Supporting Information for

Reductive Functionalization of a Rh(III)-methyl Bond by Electronic Modification of the Supporting Ligand

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Experimental

General Considerations. Unless otherwise noted, all synthetic procedures were performed under anaerobic conditions in a nitrogen filled glovebox or by using standard Schlenk techniques. Glovebox purity was maintained by periodic nitrogen purges and was monitored by an oxygen analyzer (O_2 < 15 ppm for all reactions). Tetrahydrofuran was dried by distillation from sodium/benzophenone. Pentane and diethyl ether were dried by distillation from Na/benzophenone. Benzene, hexanes, and methylene chloride were purified by passage through a column of activated alumina. Benzene-d_6, chloroform-d_1, tetrahydrofuran-d_8, and nitromethane-d_3 were stored over 4 Å molecular sieves in a nitrogen atmosphere. ^{1}H NMR spectra were recorded on a Varian Mercury Plus 300 MHz or a Varian Inova 500 MHz spectrometer, and the ^{13}C NMR spectra were recorded on a Varian Inova 500 MHz spectrometers (operating frequency 126 MHz). All ^{1}H and ^{13}C NMR spectra are referenced against residual proton signals (^{1}H NMR) or the ^{13}C resonances of the deuterated solvent (^{13}C NMR). 4,4',4"-trinitropyridine,[1] $\{(COE)_2Rh(\mu\text{–}Cl)\}_2$,[2] and $\{(ethylene)_2Rh(\mu\text{–}Cl)\}_2$[3] were prepared according to published literature procedures. All other reagents were used as purchased from commercial sources.

Synthesis of [^{t}Bu$_3$terpy]RhCl (1). Benzene solutions (10 mL) containing ^{t}Bu$_3$terpy (0.513 g, 1.27 mmol) and $[(ethylene)_2Rh(\mu\text{–}Cl)]_2$ (0.248 g, 0.638 mmol) were combined. The solution immediately changed color from orange to deep blue and was stirred for 1 h. The volatiles were reduced in vacuo to ~2 mL, and hexanes were added to precipitate a dark blue powder. The precipitate was isolated by filtration and washed with hexanes (2 x 5 mL) (0.608 g, 88%). ^{1}H NMR (C_6D_6, 500 MHz): δ = 9.88 (s, 2H, Ar–*H*), 7.69 (s, 2H, Ar–*H*), 7.57 (s, 2H, Ar–*H*), 6.92 (dd, 2H, ^3J = 6 Hz, ^4J = 2 Hz, Ar–*H*), 1.23 (s, 9H, –C(C*H*$_3$)$_3$), and 1.08 (s, 18H, –C(C*H*$_3$)$_3$) ppm. ^{13}C{^{1}H} NMR (C_6D_6, 150 HMz): δ = 158.0 (s, Ar–*C*), 157.5 (s, Ar–*C*), 154.7 (s, Ar–*C*), 152.6 (s, Ar–*C*), 128.3 (s, Ar–*C*), 124.7 (s, Ar–*C*), 118.7 (s, Ar–*C*), 117.1 (s, Ar–*C*), 36.3 (s, –*C*(CH$_3$)$_3$), 35.1 (s, –*C*(CH$_3$)$_3$), 30.0 (s, –C(*C*H$_3$)$_3$), and 29.5 (s, –C(*C*H$_3$)$_3$) ppm. Anal. Calcd. for $C_{27}H_{35}ClN_3Rh$ (539.95 g/mol): C: 60.06%; H: 6.53%; N: 7.78%, Found; C: 59.97%; H: 6.61%; N: 7.83%.

Synthesis of [(NO$_2$)$_3$terpy]RhCl (2). 4,4',4"-trinitro-2,2':6',2"-terpyridine (0.237 g, 0.644 mmol) and $\{Rh(\mu\text{–}Cl)(COE)_2\}_2$ (0.230 g, 0.321 mmol) were combined in THF (30 mL) and stirred overnight. The solvent was reduced in vacuo to 5 mL, and then pentane (15 mL) was added. The dark precipitate was collected by filtration and then washed with C_6H_6 (2 x 5 mL), THF (2 x 5 mL), and pentane (5 mL). The fine black powder was dried in vacuo for several hours to afford the complex **2** (0.334 g, yield = 98%). A suitable ^{1}H NMR spectrum could not be obtained due to poor solubility in standard NMR solvents. Anal. Calcd. for $C_{15}H_8ClN_6O_6Rh$ (506.62 g/mol): C: 35.56%; H: 1.59%; N: 16.59%, Found; C: 35.49%; H: 1.67%; N: 16.40%.

Synthesis of [^{t}Bu$_3$terpy]RhMe(Cl)(I) (3). Iodomethane (27 μL, 0.432 mmol) was added to a THF solution (10 mL) containing complex **1** (0.231 g, 0.428 mmol). Immediately after the addition, the dark blue solution turned a yellow-orange color. The reaction was allowed to stir for 2 hours and then was filtered through Celite. The filtrate was reduced to low volume in vacuo, and hexanes were added. The yellow-orange solid was collected on a fine porosity frit and rinsed with hexanes (2 x 5 mL) (0.115 g, 40% yield). ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 9.33 (d, 2H, ^3J = 6 Hz, Ar–*H*), 7.97 (m, 4H, Ar–*H*), 7.55 (dd, 2H, ^3J = 6 Hz, ^4J = 2 Hz, Ar–*H*), 1.55 (s, 9H, –C(C*H*$_3$)$_3$), 1.45 (s, 18H, –C(C*H*$_3$)$_3$), and 1.13 (d, 3H, $^2J_{Rh–H}$ = 2 Hz, Rh–C*H*$_3$) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ = 162.7 (s, Ar–*C*), 161.9 (s, Ar–*C*), 156.6 (s, Ar–*C*), 155.3 (s, Ar–*C*), 153.4 (s, Ar–*C*), 124.8 (s, Ar–*C*), 120.0 (s, Ar–*C*), 119.1 (s, Ar–*C*), 36.3

(s, –*C*(CH_3)$_3$), 35.7 (s, –*C*(CH_3)$_3$), 31.0 (s, –C(*C*H_3)$_3$), 30.7 (s, –C(*C*H_3)$_3$), and 15.8 (d, $^1J_{Rh–C}$ = 22 Hz, Rh–$^{13}CH_3$) ppm. Anal. Calcd. for $C_{28}H_{38}ClN_3IRh$: C: 49.32%; H: 5.56%; N: 6.16%, Found; C: 49.29%; H: 5.66%; N: 6.09%.

Synthesis of [^{t}Bu$_3$terpy]RhMe(Cl)$_2$ (4). In a Schlenk flask, complex **1** (0.143 g, 0.265 mmol) was dissolved in 10 mL of THF. Chloromethane was bubbled through the solution for 30 min during which time the solution changed from dark blue to yellow-orange. The volatiles were reduced in vacuo to ~1 mL. The addition of hexanes resulted in the formation of a yellow-orange precipitate. The solid was collected by filtration and washed with hexanes (3 x 2 mL) (0.120 g, 77% yield). ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 9.29 (d, 2H, ^3J = 6Hz, Ar–*H*), 7.96 (s, 2H, Ar–*H*), 7.94 (d, 2H, ^4J = 2 Hz, Ar–*H*), 7.54 (dd, 2H, ^3J = 6 Hz, ^4J = 2 Hz, Ar–*H*), 1.53 (s, 9H, –C(C*H*$_3$)$_3$), 1.43 (s, 18H, –C(C*H*$_3$)$_3$), and 0.94 (d, 3H, $^2J_{Rh–H}$ = 2 Hz, Rh–Me) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ = 162.8 (s, Ar–*C*), 162.1 (s, Ar–*C*), 156.6 (s, Ar–*C*), 155.5 (s, Ar–*C*), 153.1 (s, Ar–*C*), 124.8 (s, Ar–*C*), 119.8 (s, Ar–*C*), 119.1 (s, Ar–*C*), 36.3 (s, –*C*(CH_3)$_3$), 35.7 (s, –*C*(CH_3)$_3$), 31.0 (s, –C(*C*H_3)$_3$), 30.7 (s, –C(*C*H_3)$_3$), and 5.30 (d, $^1J_{Rh–C}$ = 22 Hz, Rh–$^{13}CH_3$) ppm. Anal. Calcd. for $C_{28}H_{38}Cl_2N_3Rh$ (590.44 g/mol): C: 56.96%; H: 6.49%; N: 7.12%, Found; C: 56.91%; H: 6.41%; N: 7.14%.

Synthesis of [^{t}Bu$_3$terpy]RhMe(Cl)(TFA) (5). A pressure tube containing a THF solution (30 mL) of complex **1** (0.125 g, 0.232 mmol) with MeTFA (0.1 mL, 0.99 mmol, ~4 equiv) was heated at 70 °C for 35 min with vigorous stirring. The solution color turned from blue to deep-yellow color, and a small amount of precipitate formed (anion exchange products). The reaction solution was allowed to cool, and then the precipitate was removed by filtration. Adding hexanes (40 mL) to the filtrate precipitates complex **5** as a pale green powder. The solid was collected by filtration, washed with hexanes (3 x 5 mL), and dried in vacuo (0.063 g, 41%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 9.20 (s, 2H, Ar–*H*), 7.96 (m, 4H, Ar–*H*), 7.53 (d, 2H, ^3J = 6 Hz, Ar–*H*), 1.54 (s, 9H, –C(C*H*$_3$)$_3$), 1.43 (s, 18H, –C(C*H*$_3$)$_3$), and 0.82 (s, 3H, Rh–CH_3) ppm. ^{19}F{^{1}H} NMR ($CDCl_3$, 282 MHz): δ = 75.4 (s, 3F, –C*F*$_3$) ppm ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ = 162-163 (br, Ar–*C*), 156-158 (br, Ar–*C*), 152.9 (s, Ar–*C*), 124.7 (s, Ar–*C*), 119.7 (br, Ar–*C*), 119.1 (s, Ar–*C*), 36.4 (s, –*C*(CH_3)$_3$), 35.8 (s, –*C*(CH_3)$_3$), 31.0 (s, –C(*C*H_3)$_3$), 30.7 (s, –C(*C*H_3)$_3$), and 0.5-1.0 (br, Rh–*C*H_3) ppm. Anal. Calcd. for $C_{30}H_{38}ClF_3N_3O_2Rh$ (668.00 g/mol): C: 53.94%; H: 5.73%; N: 6.29%, Found; C: 53.84%; H: 5.68%; N: 6.21%.

Synthesis of [(NO$_2$)$_3$terpy]RhMe(Cl)(I) (6). A pressure tube containing a suspension of complex **2** (0.343 g, 0.678 mmol) in THF (30 mL) with MeI (0.5 mL, 8.03 mmol, ~10 equiv) was heated at 70 °C for 45 min with vigorous stirring. During this time, the colorless solution turned deep brown. The pressure flask was allowed to cool to room temperature. The reaction mixture was filtered, and the filtrate was reduced in vacuo to yield a brown oil. The oil was dissolved in a minimal amount of THF, and diethyl ether was added slowly with stirring to precipitate complex **6** as a brown powder (0.289 g, 65%). ^{1}H NMR (*d*$_8$-THF, 500 MHz): δ = 9.77 (d, 2H, ^3J = 6 Hz, Ar–H), 9.69 (s, 2H, Ar–H), 9.56 (d, 2H, ^4J = 2.8 Hz, Ar–H), 8.55 (dd, 2H, ^3J = 6 Hz, ^4J = 2 Hz, Ar–H), and 1.05 (d, 3H, Rh–CH_3, $^2J_{Rh–H}$ = 2 Hz) ppm. ^{13}C{^{1}H} NMR (*d*$_8$-THF, 126 MHz): δ = 159.2 (s, Ar–*C*), 156.9 (s, Ar–*C*), 156.8 (s, Ar–*C*), 156.2 (s, Ar–*C*), 155.9 (s, Ar–*C*), 122.1 (s, Ar–*C*), 119.7 (s, Ar–*C*), 119.6 (s, Ar–*C*), and 17.1 (d, $^1J_{Rh–C}$ = 20 Hz, Rh–CH_3) ppm. Anal. Calcd. for $C_{16}H_{11}ClN_6IO_6Rh$ (648.56 g/mol): C: 29.63%; H: 1.71%; N: 12.96%, Found; C: 29.64%; H: 1.67%; N: 12.87%.

Synthesis of [^{t}Bu$_3$terpy]RhI (7). Complex **1** (0.192 g, 0.356 mmol) was dissolved in 5 mL of THF, and NaI was added (0.218 g, 1.45 mmol). After stirring for 12 h, the volatiles were removed in vacuo. The dark blue residue was reconstituted in 15 mL of benzene and filtered. The filtrate was reduced to ~5 mL,

then hexanes (20 mL) were added to precipitate a dark blue solid (0.080 g, 40%). ^{1}H NMR (C_6D_6, 500 MHz): δ = 10.36 (d, 2H, ^{3}J = 6Hz, Ar–*H*), 7.52 (d, 2H, ^{4}J = 2 Hz, Ar–*H*), 7.40 (s, 2H, Ar–*H*), 6.77 (dd, 2H, ^{3}J = 6 Hz, ^{4}J = 2 Hz, Ar–*H*), 1.16 (s, 9H, –C(CH_3)$_3$), and 1.04 (s, 18H, –C(CH_3)$_3$) ppm. ^{13}C{^{1}H} NMR (C_6D_6, 126 HMz): δ = 157.8 (s, Ar–*C*), 157.5 (s, Ar–*C*), 157.2 (s, Ar–*C*), 154.3 (s, Ar–*C*), 149.4 (s, Ar–*C*), 124.8 (s, Ar–*C*), 118.0 (s, Ar–*C*), 117.3 (s, Ar–*C*), 36.4 (s, –*C*(CH$_3$)$_3$), 35.1 (s, –*C*(CH$_3$)$_3$), 30.0 (s, –C(*C*H$_3$)$_3$), and 29.4 (s, –C(*C*H$_3$)$_3$) ppm. Anal. Calcd. for $C_{27}H_{35}IN_3Rh$ (631.41 g/mol): C, 51.36; H, 5.59; N, 6.66. Found: C, 51.31; H, 5.67; N, 6.57.

