C      0.862460    -0.414471    -0.299478
  N      1.137373     0.029036     1.101324
  C      0.054216     0.002756     1.910310
  N     -1.007886    -0.218562     1.117186
  C      2.460514     0.169401     1.615826
  C      1.401620    -1.802207    -0.592035
  C      1.452376    -2.805570     0.376600
  C      1.930593    -4.072556     0.061352
  C      2.368362    -4.356090    -1.228479
  C      2.330729    -3.360975    -2.199399
  C      1.855827    -2.093844    -1.879169
  C     -2.339137    -0.292917     1.630774
  C     -2.636872    -1.322218     2.523739
  C     -3.918608    -1.483619     3.028409
  C     -4.930245    -0.620080     2.622826
  C     -4.635597     0.416769     1.749084
  C     -3.340406     0.618653     1.254499
  C     -3.078164     1.827716     0.427619
  H      1.307558     0.274840    -1.011063
  H     -0.871941     0.784548    -0.726448
  H     -5.411001     1.119315     1.469032
  H     -5.938848    -0.740661     2.998450
  H     -4.127908    -2.287540     3.723294
  H     -1.841674    -1.996357     2.812897
  H     -1.661774     0.243260    -2.796497
  H     -2.889172    -1.279742    -4.296830
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  H     -3.443760    -3.579738    -3.548164
  H     -2.744929    -4.333696    -1.292569
  H     -1.496213    -2.822244     0.188420
  H      1.836934    -1.320738    -2.639009
  H      2.676924    -3.568304    -3.204793
  H      2.743410    -5.342600    -1.472434
  H      1.966971    -4.838531     0.826781
  H      1.125288    -2.593016     1.386284
  C      3.453462     0.902336     0.937822
  C      4.743698     0.932620     1.484870
  C      5.047282     0.306188     2.683835
  C      4.045462    -0.373722     3.368565
  C      2.770417    -0.447953     2.831267
  C      3.202991     1.702319    -0.293064
  H      5.507668     1.499615     0.967058
  H      6.051029     0.361649     3.086510
  H      4.258439    -0.859726     4.312872
  H      1.983249    -0.979819     3.346707
  C     -3.833678     2.091861    -0.719565
  C     -3.635969     3.259830    -1.448931
  C     -2.683265     4.187076    -1.039598
  C     -1.927655     3.936064     0.102479
  C     -2.120578     2.766806     0.828990
  H     -4.572318     1.370138    -1.046430
  H     -4.228327     3.445273    -2.336981
  H     -2.533772     5.100014    -1.603208
  H     -1.193454     4.659339     0.437075
  H     -1.538202     2.581287     1.722851
  C      3.977642     1.505160    -1.441465
  C      3.781635     2.285240    -2.576699
  C      2.808654     3.279160    -2.582814
  C      2.035454     3.489000    -1.444103
  C      2.231573     2.710032    -0.309817
  H      4.728681     0.724525    -1.446523
  H      4.388966     2.113902    -3.457457
  H      2.655366     3.887432    -3.465854
  H      1.279332     4.264591    -1.437084
  H      1.632213     2.882369     0.575068
49
nhc-rh-co-me-me2 SCF Done: -1644.72650150 A.U.
  C     -2.974757     0.033979    -1.066572
  C     -2.470638    -0.801188    -0.071359
  C     -3.278389    -1.221260     0.997352
  C     -4.603514    -0.780727     1.021520
  C     -5.113217     0.048411     0.029734
  C     -4.294913     0.462748    -1.014330
  N     -1.113260    -1.261058    -0.149385
  C     -0.788625    -2.634604    -0.632628
  C      0.722851    -2.708696    -0.308395
  N      1.068120    -1.262694    -0.185253
  C     -0.018704    -0.491320    -0.054109
  C      2.425356    -0.805358    -0.072152
  C      3.151457    -1.021568     1.108878
  C      4.477887    -0.584774     1.142635
  C      5.065369     0.045948     0.052891
  C      4.325798     0.262521    -1.103708
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  C      3.006766    -0.166967    -1.165245
  C      2.546219    -1.681443     2.321176
  C      1.601547    -3.459747    -1.296178
  C     -1.176726    -2.797952    -2.099866
  Rh     0.003938     1.587752     0.109537
  C      0.040914     3.514895     0.069512
  O      0.065659     4.650440     0.012406
  C     -2.755120    -2.098763     2.105257
  Cl     0.065555     1.624688    -2.307226
  C     -0.062814     1.482468     1.957234
  O     -0.106782     1.399929     3.101077
  H     -1.330690    -3.364842    -0.031845
  H      0.841733    -3.164687     0.679894
  H      5.053187    -0.732068     2.049555
  H      6.094578     0.378172     0.113452
  H      4.766917     0.768531    -1.953042
  H      2.403498     0.016875    -2.043756
  H     -5.240638    -1.085209     1.843973
  H     -6.143866     0.377877     0.080033
  H     -4.676679     1.118683    -1.786458
  H     -2.318199     0.360338    -1.862152
  H     -0.932728    -3.801085    -2.453231
  H     -2.251385    -2.655422    -2.215771
  H     -0.669327    -2.067454    -2.731373
  H      2.641724    -3.439037    -0.970365
  H      1.290982    -4.504935    -1.351536
  H      1.551968    -3.028499    -2.295410
  H      3.116404    -1.431023     3.215777
  H      1.515157    -1.364912     2.482822
  H      2.547463    -2.772085     2.231985
  H     -3.399086    -2.030999     2.982067
  H     -2.721855    -3.152109     1.810059
  H     -1.746319    -1.810945     2.403739
63
nhc-rh-co-ph-me2 SCF Done: -2028.30851186 A.U.
  C      1.840506     2.681947    -0.429831
  C      1.271200     2.180832     0.738427
  C      1.630630     2.694693     1.994522
  C      2.564389     3.732806     2.028279
  C      3.129344     4.241951     0.865752
  C      2.772242     3.709707    -0.366933
  N      0.295414     1.127412     0.662205
  C     -1.152973     1.390798     0.879395
  C     -1.678427    -0.071833     1.070096
  N     -0.583321    -0.862270     0.434305
  C      0.539998    -0.139703     0.300805
  C     -3.077205    -0.376462     0.595105
  C     -3.390481    -0.594531    -0.747453
  C     -4.701832    -0.843341    -1.133194
  C     -5.720815    -0.872925    -0.185784
  C     -5.419843    -0.658205     1.154188
  C     -4.104987    -0.418429     1.539144
  C     -1.778251     2.224284    -0.221817
  C     -1.436343     2.064067    -1.565819
  C     -2.057226     2.833424    -2.543591
  C     -3.025783     3.769336    -2.193951
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  C     -3.368508     3.937761    -0.856894
  C     -2.743731     3.171485     0.120940
  Rh     2.351926    -0.848641    -0.457825
  C      2.916758    -1.292737     1.249055
  O      3.250689    -1.561273     2.313293
  C     -0.667848    -2.279918     0.202169
  C     -0.608640    -2.738633    -1.112075
  C     -0.693763    -4.096467    -1.386658
  C     -0.850187    -4.999701    -0.342644
  C     -0.896996    -4.538479     0.966483
  C     -0.800503    -3.178437     1.271764
  C     -0.808179    -2.739267     2.713374
  C      1.066610     2.153645     3.283353
  Cl     1.538791    -0.229993    -2.653619
  C      3.968244    -1.461450    -1.310705
  O      4.909396    -1.815317    -1.841802
  H     -1.285280     1.925030     1.818715
  H     -1.647767    -0.277820     2.142511
  H     -0.993747    -5.248219     1.780080
  H     -0.920816    -6.061770    -0.543123
  H     -0.636605    -4.441643    -2.411152
  H     -0.464707    -2.024257    -1.910910
  H     -3.875831    -0.262773     2.588021
  H     -6.204049    -0.685199     1.900820
  H     -6.741813    -1.067290    -0.490505
  H     -4.928084    -1.014723    -2.178339
  H     -2.609745    -0.572244    -1.494253
  H     -3.010957     3.313310     1.162527
  H     -4.115078     4.669511    -0.573272
  H     -3.505107     4.368709    -2.958350
  H     -1.777123     2.701824    -3.581595
  H     -0.678515     1.347207    -1.859462
  H      2.861507     4.136685     2.989350
  H      3.854728     5.044157     0.925461
  H      3.215259     4.087836    -1.279496
  H      1.567064     2.245948    -1.379777
  H     -0.580987    -3.581812     3.366414
  H     -0.065269    -1.962924     2.904724
  H     -1.785389    -2.350690     3.014146
  H      1.720980     2.402257     4.118869
  H      0.083246     2.578364     3.508133
  H      0.958251     1.068673     3.253589
63
nhc-rh-co-me-ph2 SCF Done: -2028.31586675 A.U.