Synthesis of [^{t}Bu$_3$terpy]RhMe(I)$_2$ (8). Complex **7** (0.0348 g, 0.0567 mmol) was dissolved in 5 mL of THF and MeI (4 μL, 0.0641 mmol) was added. The solution color changed immediately from blue to yellow-orange. After 2 h, the volatiles were taken to low volume in vacuo, and hexanes (20 mL) were added. The yellow-orange solid was filtered through a fine porosity frit and washed with hexanes (3 x 2 mL) (0.035 g, 80%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 9.78 (d, 2H, ^{3}J = 6Hz, Ar–*H*), 7.98 (s, 2H, Ar–*H*), 7.97 (d, 2H, ^{4}J = 2 Hz, Ar–*H*), 7.46 (dd, 2H, ^{3}J = 6 Hz, ^{4}J = 2 Hz, Ar–*H*), 1.55 (s, 9H, –C(CH_3)$_3$), 1.44 (s, 18H, –C(CH_3)$_3$), and 1.31 (d, 3H, $^{2}J_{Rh–H}$ = 2 Hz, Rh−CH$_3$) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$, 126 HMz): δ = 162.4 (s, Ar–*C*), 162.1 (s, Ar–*C*), 157.5 (s, Ar–*C*), 156.2 (s, Ar–*C*), 155.0 (s, Ar–*C*), 125.3 (s, Ar–*C*), 120.2 (s, Ar–*C*), 119.4 (s, Ar–*C*), 36.4 (s, –*C*(CH$_3$)$_3$), 35.7 (s, –*C*(CH$_3$)$_3$), 31.0 (s, –C(*C*H$_3$)$_3$), 30.7 (s, –C(*C*H$_3$)$_3$), and 13.1 (d, $^{1}J_{Rh–C}$ = 21 Hz, Rh−CH$_3$) ppm. Anal. Calcd. for $C_{28}H_{38}I_2N_3Rh$ (773.35 g/mol): C, 43.49; H, 4.95; N, 5.43. Found: C, 43.39; H, 4.86; N, 5.26.

Solution Calormetric Experiments. In the glove box, a stock solution was prepared from 1.4164 g of CH_3I and 20 mL THF that had been freshly distilled from Na/benzophenone under argon. Two mL of the CH_3I/THF solution (1 mmol CH_3I) was transferred to the inner chamber of the Calvet mixing cell of the Setaram C-80 Calvet calorimeter and capped. To the outer chamber was added 2 mL of a THF solution containing 34.8 mg of complex **7** (0.055 mmol). Following equilibration, the reaction was initiated by rotating the calorimeter. Following return to baseline the thermogram was integrated and gave a value of -24.3 kcal/mol. The Calvet cell was taken into the glove box, the THF solvent evaporated to dryness and the solid residue dissolved in C_6D_6. An NMR spectrum confirmed quantitative addition of CH_3I, and no starting material was present in the spectrum. The value of –23.5 ± 0.8 kcal/mol is the average of three independent runs.

Computational Methods. The thermodynamics and kinetics of oxidative addition by substituted terpyridine ligated rhodium complexes was studied using DFT. All optimization and frequency calculations were performed by the Gaussian 09 software package.[4] Ground and transition states were determined by whether 0 or 1 imaginary frequency was observed in the energy Hessian. Optimization and frequency calculations were performed with implicit solvation using the CPCM[5,6] method as employed by Gaussian 09. To most closely model experimental conditions, for the thermodynamics of oxidative addition THF (ε = 7.4257) was used as solvent and for the kinetic studies of RE nitromethane (ε = 36.562) was used as solvent. The systems were modeled by the B3LYP[7,8] exchange-correlation functional with the CEP-31G(d)[9,10] basis set. Free energies are reported at STP in kcal/mol. All complexes reported were calculated as singlets.

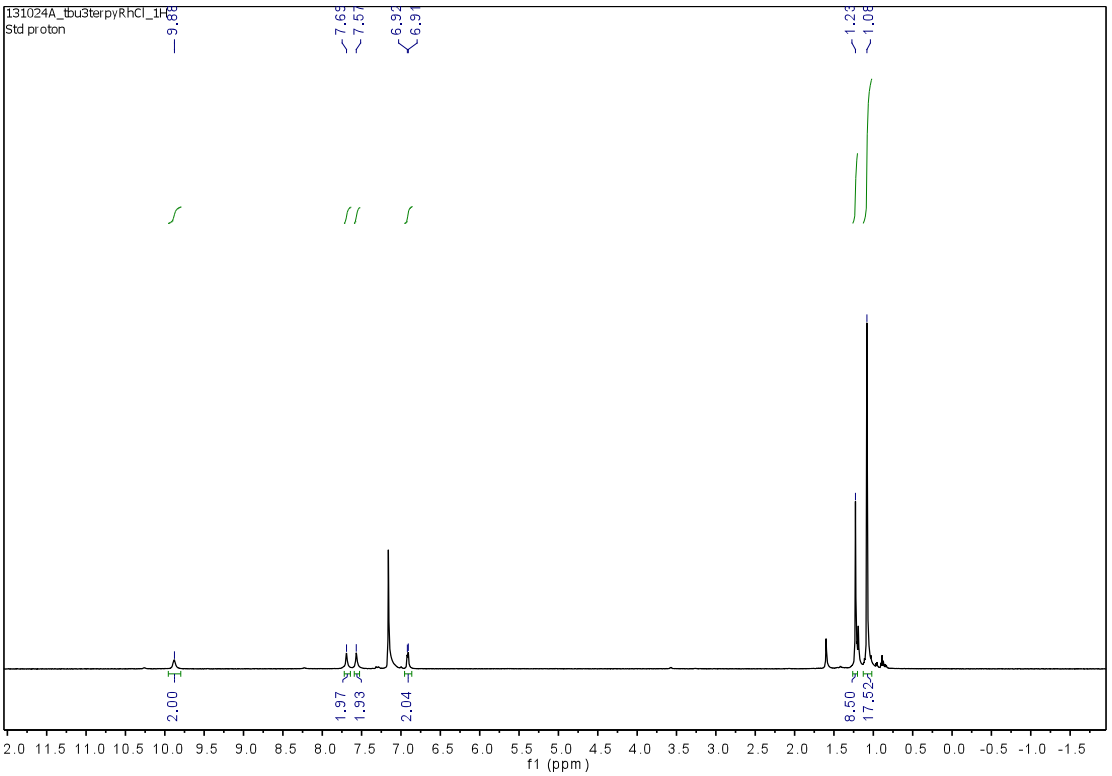

Figure S1. ^{1}H NMR (C_6D_6, 500 MHz) spectrum of **1**.

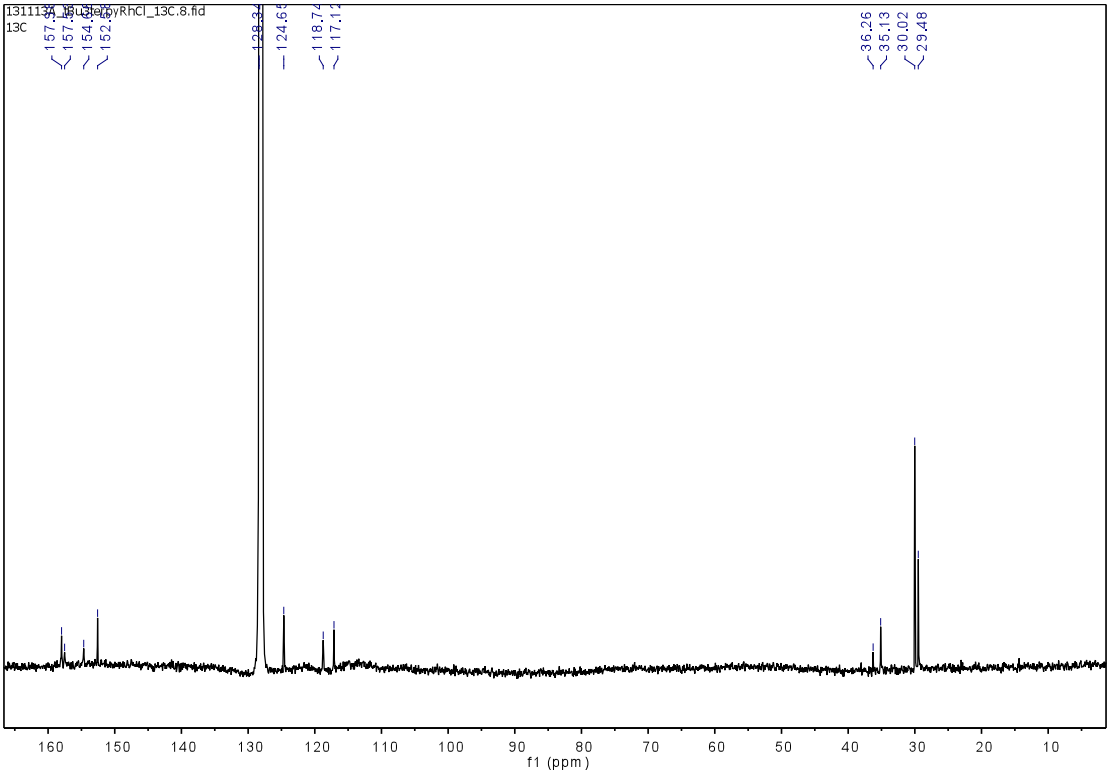

Figure S2. $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz) spectrum of **1**.

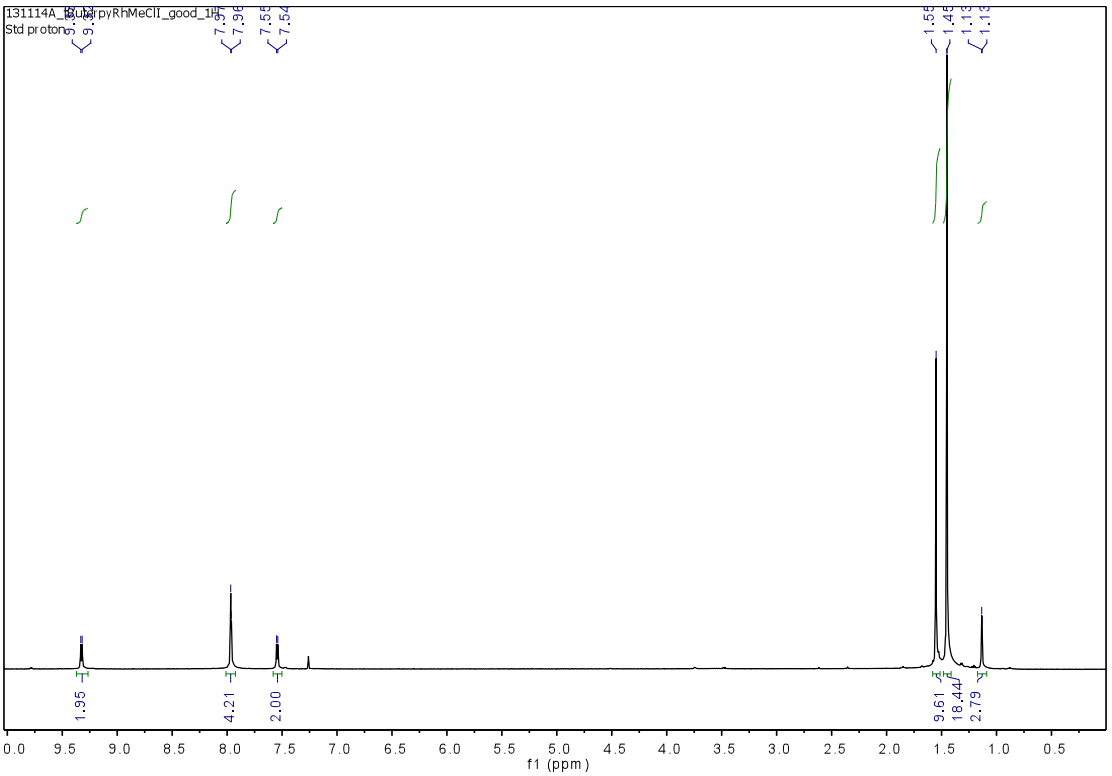

Figure S3. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **3**.

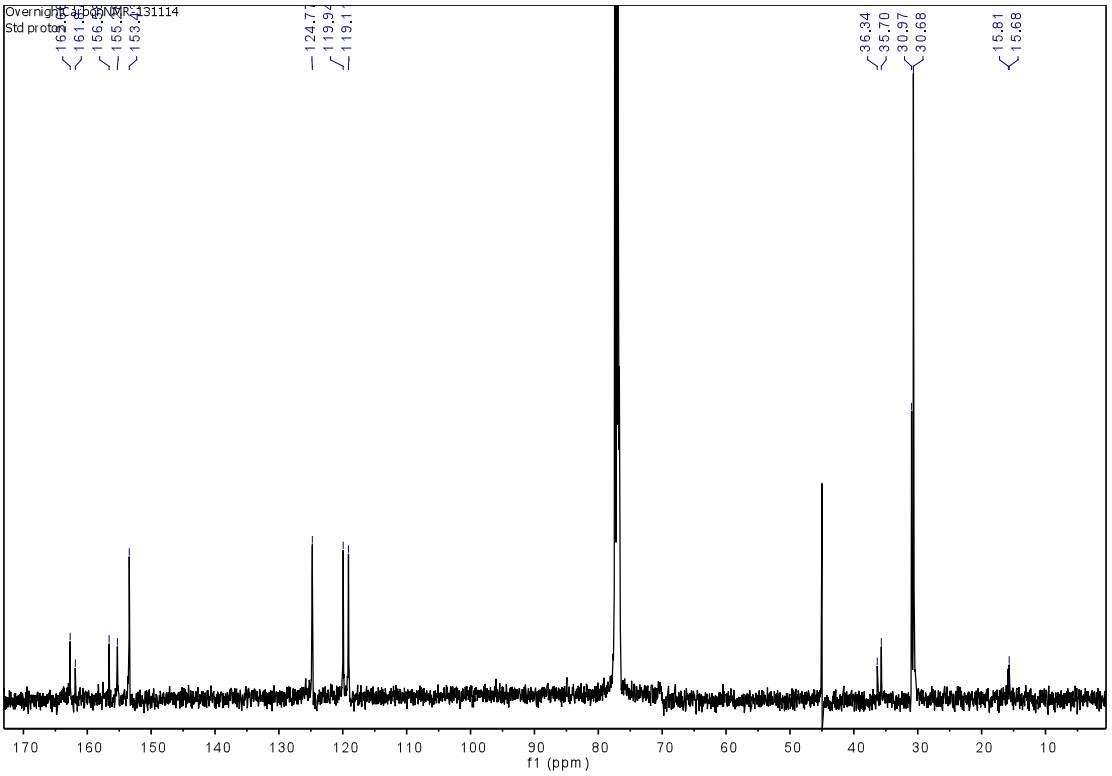

Figure S4. ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz) spectrum of **3**.

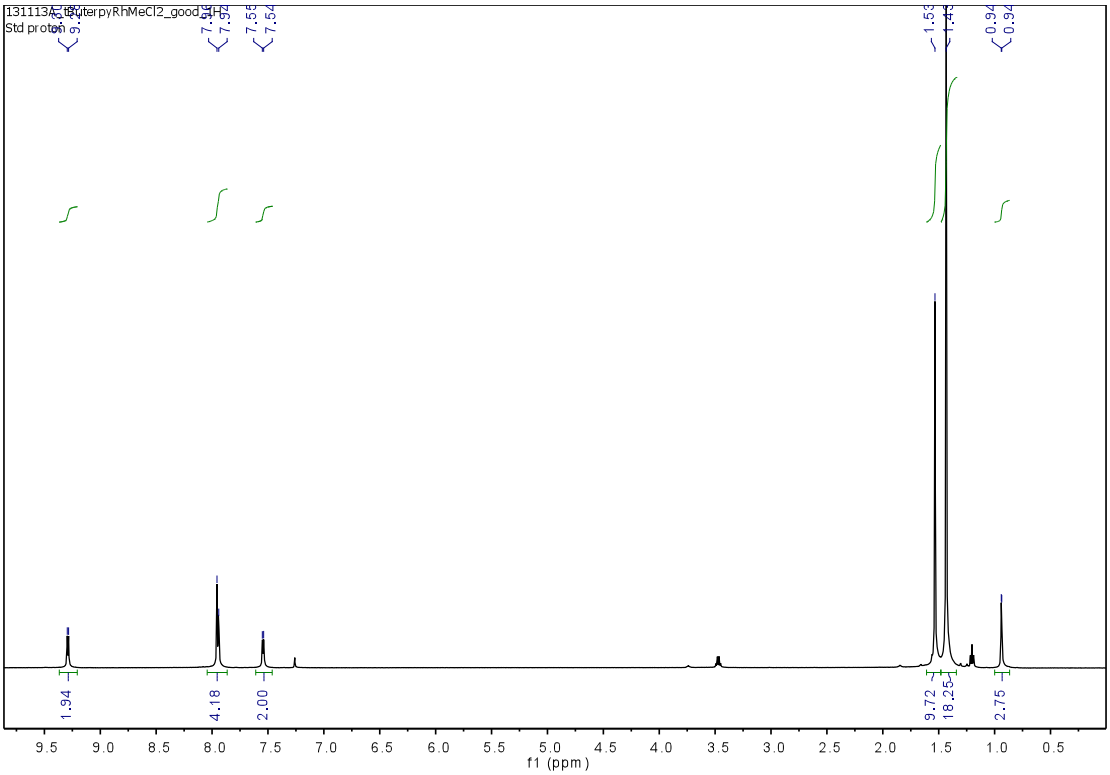

Figure S5. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **4**.

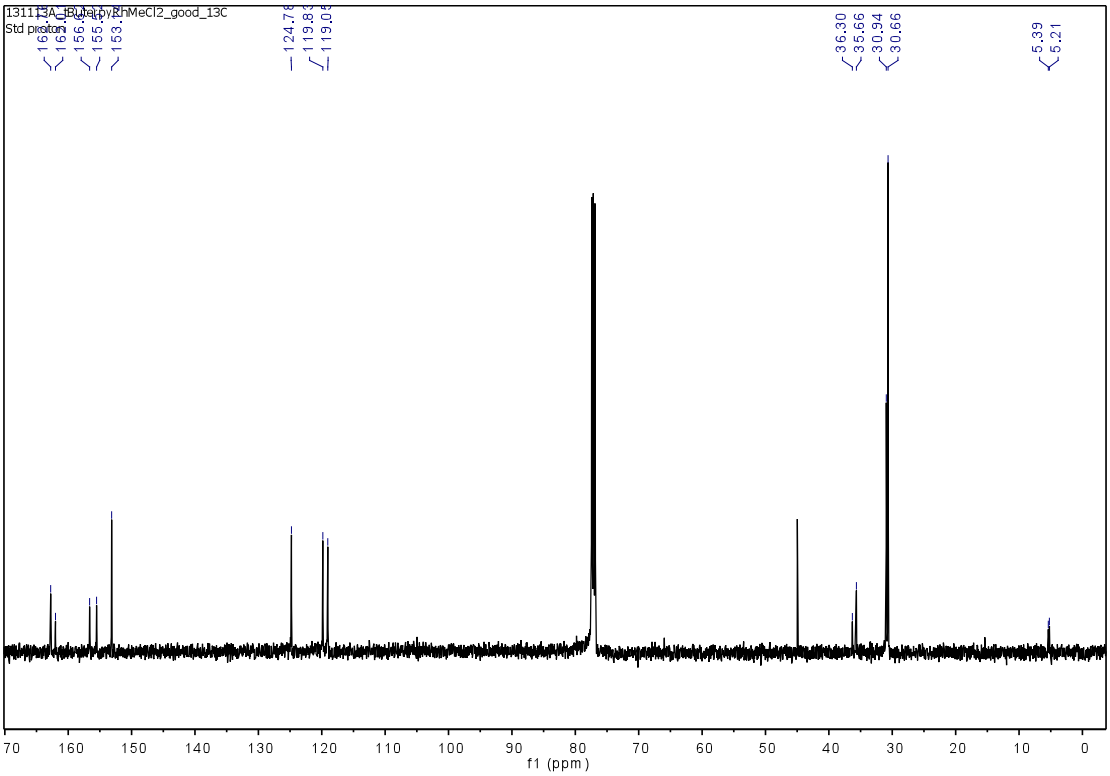

Figure S6. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz) spectrum of **4**.

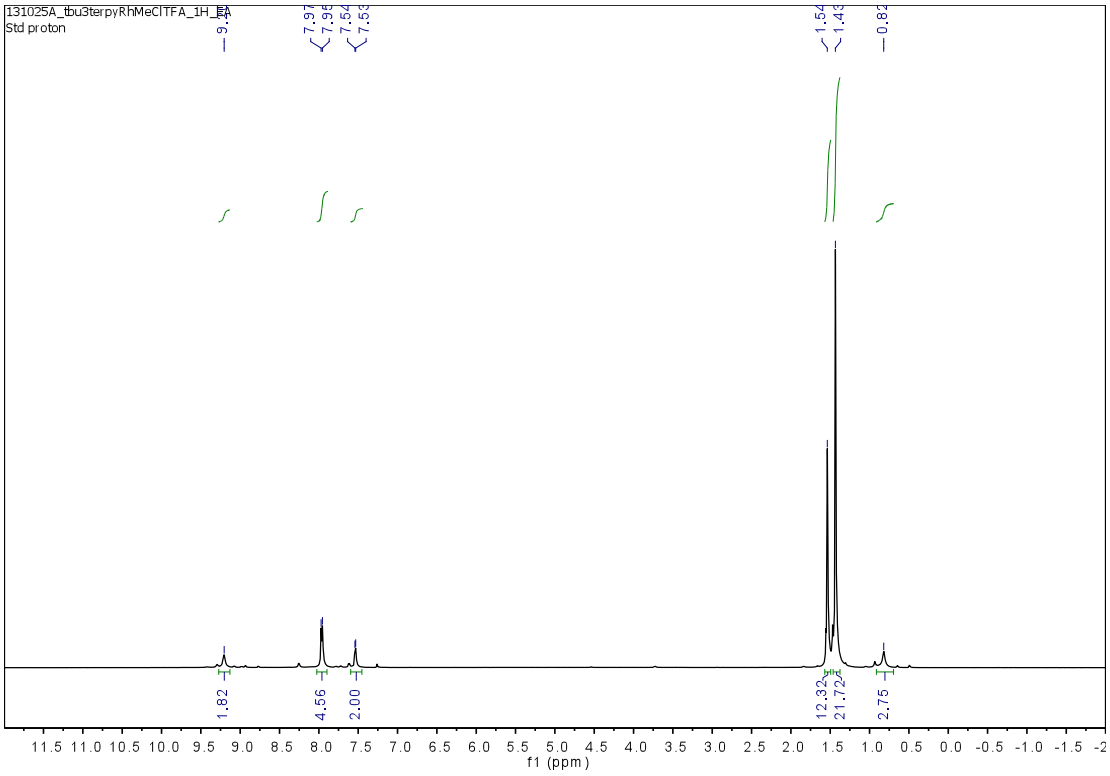

Figure S7. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **5**.

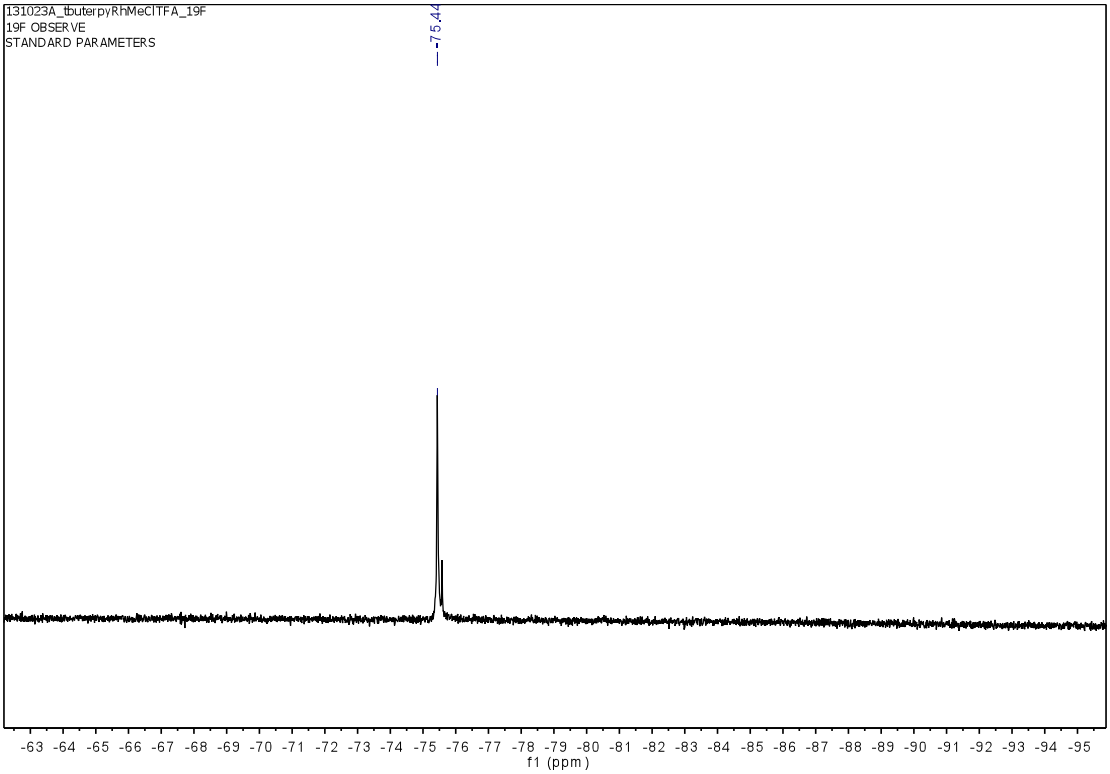

Figure S8. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 282 MHz) spectrum of **5**.

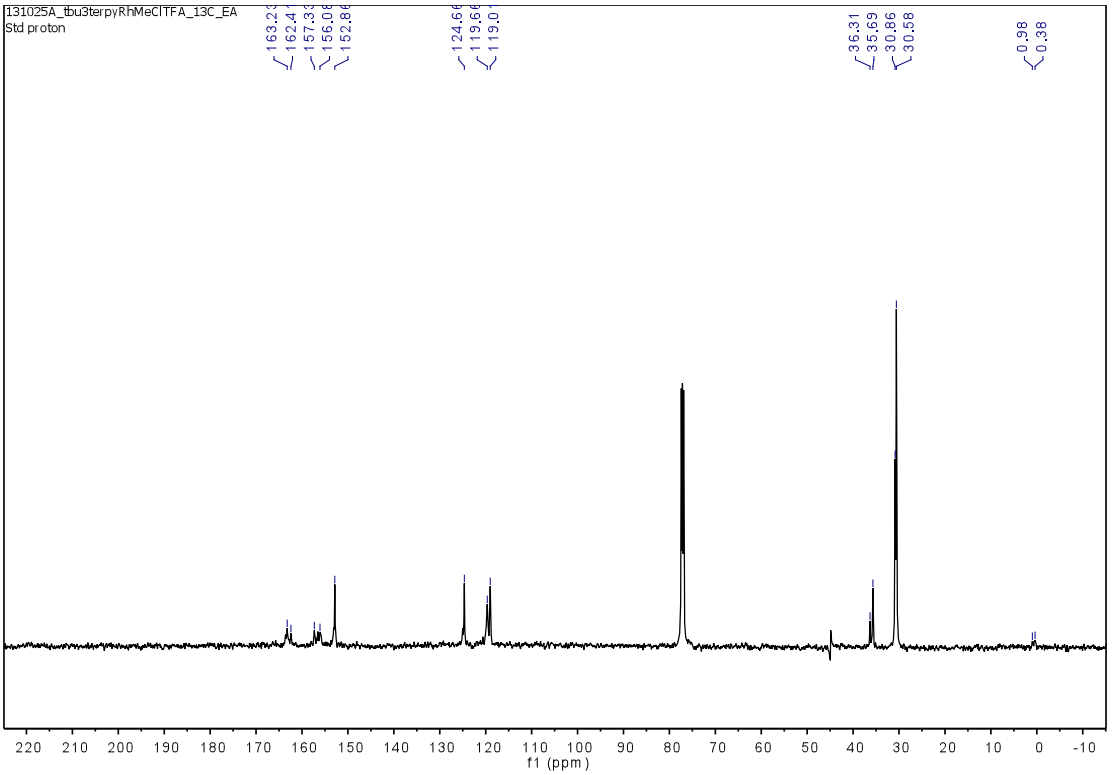

Figure S9. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz) spectrum of **5**.

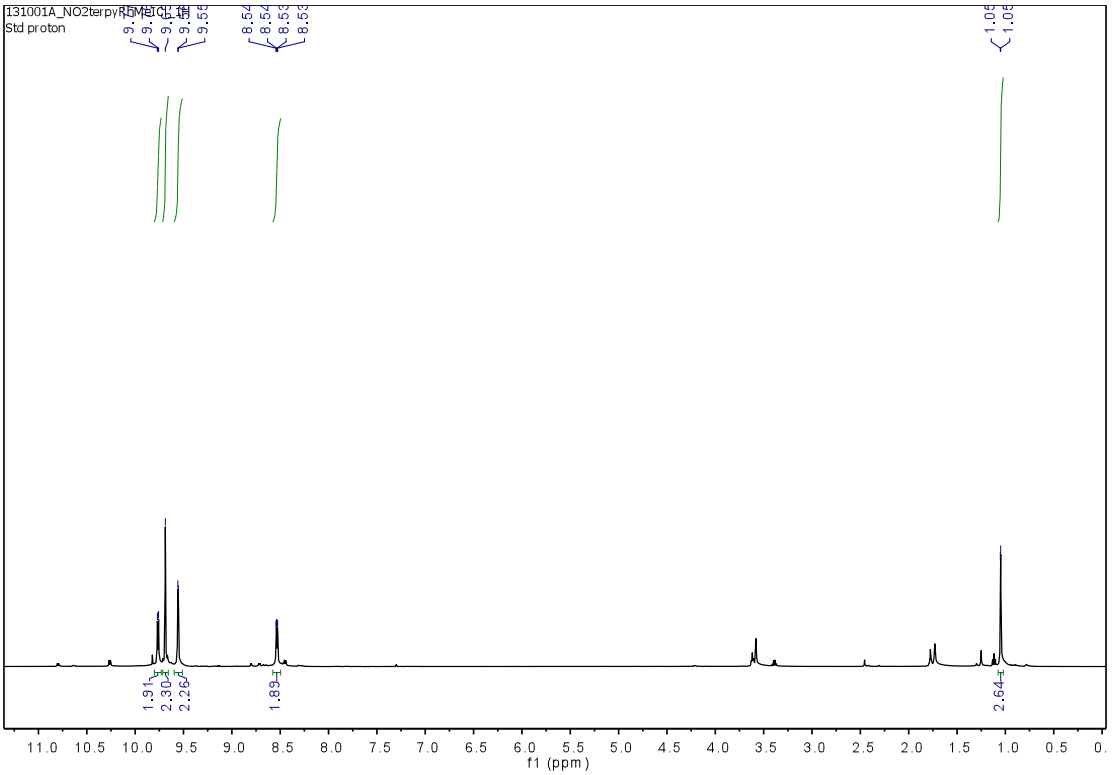

Figure S10. ^{1}H NMR (d_8-THF, 500 MHz) spectrum of **6**.