  C      1.469864     2.514448    -1.520767
  C      2.252737     2.709967    -0.379445
  C      2.394358     4.010081     0.118579
  C      1.761497     5.083157    -0.500051
  C      0.987028     4.875843    -1.636770
  C      0.847140     3.588660    -2.146526
  C      3.001931     1.580789     0.241343
  C      2.394642     0.459391     0.835264
  C      3.178645    -0.564213     1.366234
  C      4.563757    -0.502103     1.301634
  C      5.179174     0.605272     0.731852
  C      4.401052     1.631868     0.214543
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  N      0.970723     0.377185     0.999186
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  C     -1.140463     0.654563     2.002624
  N     -1.093530    -0.328208     0.879537
  C      0.163478    -0.544543     0.452443
  C     -2.241129    -1.127002     0.559274
  C     -3.424845    -0.522484     0.093876
  C     -4.531349    -1.347540    -0.144125
  C     -4.476215    -2.720140     0.054020
  C     -3.302133    -3.299598     0.517943
  C     -2.196482    -2.502859     0.783619
  C     -3.573038     0.938882    -0.150471
  C     -4.608101     1.645255     0.475117
  C     -4.793116     3.002611     0.236900
  C     -3.948130     3.678400    -0.637029
  C     -2.920337     2.986115    -1.269978
  C     -2.732619     1.629588    -1.029551
  C     -1.362526    -0.064043     3.331629
  C      0.936043     1.776551     3.100212
  Rh     0.779914    -2.108350    -0.810052
  C      1.399157    -3.612235    -1.843092
  O      1.775705    -4.513230    -2.425377
  C      0.345257    -1.102426    -2.298719
  O      0.052389    -0.485836    -3.222085
  Cl     1.234140    -3.460800     1.151040
  H     -1.952059     1.357821     1.826739
  H      0.065270     2.259222     1.204688
  H      4.876548     2.487639    -0.248683
  H      6.259233     0.669387     0.682555
  H      5.153958    -1.314668     1.706100
  H      2.689521    -1.416491     1.816526
  H     -5.441515    -0.894380    -0.516911
  H     -5.346113    -3.330925    -0.153934
  H     -3.242782    -4.367224     0.688065
  H     -1.289344    -2.942989     1.173754
  H     -1.398689     0.652769     4.153287
  H     -2.314668    -0.595091     3.311803
  H     -0.574836    -0.791491     3.533593
  H      1.876023     2.276142     2.868507
  H      0.318871     2.479141     3.663272
  H      1.154523     0.918734     3.735474
  H      3.005923     4.179620     0.996895
  H      1.880844     6.082063    -0.098115
  H      0.503853     5.712346    -2.126728
  H      0.264964     3.418829    -3.044263
  H      1.376827     1.521992    -1.939341
  H     -1.941079     1.098668    -1.541413
  H     -2.261677     3.502486    -1.956407
  H     -4.090649     4.735290    -0.826151
  H     -5.597023     3.531096     0.735019
  H     -5.265149     1.125334     1.161990
77
nhc-rh-co-ph-ph2 SCF Done: -2411.89843248 A.U.