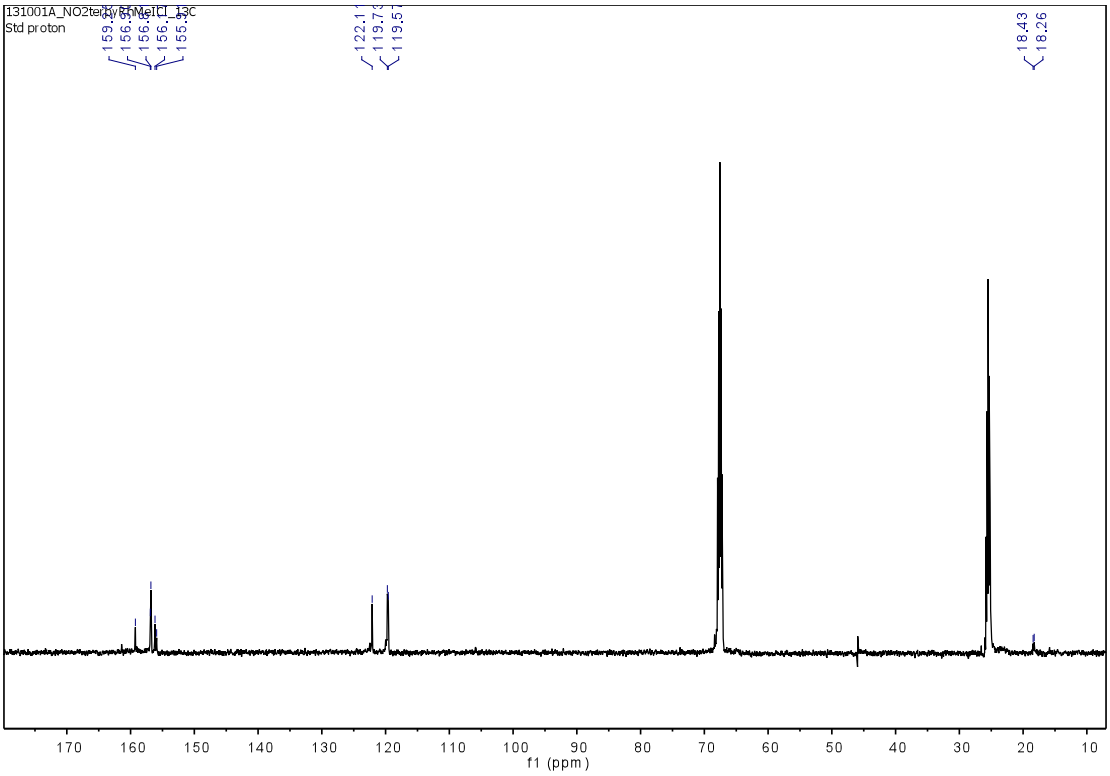

Figure S11. $^{13}C\{^{1}H\}$ NMR (d_8-THF, 126 MHz) spectrum of **6**.

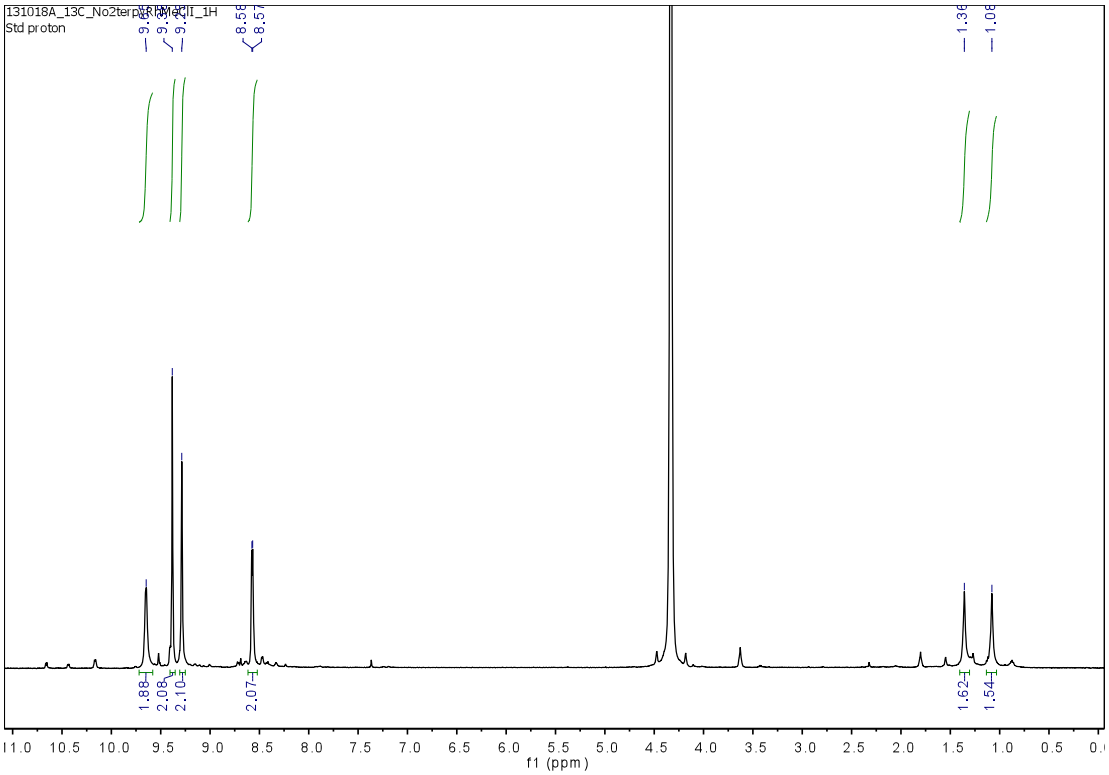

Figure S12. ^{1}H NMR (CD_3NO_2, 500 MHz) spectrum of **6***.

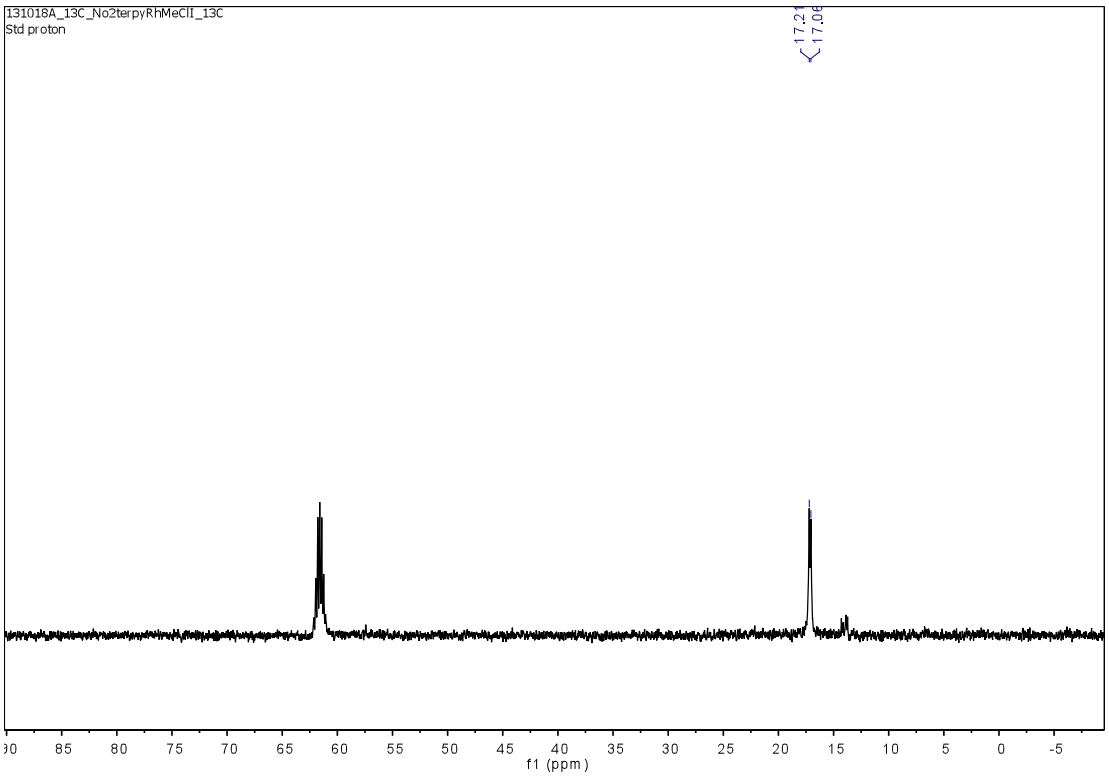

Figure S13. $^{13}C\{^{1}H\}$ NMR (CD_3NO_2, 126 MHz) spectrum of **6***.

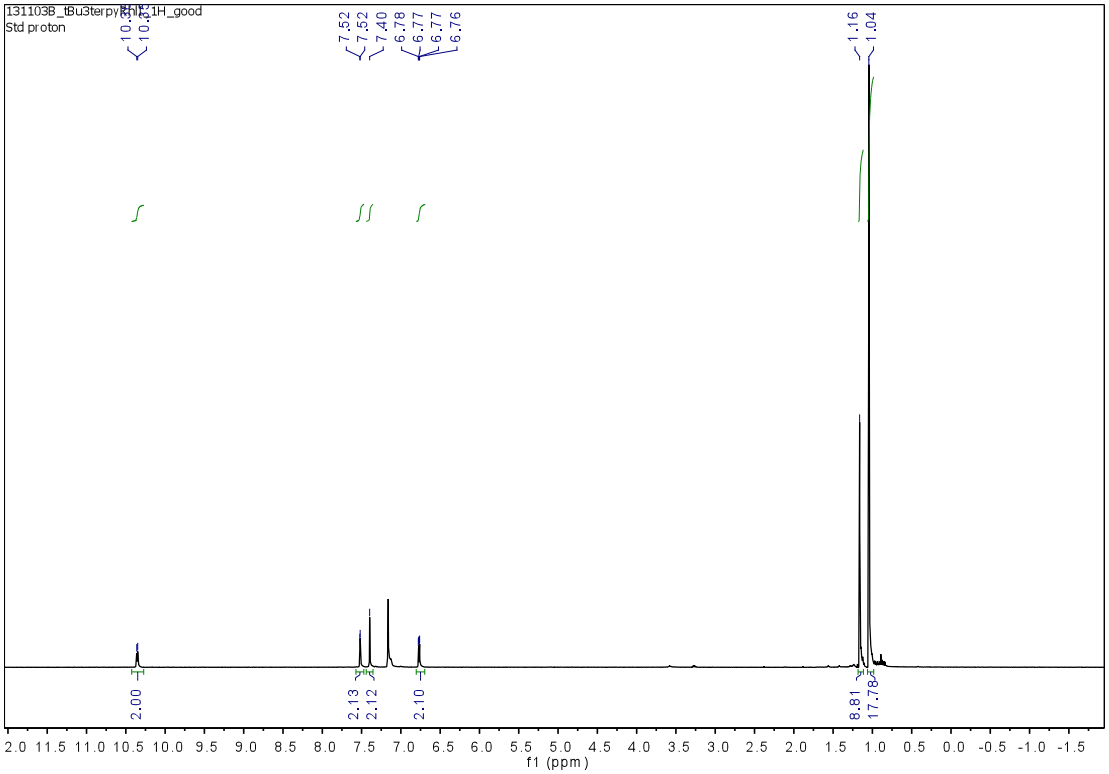

Figure S14. ^{1}H NMR (C_6D_6, 500 MHz) spectrum of **7**.

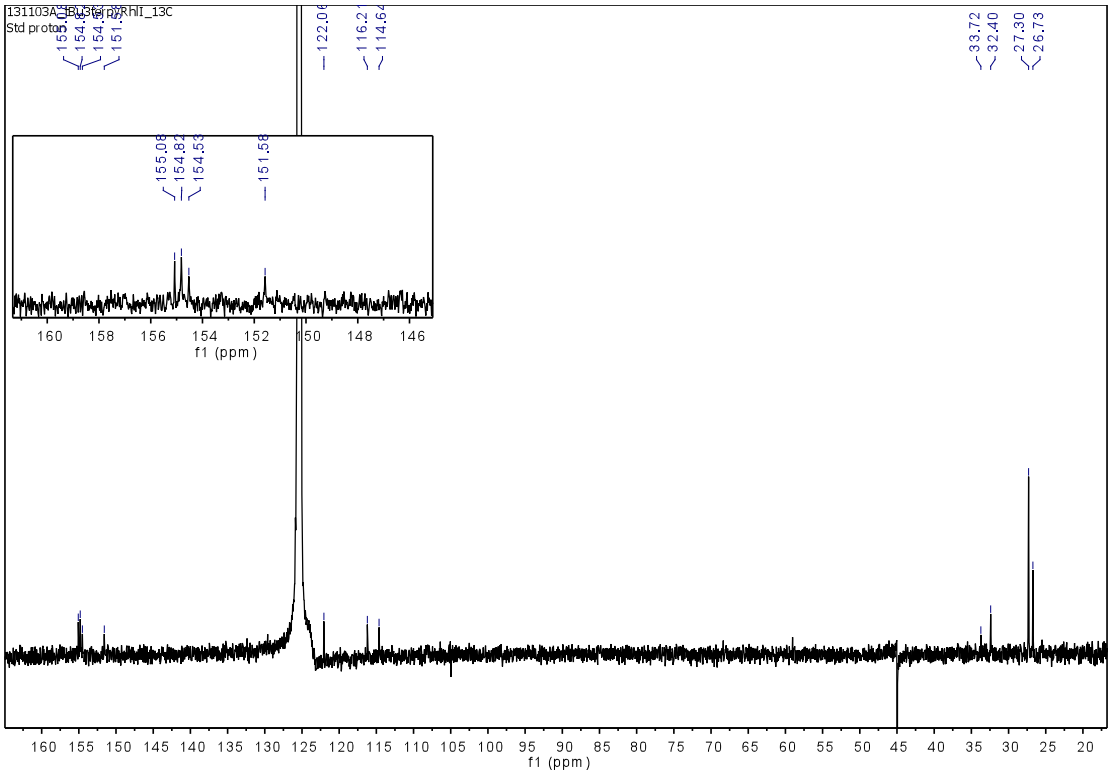

Figure S15. $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz) spectrum of **7**.

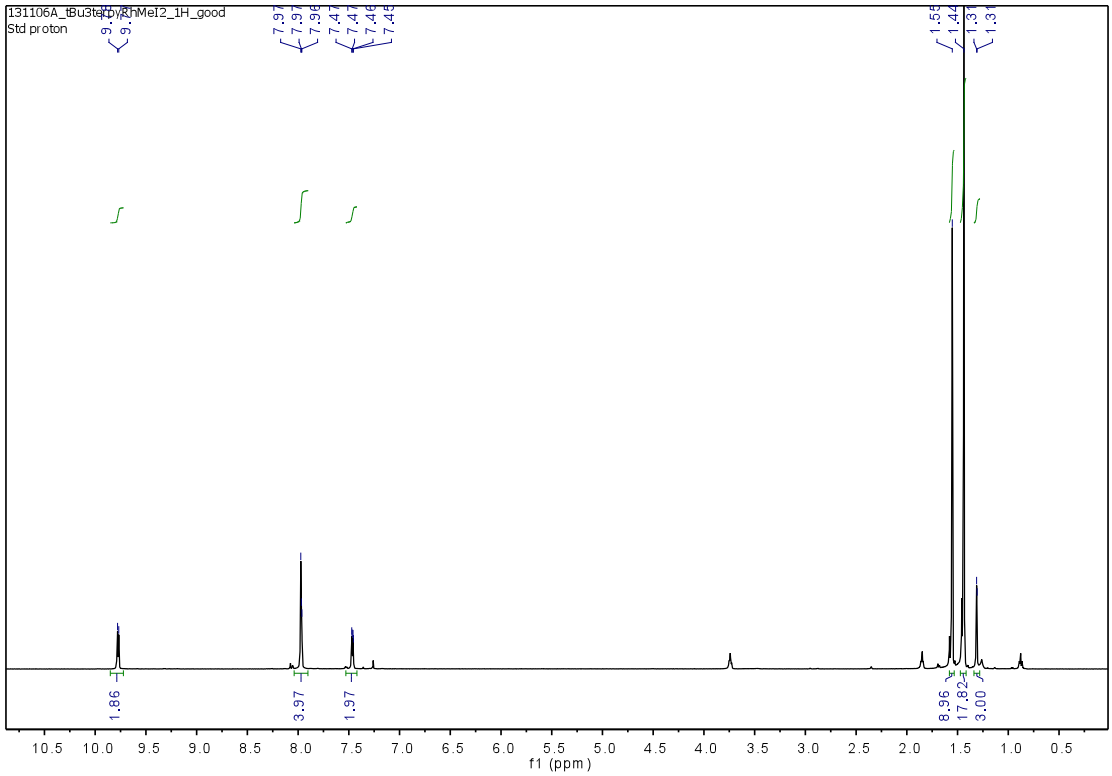

Figure S16. ^{1}H NMR (C_6D_6, 500 MHz) spectrum of **8**.

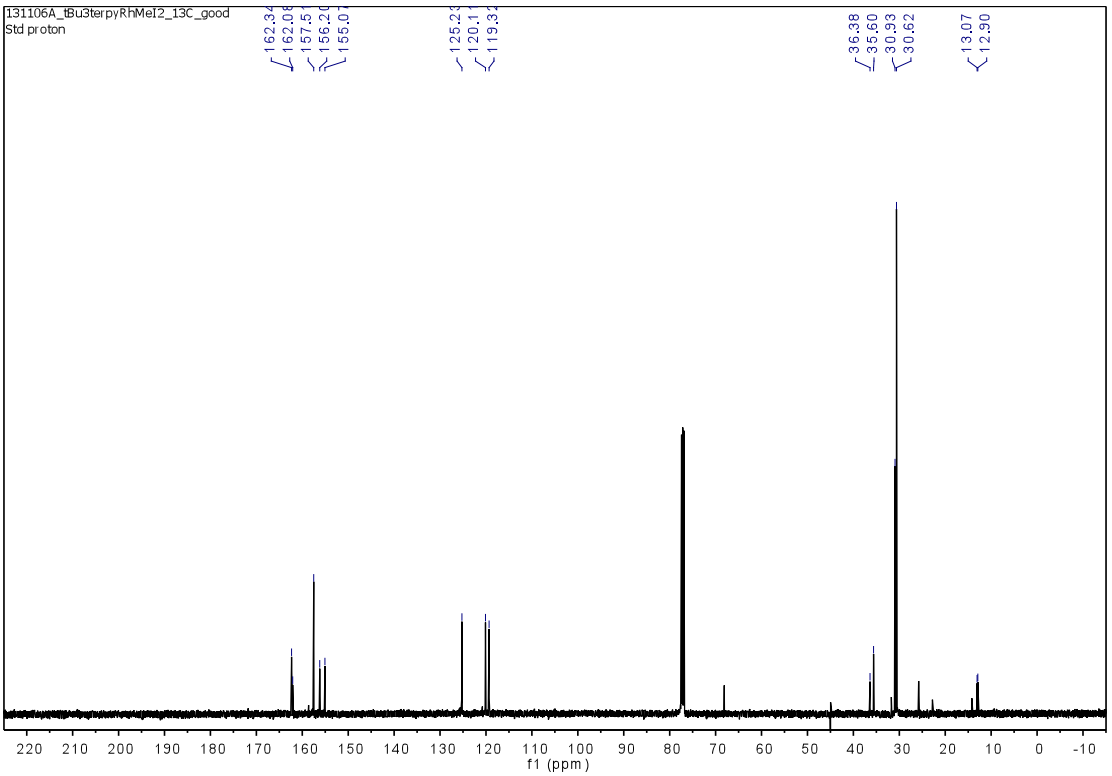

Figure S17. $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz) spectrum of **8**.

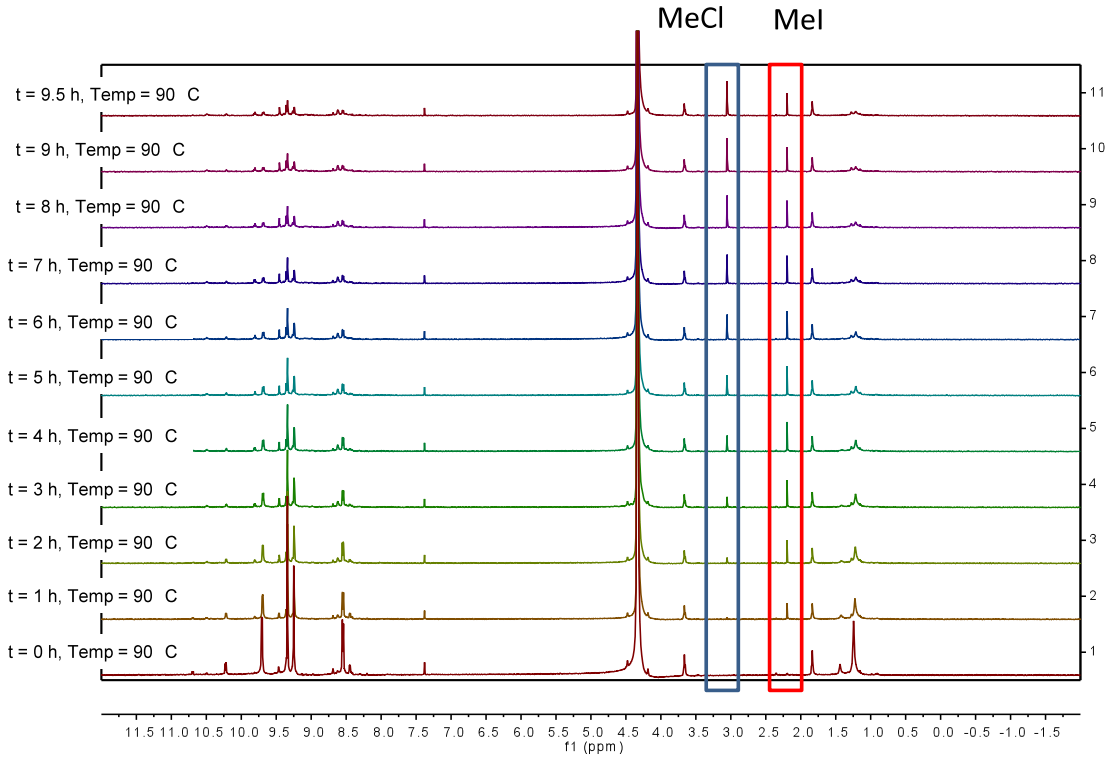

Figure S18. Reductive functionalization of complex **6** upon heating at 90 ºC in CD_3NO_2 (0.5 mL).

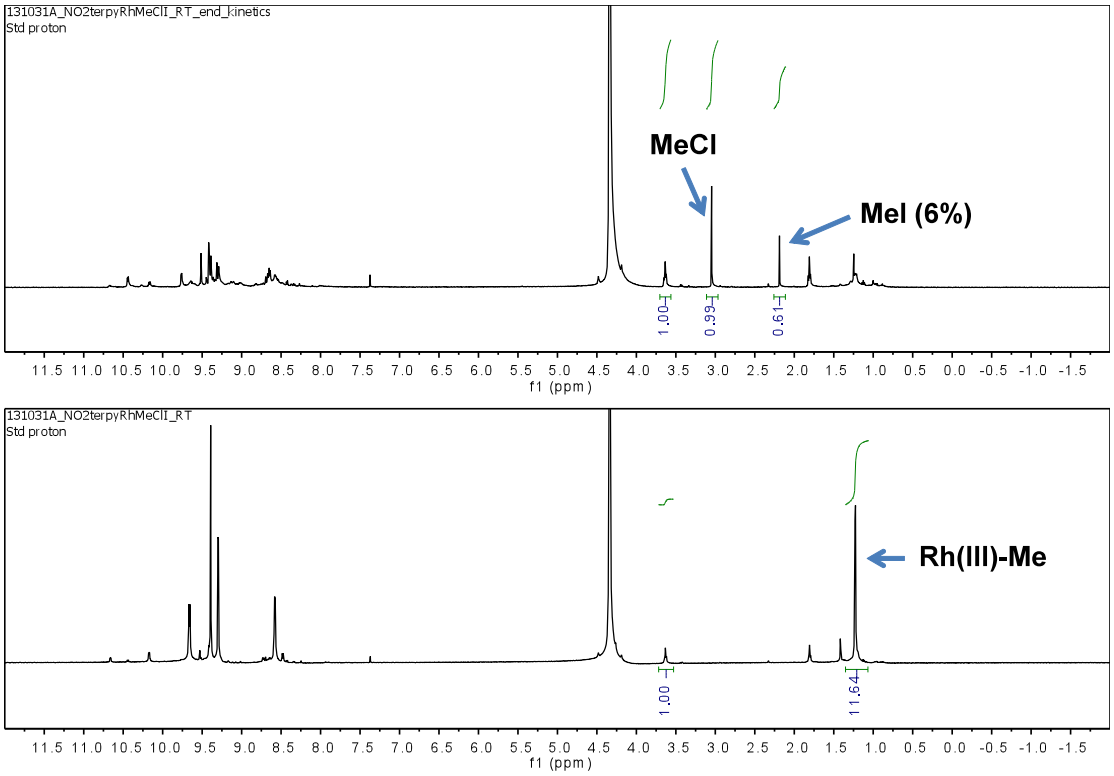

Figure S19. Reductive functionalization of complex **6** before (bottom) and after heating at 90 ºC (top) in CD_3NO_2 (0.5 mL).

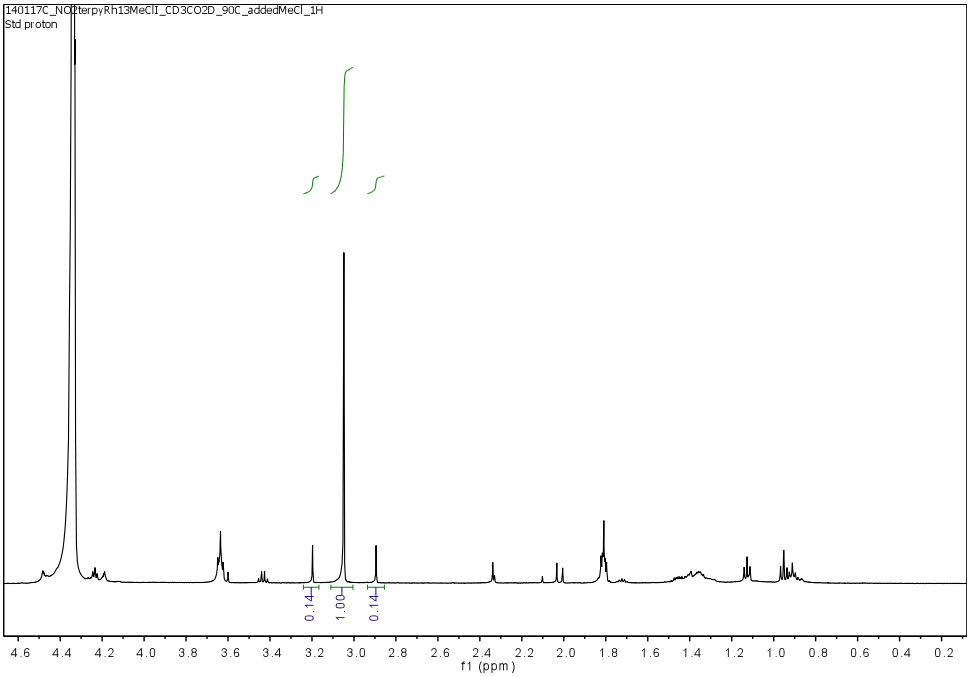

Figure S20. Reductive functionalization of complex **6*** after heating at 90 ºC in CD_3NO_2 and one equivalent of MeCl.