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  C     -3.612197     1.607441    -0.902502
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C	-1.375908	0.670137	-0.318305
C	-0.137696	1.605094	-0.507961
N	0.959497	0.700450	-0.063637
C	0.596163	-0.594016	-0.082608
N	-0.727550	-0.676676	-0.294848
C	2.291588	1.200148	0.139101
C	0.105214	2.183601	-1.888418
C	0.700092	1.449910	-2.916299
C	0.881705	2.019797	-4.171614
C	0.472392	3.326706	-4.417493
C	-0.117055	4.065681	-3.397493
C	-0.293053	3.496892	-2.140814
C	-1.487133	-1.895879	-0.368998
C	-1.227242	-2.766683	-1.426794
C	-1.968519	-3.927927	-1.590553
C	-3.005550	-4.213004	-0.711727
C	-3.269845	-3.345401	0.338345
C	-2.514842	-2.184142	0.546170
Rh	1.898530	-2.233768	0.101989
Cl	2.136429	-2.252074	-2.316573
C	-2.833578	-1.367831	1.752326
C	1.776040	-2.150742	1.944848
O	1.716797	-2.082318	3.089044
C	3.077086	-3.757609	0.117953
O	3.767270	-4.660682	0.094655
H	-0.228218	2.430321	0.193293
H	-1.769195	0.852668	0.683643
H	-4.059562	-3.576925	1.042301
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H	-1.740399	-4.595512	-2.411825
H	-0.429854	-2.529070	-2.116361
H	-3.647175	2.014768	0.101625
H	-5.509008	2.445379	-1.456505
H	-5.457911	1.488159	-3.744819
H	-3.521033	0.114992	-4.455394
H	-1.652362	-0.285207	-2.913598
H	-0.745899	4.080860	-1.347244
H	-0.432988	5.086318	-3.576218
H	0.618136	3.768194	-5.395868
H	1.348927	1.438815	-4.957382
H	1.030896	0.432261	-2.746551
C	2.540936	2.213072	1.084855
C	3.851605	2.692997	1.200970
C	4.888036	2.186634	0.429988
C	4.625019	1.187668	-0.497854
C	3.330831	0.710254	-0.651385
C	1.503312	2.812346	1.969525
H	4.054357	3.462540	1.935372
H	5.892720	2.571046	0.555579
H	5.417384	0.785803	-1.116622
H	3.118929	-0.043317	-1.395547
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  H     -4.815142    -0.864563     1.092492
  H     -5.420646     0.335498     3.162312
  H     -3.791762     0.503762     5.024257
  H     -1.553504    -0.543679     4.792346
  H     -0.953371    -1.734377     2.725083
  C      1.298398     4.197820     1.954211
  C      0.368238     4.791660     2.799785
  C     -0.372364     4.010281     3.680716
  C     -0.173670     2.633386     3.709331
  C      0.755552     2.038398     2.862761
  H      1.866250     4.809204     1.263372
  H      0.222495     5.864764     2.769295
  H     -1.096541     4.470338     4.341782
  H     -0.742174     2.018158     4.394783
  H      0.915261     0.968921     2.908193
23
nhc-me SCF Done: -384.759603431 A.U.
  C      0.220295    -1.461992    -0.258573
  N      1.182534    -0.612744     0.139946
  C      0.710205     0.758750     0.450212
  C     -0.812570     0.505071     0.578686
  N     -0.942828    -0.791429    -0.130400
  C      2.592185    -0.930210     0.088579
  C      1.133331     1.762627    -0.624840
  C     -1.739433     1.595144     0.056342
  C     -2.228125    -1.446514    -0.234740
  H      1.121304     1.078583     1.412222
  H     -1.050675     0.332757     1.638403
  H      0.750817     2.760916    -0.403776
  H      2.221195     1.834367    -0.670617
  H      0.773157     1.462095    -1.610085
  H     -2.782927     1.322639     0.221824
  H     -1.563977     2.535676     0.583117
  H     -1.599938     1.766417    -1.011606
  H     -2.066059    -2.428812    -0.671820
  H     -2.696345    -1.571994     0.750548
  H     -2.917048    -0.884333    -0.870701
  H      2.685433    -1.996776    -0.101729
  H      3.113176    -0.386951    -0.706989
  H      3.078611    -0.692628     1.040391
37
nhc-ph SCF Done: -768.347704085 A.U.
  C      2.408004    -0.417253    -1.292085
  C      1.453819    -0.620336    -0.293473
  C      1.696222    -0.094885     0.977400
  C      2.856545     0.624947     1.236553
  C      3.794344     0.833413     0.229330
  C      3.567165     0.308962    -1.038202
  C      0.195730    -1.391446    -0.617562
  N     -0.297469    -2.287262     0.456286
  C     -1.642322    -2.400338     0.490180
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  C     -1.603396     2.398692     1.431943
  C     -1.253811     3.468536     0.613564
  C     -0.864621     3.228821    -0.699897
  C     -0.826649     1.926793    -1.187720
  C     -3.529801    -1.230408    -0.572196
  H     -1.230333    -0.506891    -2.012216
  H      0.409339    -2.010222    -1.499587
  H      2.243537    -0.835173    -2.279596
  H      4.294293     0.457290    -1.827472
  H      4.697864     1.394923     0.433404
  H      3.029419     1.024344     2.228649
  H      0.973370    -0.255823     1.766516
  H     -0.526797     1.748713    -2.214653
  H     -0.596091     4.054993    -1.347168
  H     -1.290451     4.481663     0.995083
  H     -1.914485     2.577327     2.454320
  H     -1.841080     0.269909     1.582158
  H     -4.084427    -1.991593    -0.028813
  H     -3.837789    -0.240981    -0.222289
  H     -3.767589    -1.306350    -1.638147
  H     -0.001328    -3.900303     1.706271
  H      0.927784    -3.988263     0.195425
  H      1.441583    -2.883646     1.483345
29
nhc-rh-co-me SCF Done: -1182.47964425 A.U.