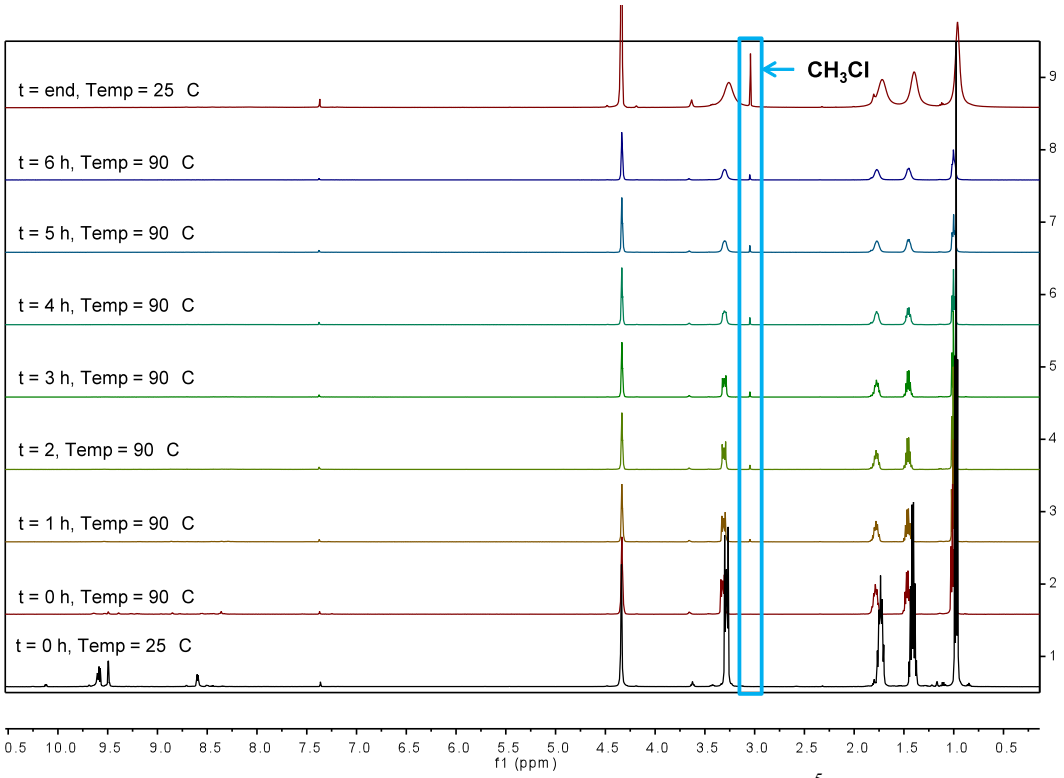

Figure S21. Reductive functionalization of complex **6** (0.0185 g, 2.71 x10^{-5} mol) with Bu_4NCl (0.023 g, 8.3 x10^{-5} mol) in CD_3NO_2 (0.5 mL).

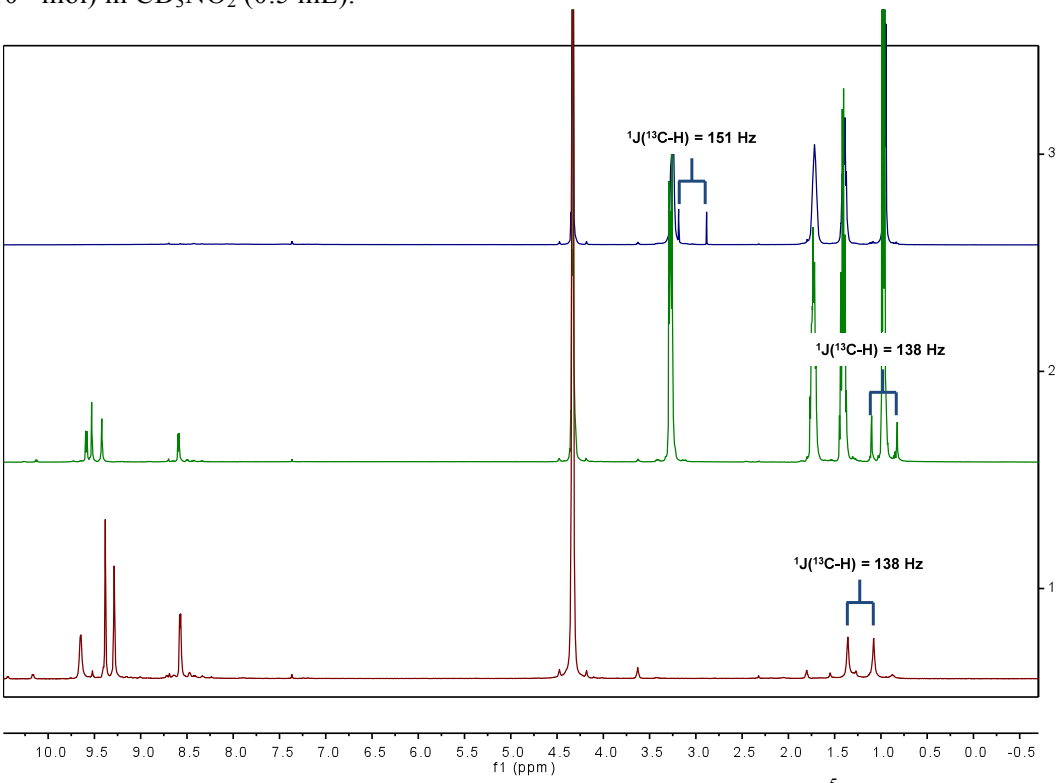

Figure S22. Reductive functionalization of complex **6*** (0.0116 g, 1.70 x10^{-5} mol) with Bu_4NCl (0.018 g, 6.5 x10^{-5} mol) in CD_3NO_2 (0.5 mL). ^1H NMR Spectra (1) **6*** (2) **6*** and Bu_4NCl and (3) **6*** and Bu_4NCl after heating at 90° C overnight.

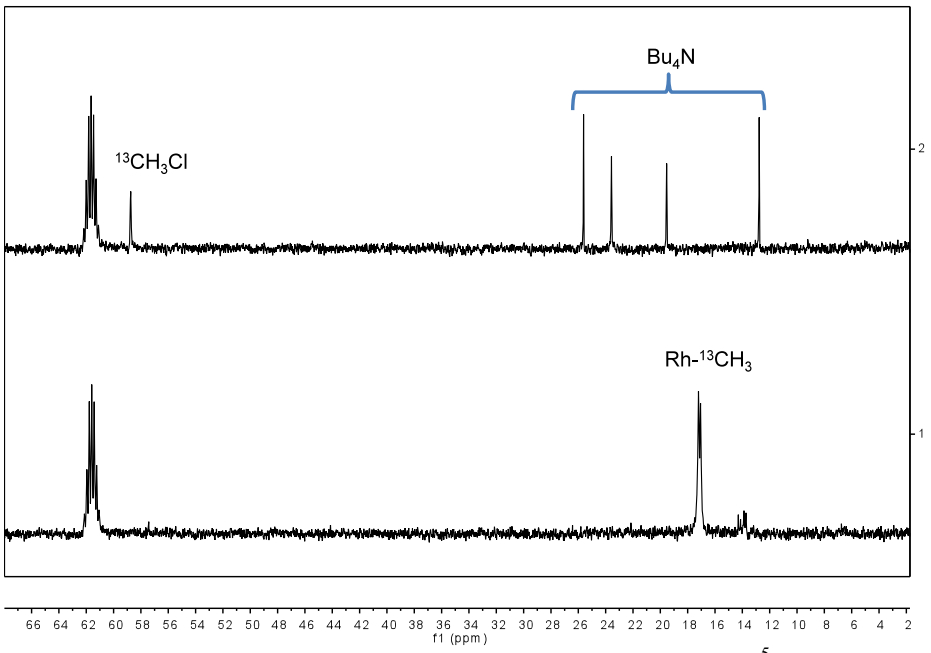

Figure S23. Reductive functionalization of complex **6*** (0.0116 g, 1.70 x10^{-5} mol) with Bu_4NCl (0.018 g, 6.5 x10^{-5} mol) in CD_3NO_2 (0.5 mL). $^{13}C\{^1H\}$ NMR Spectra (1) **6*** and (2) **6*** and Bu_4NCl after heating at 90° C overnight.

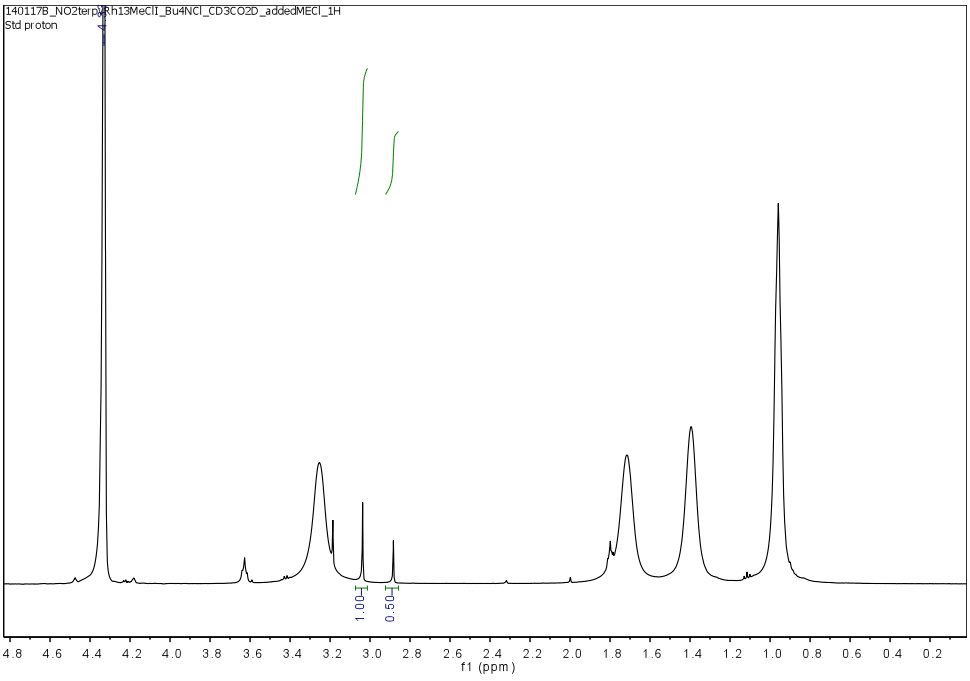

Figure S24. Reductive functionalization of complex **6*** with Bu_4NCl in CD_3NO_2 (0.5 mL) and one equivalent of MeCl added.

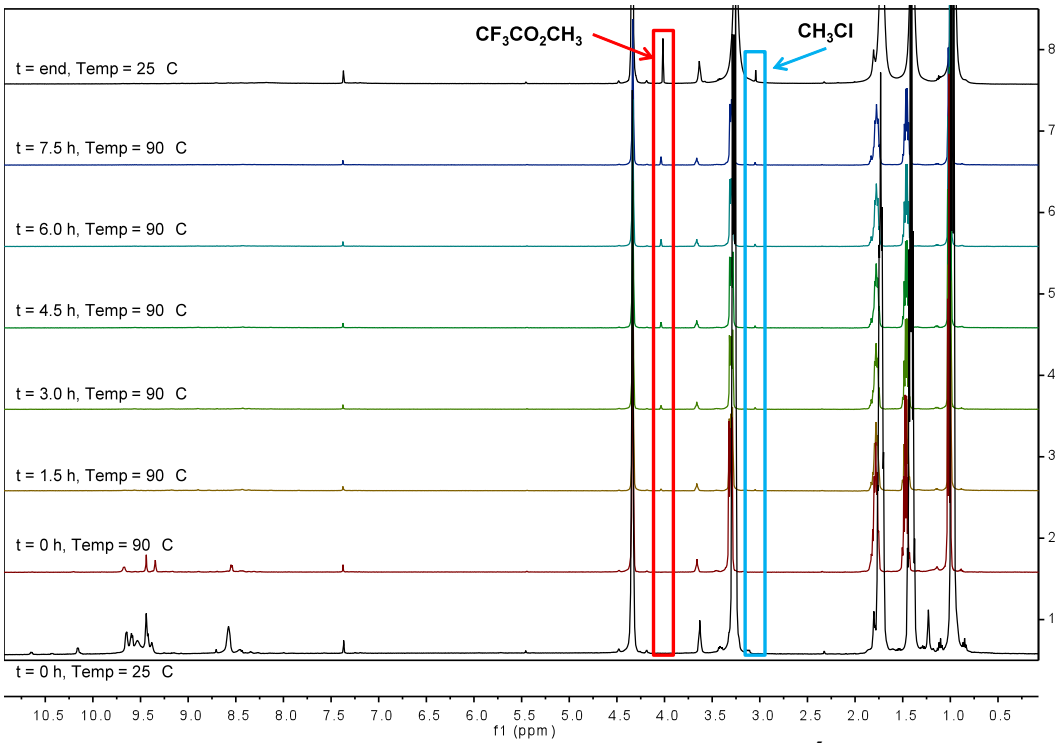

Figure S25. Reductive functionalization of complex **6** (0.0185 g, 2.71 x10^{-5} mol) with Bu_4NTFA (0.029 g, 8.2 x10^{-5} mol) in CD_3NO_2 (0.5 mL).

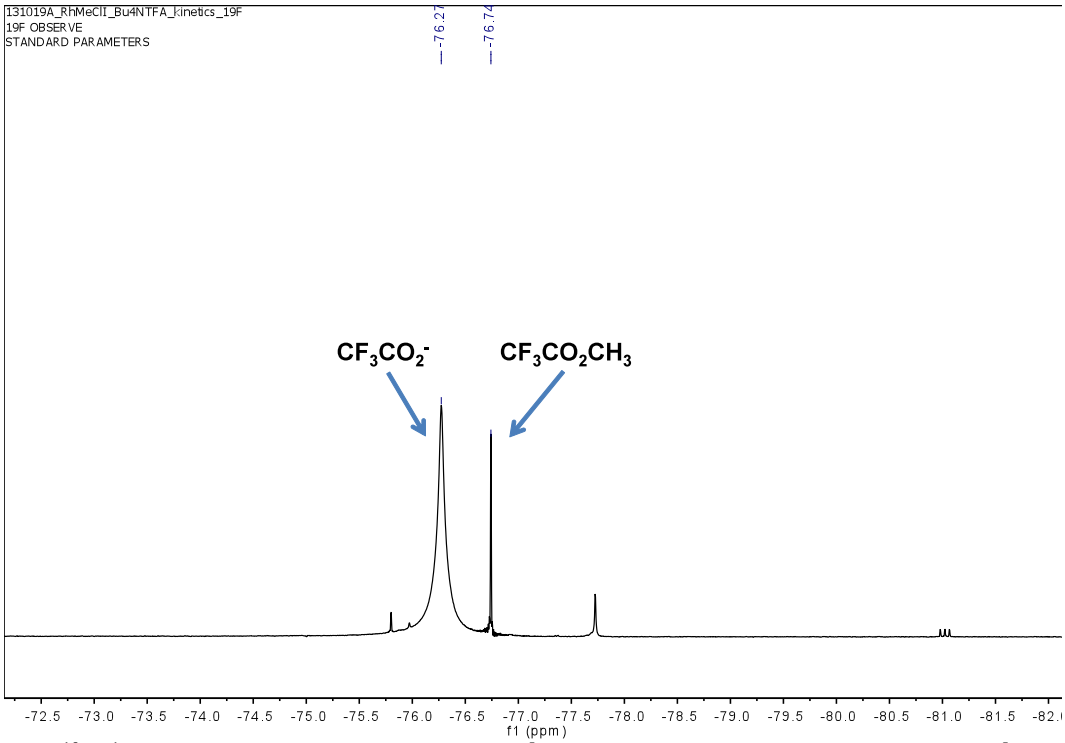

Figure S26. $^{19}F\{^1H\}$ NMR of **6** (0.0185 g, 2.71 x10^{-5} mol) with Bu_4NTFA (0.029 g, 8.2 x10^{-5} mol) in CD_3NO_2 (0.5 mL) after heating at 90° C overnight.

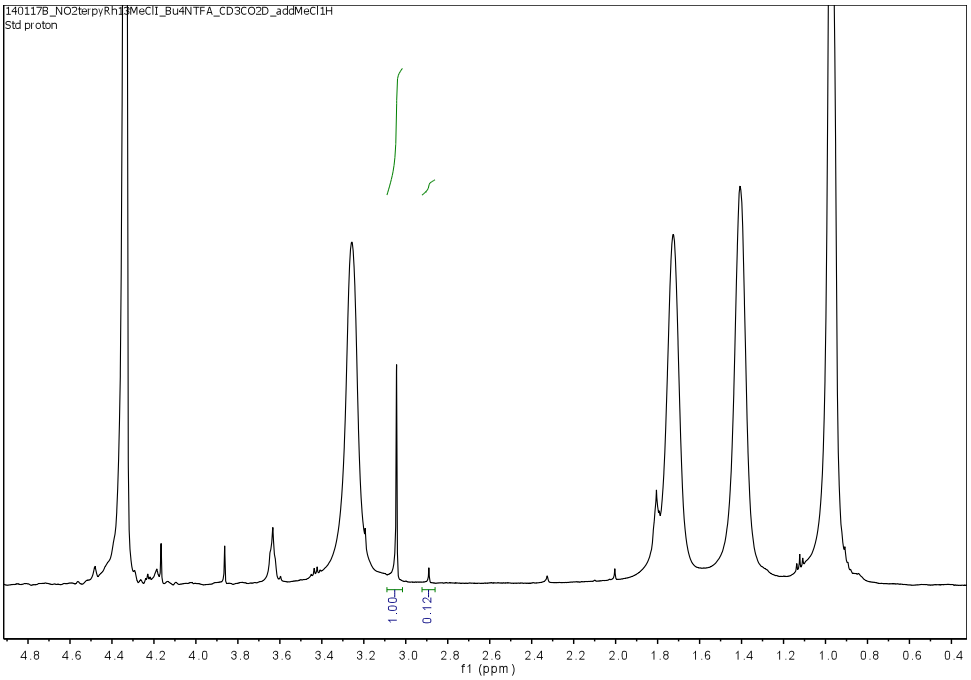

Figure S27. Reductive functionalization of complex **6*** with [Bu_4N][TFA] in CD_3NO_2 (0.5 mL) and one equivalent of MeCl added.

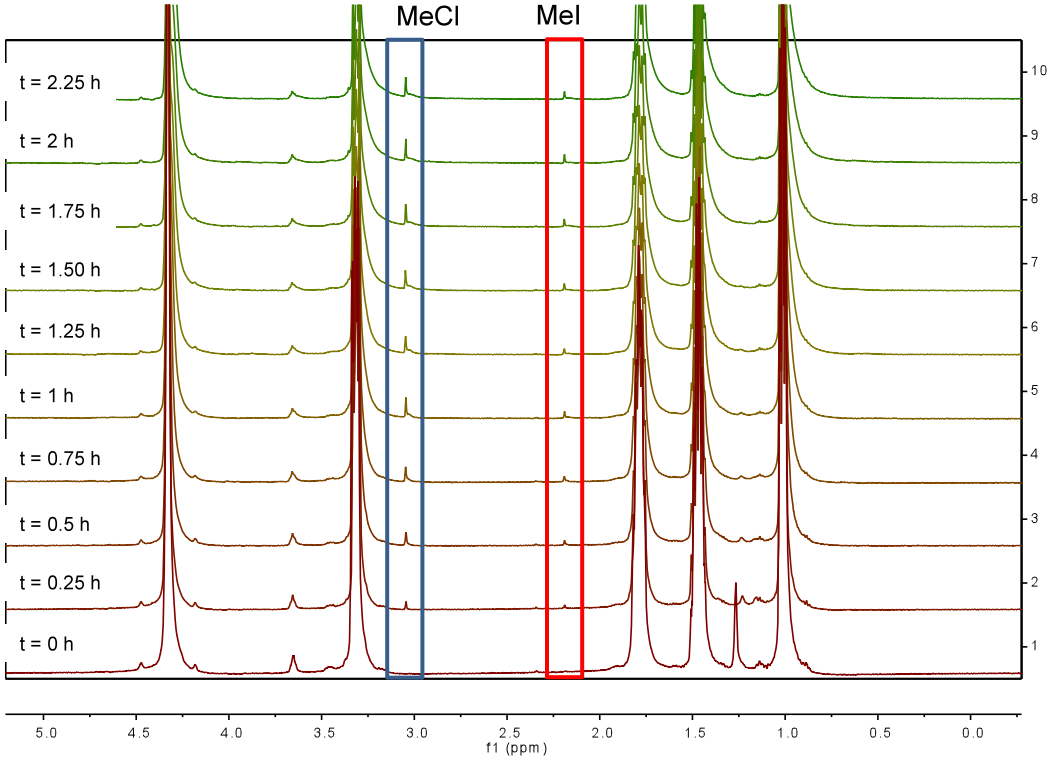

Figure S28. ^{1}H NMR spectra of complex **6** (0.0185 g, 2.71 x10^{-5} mol) with Bu_4NI (0.021 g, 5.7 x10^{-5} mol) in CD_3NO_2 (0.5 mL) at 90 °C.

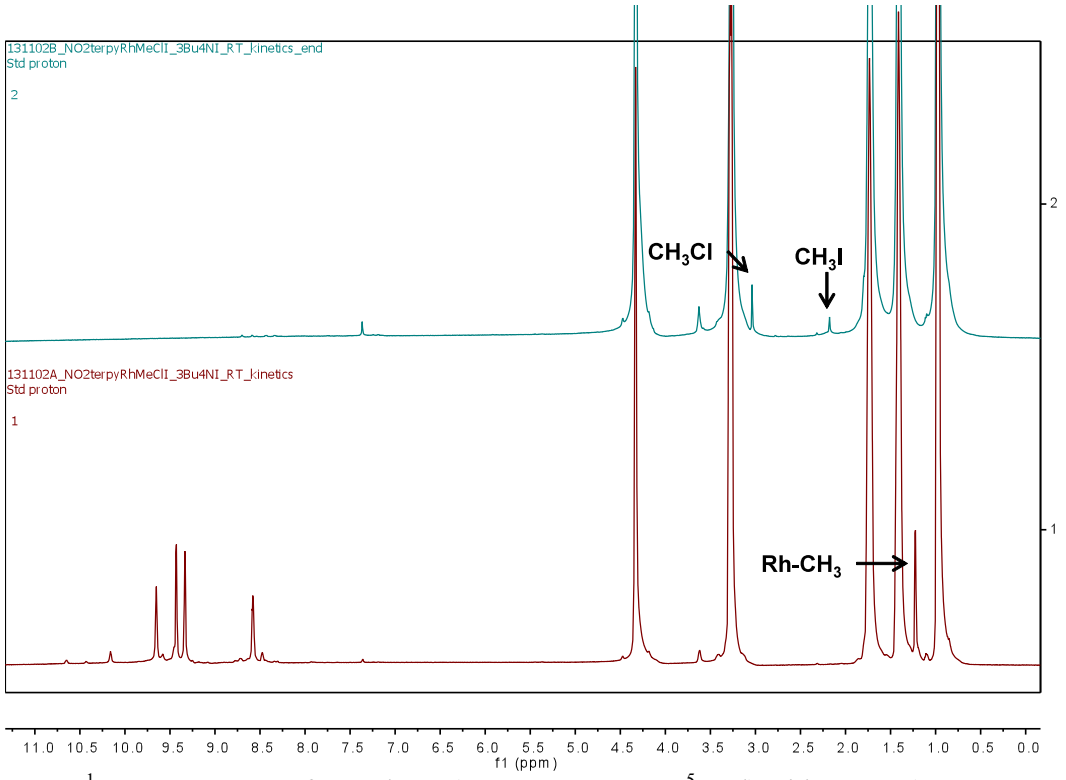

Figure S29. ^{1}H NMR spectra of complex **6** (0.0185 g, 2.71 x10^{-5} mol) with Bu_4NI (0.021 g, 5.7 x10^{-5} mol) in CD_3NO_2 (0.5 mL) before and after heating at 90 °C for 8h.

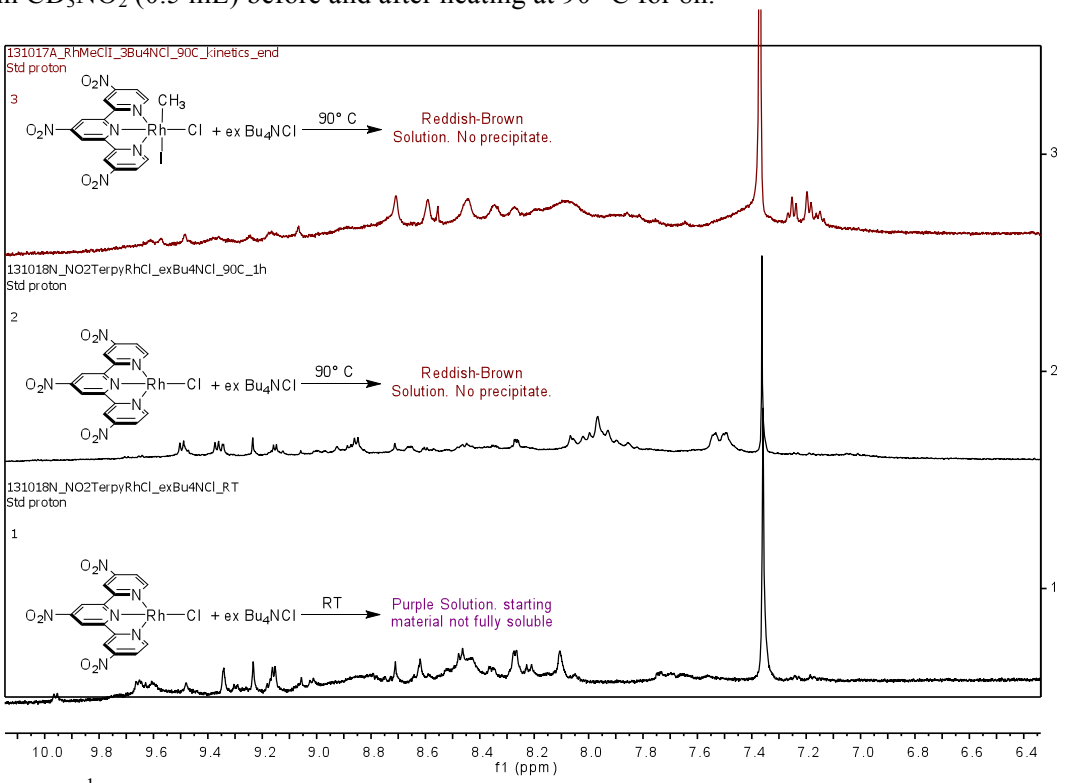

Figure S30. ^{1}H NMR spectra in CD_3NO_2 of (1) **2** and Bu_4NCl at room temperature, (2) **2** and Bu_4NCl after heating for 1h at 90° C, and (3) **6** and Bu_4NCl after 90°C heating overnight.

Table S1. Computed Free Energies (298.15 K, 1 atm) for Eq 8 (B3LYP/CEP-31G(d)/CPCM-THF) and Terpy Congener

$$LRhI + MeI \Rightarrow LRhMeI_2;\ L = terpy,\ {}^{t}Bu_3terpy$$

a.u. = atomic units of energy

G(MeI) a.u.	G(LRhI) a.u.	G(LRhMeI2) a.u.	ΔG_{rxn} kcal/mol	L
-18.8910	-242.5475	-261.4518	-8.4	terpy
-18.8910	-324.5005	-343.4046	-8.2	$^{t}Bu_3$terpy

Table S2. Computed Enthalpies (298.15 K, 1 atm) for Eq 8 (B3LYP/CEP-31G(d)/CPCM-THF)

$$LRhI + MeI \Rightarrow LRhMeI_2;\ L = terpy,\ {}^{t}Bu_3terpy$$

a.u. = atomic units of energy

H(MeI) a.u.	H(LRhI) a.u.	H(LRhMeI2) a.u.	ΔH_{rxn} kcal/mol	L
-18.8611	-324.3987	-343.2940	-21.4	$^{t}Bu_3$terpy

Table S3. Cartesian Coordinates (Å) for B3LYP/CEP-31G(d) optimized stationary points. The first column identifies the element by atomic number (Z).

CH_3Cl (in THF)

6	-1.157027000	-0.000094000	0.000000000
1	-1.493478000	0.564233000	-0.879121000
1	-1.493501000	0.479716000	0.927890000
1	-1.493392000	-1.043518000	-0.048782000
17	0.671914000	0.000008000	0.000001000

CH_3I (in THF)

6	-1.843488000	-0.000084000	-0.000050000
1	-2.166599000	0.771853000	-0.707743000
1	-2.166750000	0.227882000	1.022000000
1	-2.168433000	-0.998576000	-0.313825000
53	0.331372000	-0.000012000	-0.000002000

CH_3TFA (in THF)

8	1.308590000	-0.643945000	-0.000042000
6	0.487820000	0.407712000	-0.000102000
8	0.785735000	1.590578000	-0.000168000
6	-1.002472000	-0.090484000	0.000106000
9	-1.261011000	-0.845588000	1.097705000
9	-1.260564000	-0.848126000	-1.096239000

9	-1.851749000	0.955127000	-0.001334000
6	2.743646000	-0.333732000	0.000042000
1	3.243211000	-1.308892000	0.000626000
1	2.994222000	0.240623000	-0.902918000
1	2.993923000	0.241521000	0.902518000

[terpy]RhCl **1'** (in THF)

45	-0.000028000	-0.843108000	0.000059000
17	-0.000097000	-3.269794000	0.000822000
7	2.039541000	-0.497045000	-0.000176000
6	2.364908000	0.846725000	-0.000119000
6	3.710211000	1.285815000	-0.000315000
6	4.750225000	0.331243000	-0.000542000
6	4.409642000	-1.042574000	-0.000564000
6	3.045139000	-1.406311000	-0.000383000
7	-2.039509000	-0.497004000	-0.000055000
6	-2.364862000	0.846782000	-0.000148000
6	-3.710156000	1.285893000	-0.000429000
6	-4.750195000	0.331349000	-0.000623000
6	-4.409633000	-1.042474000	-0.000511000
6	-3.045140000	-1.406244000	-0.000225000
7	0.000028000	1.099324000	-0.000091000
6	1.196147000	1.767360000	0.000108000
6	1.224846000	3.180941000	0.000469000
6	-1.196085000	1.767391000	0.000071000
6	-1.224743000	3.180968000	0.000451000
6	0.000061000	3.890640000	0.000672000
1	3.938362000	2.352406000	-0.000321000
1	5.794292000	0.651596000	-0.000674000
1	5.173897000	-1.821455000	-0.000729000
1	2.728627000	-2.451014000	-0.000360000
1	2.173346000	3.719361000	0.000638000
1	-3.938276000	2.352491000	-0.000515000
1	-5.794255000	0.651721000	-0.000825000
1	-5.173899000	-1.821343000	-0.000641000
1	-2.728647000	-2.450952000	-0.000063000
1	-2.173227000	3.719417000	0.000650000
1	0.000072000	4.982172000	0.000973000