  C     -0.735141    -0.009573     0.060104
  N     -1.463946     0.405244     1.096540
  C     -2.910244     0.163433     0.907937
  C     -2.883351    -0.853428    -0.262195
  N     -1.537343    -0.609187    -0.831434
  C     -0.951011     1.099309     2.261752
  C     -3.664670     1.468406     0.650509
  C     -4.010555    -0.756533    -1.278843
  C     -1.051290    -1.413875    -1.938902
  Rh     1.340024     0.110618    -0.075533
  C      1.241775     1.761299    -0.919728
  O      1.162583     2.780843    -1.439610
  C      3.270175     0.030515    -0.097608
  O      4.404545    -0.046189    -0.093258
  Cl     1.305692    -2.018339     1.019944
  H     -3.311033    -0.311712     1.806386
  H     -2.876444    -1.867773     0.157477
  H     -4.728173     1.278698     0.499103
  H     -3.572682     2.135387     1.508800
  H     -3.275363     1.988088    -0.226263
  H     -3.913405    -1.536217    -2.035043
  H     -4.974518    -0.902519    -0.787847
  H     -4.021692     0.209758    -1.783522
  H     -0.016769    -1.143477    -2.136845
  H     -1.087361    -2.478904    -1.689046
  H     -1.647568    -1.231590    -2.833899
  H      0.135289     1.055393     2.239409
  H     -1.267002     2.145709     2.279539
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43
nhc-rh-co-ph SCF Done: -1566.06641673 A.U.
  C      3.431898    -2.329549    -0.744319
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  C      2.781340    -1.208399     1.278153
  C      3.952751    -1.638093     1.890334
  C      4.872758    -2.407294     1.183920
  C      4.609701    -2.752564    -0.136914
  C      1.258784    -1.084477    -0.757415
  N      0.037545    -1.073057     0.076250
  C     -0.788173    -0.077688    -0.280580
  N     -0.148596     0.760405    -1.094436
  C      1.253528     0.375236    -1.339429
  C     -0.422526    -2.308721     0.693652
  C      2.244437     1.364128    -0.752951
  C      1.977072     2.068309     0.421713
  C      2.910434     2.958936     0.940716
  C      4.125499     3.156873     0.292626
  C      4.398774     2.463542    -0.881662
  C      3.460992     1.578091    -1.401491
  C     -0.726550     1.927181    -1.735864
  Rh    -2.808252     0.033187     0.212522
  Cl    -3.111189    -1.274031    -1.772299
  C     -4.721424     0.013178     0.481600
  O     -5.850612    -0.017057     0.609639
  C     -2.446285     1.041922     1.727502
  O     -2.200822     1.665308     2.659028
  H      1.426886     0.321592    -2.416128
  H      1.075171    -1.770421    -1.592652
  H      3.224722    -2.617117    -1.769448
  H      5.314443    -3.359410    -0.692061
  H      5.785085    -2.740800     1.662854
  H      4.147687    -1.371166     2.921811
  H      2.070345    -0.613162     1.836374
  H      3.678742     1.048058    -2.322177
  H      5.338642     2.616531    -1.397774
  H      4.851156     3.852188     0.696198
  H      2.685843     3.501128     1.851155
  H      1.031193     1.928944     0.930551
  H     -1.746004     2.049840    -1.377676
  H     -0.143642     2.820686    -1.504404
  H     -0.751359     1.785538    -2.819157
  H     -1.311076    -2.094414     1.283097
  H     -0.683764    -3.048044    -0.069148
  H      0.357545    -2.711331     1.338546
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