[$(NO_2)_3$terpy]RhCl **2'** (in THF)

45	-0.000011000	-1.487371000	0.000176000
7	-2.032999000	-1.154557000	-0.000149000
6	-2.363799000	0.188755000	-0.000103000
6	-3.704955000	0.625962000	-0.000170000
6	-4.710702000	-0.358405000	-0.000251000
6	-4.393379000	-1.733153000	-0.000224000
6	-3.026379000	-2.077666000	-0.000248000
7	2.032994000	-1.154532000	0.000178000
6	2.363796000	0.188755000	-0.000027000
6	3.704955000	0.625970000	-0.000058000

6	4.710709000	-0.358394000	-0.000275000
6	4.393379000	-1.733160000	-0.000261000
6	3.026368000	-2.077662000	0.000057000
7	-0.000011000	0.443037000	0.000213000
6	-1.199771000	1.112275000	0.000292000
6	-1.237605000	2.518628000	0.000415000
6	1.199746000	1.112281000	0.000301000
6	1.237584000	2.518648000	0.000378000
6	-0.000023000	3.203781000	0.000370000
1	-3.965088000	1.682440000	-0.000023000
1	-5.165469000	-2.500078000	-0.000148000
1	-2.703158000	-3.119417000	-0.000260000
1	-2.171722000	3.076748000	0.000490000
1	3.965031000	1.682444000	-0.000082000
1	5.165430000	-2.500086000	-0.000408000
1	2.703047000	-3.119370000	0.000140000
1	2.171681000	3.076782000	0.000264000
17	0.000040000	-3.880554000	0.000528000
7	-6.131228000	0.064414000	-0.000370000
8	-7.001840000	-0.830768000	-0.000640000
8	-6.373785000	1.290315000	-0.000200000
7	-0.000025000	4.674469000	0.000210000
8	-1.106835000	5.260498000	-0.000491000
8	1.106786000	5.260494000	0.000563000
7	6.131250000	0.064444000	-0.000485000
8	7.001882000	-0.830728000	-0.000689000
8	6.373870000	1.290319000	-0.000445000

[terpy]RhMe(Cl)(I) **3'** (in THF)

45	-0.000002000	-0.472900000	-0.703751000
17	0.000001000	-2.790965000	-1.436560000
7	2.048631000	-0.134979000	-0.636075000
6	2.365782000	1.150903000	-0.257770000
6	3.709274000	1.570649000	-0.139438000
6	4.744571000	0.651706000	-0.423902000
6	4.403535000	-0.661419000	-0.817938000
6	3.036602000	-1.011778000	-0.909903000
7	-2.048636000	-0.134987000	-0.636065000
6	-2.365791000	1.150895000	-0.257761000
6	-3.709283000	1.570638000	-0.139426000
6	-4.744578000	0.651692000	-0.423886000
6	-4.403540000	-0.661433000	-0.817920000
6	-3.036606000	-1.011789000	-0.909888000
7	-0.000004000	1.422850000	-0.163772000
6	1.196347000	2.039316000	0.013910000
6	1.228358000	3.393364000	0.422047000
6	-1.196357000	2.039313000	0.013915000
6	-1.228371000	3.393360000	0.422052000
6	-0.000007000	4.064515000	0.628230000
53	0.000014000	-1.196465000	2.187867000
1	3.943479000	2.590005000	0.168754000

1	5.789398000	0.957029000	-0.338232000
1	5.166127000	-1.406624000	-1.047930000
1	2.710696000	-2.011416000	-1.202244000
1	2.174238000	3.911706000	0.578370000
6	-0.000016000	0.071418000	-2.716873000
1	-3.943490000	2.589994000	0.168765000
1	-5.789406000	0.957013000	-0.338214000
1	-5.166131000	-1.406641000	-1.047909000
1	-2.710698000	-2.011427000	-1.202229000
1	-2.174251000	3.911699000	0.578379000
1	0.900575000	-0.349532000	-3.189478000
1	-0.900578000	-0.349590000	-3.189478000
1	-0.000008000	5.108223000	0.947755000
1	-0.000052000	1.170813000	-2.814246000

[terpy]RhMe(Cl)(I) **3'-iso** (in THF)

45	-0.000002000	-0.216679000	-0.083054000
53	-0.000018000	-2.992857000	-0.109392000
7	2.059641000	0.138192000	-0.103168000
6	2.366336000	1.480976000	-0.106735000
6	3.704365000	1.933975000	-0.097366000
6	4.752780000	0.987298000	-0.085950000
6	4.426430000	-0.386369000	-0.084934000
6	3.063596000	-0.764064000	-0.094933000
7	-2.059639000	0.138212000	-0.103182000
6	-2.366319000	1.480999000	-0.106741000
6	-3.704342000	1.934014000	-0.097361000
6	-4.752768000	0.987351000	-0.085946000
6	-4.426434000	-0.386321000	-0.084943000
6	-3.063605000	-0.764032000	-0.094950000
7	0.000010000	1.762231000	-0.113286000
6	1.194256000	2.404471000	-0.114498000
6	1.227251000	3.819136000	-0.120177000
6	-1.194230000	2.404483000	-0.114501000
6	-1.227211000	3.819148000	-0.120181000
6	0.000024000	4.521827000	-0.123960000
17	-0.000006000	-0.086316000	2.509859000
1	3.924019000	3.001687000	-0.096524000
1	5.793414000	1.317758000	-0.077061000
1	5.196156000	-1.159169000	-0.074986000
1	2.759443000	-1.811711000	-0.092785000
1	2.172936000	4.360808000	-0.120084000
6	0.000018000	-0.253054000	-2.171405000
1	-3.923981000	3.001730000	-0.096508000
1	-5.793399000	1.317822000	-0.077046000
1	-5.196169000	-1.159112000	-0.074995000
1	-2.759466000	-1.811683000	-0.092814000
1	-2.172889000	4.360830000	-0.120094000
1	0.898722000	-0.781161000	-2.526372000
1	-0.898760000	-0.781018000	-2.526401000
1	0.000029000	5.613343000	-0.128555000

1	0.000107000	0.779761000	-2.563217000

[terpy]RhMe(Cl)$_2$ **4'** (in THF)

45	0.000013000	-0.737663000	-0.125733000
17	0.000023000	-3.171442000	-0.247556000
7	2.049391000	-0.396350000	-0.130219000
6	2.365689000	0.943294000	-0.097511000
6	3.708614000	1.380497000	-0.074211000
6	4.744853000	0.419565000	-0.084959000
6	4.404946000	-0.951096000	-0.118096000
6	3.037934000	-1.313558000	-0.140842000
7	-2.049377000	-0.396344000	-0.130259000
6	-2.365667000	0.943298000	-0.097555000
6	-3.708591000	1.380508000	-0.074247000
6	-4.744832000	0.419579000	-0.084997000
6	-4.404930000	-0.951084000	-0.118138000
6	-3.037920000	-1.313551000	-0.140883000
7	0.000012000	1.231194000	-0.095937000
6	1.195870000	1.872266000	-0.081319000
6	1.228288000	3.286459000	-0.049723000
6	-1.195845000	1.872268000	-0.081334000
6	-1.228261000	3.286461000	-0.049747000
6	0.000013000	3.988347000	-0.034902000
1	3.941539000	2.445186000	-0.045622000
1	5.789338000	0.737348000	-0.065951000
1	5.167973000	-1.730574000	-0.124747000
1	2.713527000	-2.355273000	-0.164046000
1	2.173945000	3.828343000	-0.035566000
6	0.000005000	-0.729734000	-2.207377000
1	-3.941512000	2.445197000	-0.045650000
1	-5.789316000	0.737364000	-0.065987000
1	-5.167963000	-1.730557000	-0.124792000
1	-2.713513000	-2.355265000	-0.164093000
1	-2.173918000	3.828346000	-0.035612000
1	0.899439000	-1.257385000	-2.561777000
1	-0.898718000	-1.258634000	-2.561713000
1	0.000014000	5.079641000	-0.010973000
1	-0.000715000	0.305245000	-2.593050000
17	-0.000134000	-0.698838000	2.480940000

[terpy]RhMe(Cl)(TFA) **5'** (in THF)

45	-0.088059000	-0.018582000	-0.047850000
8	2.019019000	0.036381000	0.080952000
7	-0.159655000	2.049983000	-0.082780000
6	-1.442593000	2.539153000	-0.146969000
6	-1.697088000	3.928600000	-0.152043000
6	-0.606480000	4.825579000	-0.091911000
6	0.705538000	4.305387000	-0.024889000
6	0.882358000	2.902248000	-0.021804000
7	-0.704617000	-2.024302000	-0.069561000

6	-2.075159000	-2.152008000	-0.103270000
6	-2.701919000	-3.417120000	-0.068468000
6	-1.901288000	-4.579277000	0.002597000
6	-0.497541000	-4.435345000	0.030861000
6	0.059924000	-3.135089000	-0.010101000
7	-2.033021000	0.226831000	-0.161561000
6	-2.511336000	1.498979000	-0.192781000
6	-3.906696000	1.720781000	-0.249954000
6	-2.832484000	-0.868879000	-0.168210000
6	-4.237643000	-0.710329000	-0.224129000
6	-4.768519000	0.599277000	-0.267785000
1	-2.720243000	4.302618000	-0.196668000
1	-0.781331000	5.903379000	-0.093810000
1	1.578085000	4.957816000	0.027413000
1	1.867231000	2.436607000	0.038064000
1	-4.312776000	2.731735000	-0.276564000
6	0.100243000	-0.066082000	-2.118780000
1	-3.789154000	-3.495425000	-0.091031000
1	-2.365906000	-5.566947000	0.033909000
1	0.165665000	-5.299962000	0.081670000
1	1.136448000	-2.964185000	-0.016269000
1	-4.900281000	-1.575335000	-0.231450000
1	-0.887808000	-0.122579000	-2.606909000
1	0.624654000	0.844716000	-2.451186000
1	-5.849290000	0.745675000	-0.311087000
1	0.696947000	-0.954250000	-2.378459000
8	2.839274000	-1.942544000	-0.757158000
6	2.923309000	-0.795066000	-0.288643000
6	4.366465000	-0.184387000	-0.068269000
9	5.346946000	-0.988093000	-0.548373000
9	4.500449000	1.025134000	-0.688773000
9	4.622358000	0.017307000	1.255974000
17	-0.262777000	0.001551000	2.532378000

[terpy]RhMe(Cl)(TFA) **5'-iso** (in THF)

45	-0.092632000	-0.584729000	-0.914693000
17	-0.121411000	0.084189000	-3.250304000
7	-2.137880000	-0.593281000	-0.535256000
6	-2.435691000	-0.936024000	0.764371000
6	-3.769525000	-0.962795000	1.228213000
6	-4.814276000	-0.628935000	0.336361000
6	-4.492522000	-0.276706000	-0.993072000
6	-3.133505000	-0.272019000	-1.385635000
7	1.955077000	-0.787784000	-0.642309000
6	2.285502000	-1.200159000	0.628018000
6	3.630232000	-1.394517000	1.008392000
6	4.654297000	-1.150207000	0.065082000
6	4.300107000	-0.720296000	-1.232618000
6	2.930020000	-0.554479000	-1.543406000
7	-0.070677000	-1.150650000	0.973726000
6	-1.256538000	-1.264932000	1.622029000

6	-1.273248000	-1.664017000	2.978957000
6	1.129608000	-1.406089000	1.550250000
6	1.177957000	-1.815801000	2.902544000
6	-0.039044000	-1.940059000	3.613234000
1	-3.989389000	-1.232910000	2.261413000
1	-5.851845000	-0.642543000	0.676251000
1	-5.262840000	-0.008232000	-1.717116000
1	-2.821223000	-0.005032000	-2.396715000
1	-2.210195000	-1.760371000	3.527133000
6	-0.172969000	-2.565982000	-1.523489000
1	3.876392000	-1.720102000	2.019441000
1	5.701197000	-1.290363000	0.342087000
1	5.053584000	-0.515120000	-1.994143000
1	2.592067000	-0.227457000	-2.528273000
1	2.127691000	-2.026448000	3.393686000
1	-0.096030000	-3.247787000	-0.657846000
1	-1.128333000	-2.740703000	-2.044286000
1	-0.025928000	-2.251356000	4.659414000
1	0.660511000	-2.757478000	-2.217845000
8	-0.147454000	1.607752000	-0.353504000
6	0.540791000	2.167371000	0.564918000
8	1.388485000	1.704161000	1.353696000
6	0.211788000	3.715190000	0.673672000
9	-1.110270000	3.926458000	0.953340000
9	0.478031000	4.371568000	-0.493747000
9	0.922793000	4.341632000	1.648358000

[$(NO_2)_3$terpy]RhMe(Cl)(I) **6'** (in THF)

45	0.000004000	-1.131768000	-0.586343000
17	-0.000046000	-3.510453000	-1.009880000
7	2.042391000	-0.796230000	-0.558552000
6	2.363333000	0.530507000	-0.366626000
6	3.703042000	0.965302000	-0.310757000
6	4.705614000	-0.012110000	-0.456326000
6	4.391952000	-1.370244000	-0.647760000
6	3.021868000	-1.713965000	-0.692894000
7	-2.042396000	-0.796238000	-0.558506000
6	-2.363320000	0.530513000	-0.366647000
6	-3.703024000	0.965324000	-0.310763000
6	-4.705607000	-0.012080000	-0.456320000
6	-4.391964000	-1.370224000	-0.647699000
6	-3.021883000	-1.713967000	-0.692810000
7	0.000011000	0.814528000	-0.309796000
6	1.197823000	1.449973000	-0.222745000
6	1.239275000	2.845210000	-0.011265000
6	-1.197804000	1.449968000	-0.222699000
6	-1.239271000	2.845214000	-0.011302000
6	0.000006000	3.510483000	0.091011000
1	3.966399000	2.010301000	-0.161212000
1	5.164517000	-2.128861000	-0.757311000
1	2.693485000	-2.744134000	-0.835893000

1	2.170939000	3.400358000	0.073861000
6	0.000022000	-0.890207000	-2.668608000
1	-3.966369000	2.010326000	-0.161232000
1	-5.164539000	-2.128833000	-0.757226000
1	-2.693505000	-2.744148000	-0.835737000
1	-2.170928000	3.400412000	0.073643000
1	0.900461000	-1.379434000	-3.066965000
1	-0.900743000	-1.378858000	-3.066942000
1	0.000355000	0.182798000	-2.922653000
53	-0.000023000	-1.476986000	2.331322000
7	-6.132468000	0.409496000	-0.407125000
8	-6.998821000	-0.477824000	-0.532198000
8	-6.369843000	1.623683000	-0.246018000
7	0.000036000	4.982366000	0.311547000
8	1.106096000	5.552100000	0.395642000
8	-1.105991000	5.552055000	0.396002000
7	6.132478000	0.409439000	-0.407081000
8	6.998818000	-0.477889000	-0.532199000
8	6.369870000	1.623610000	-0.245871000

[$(NO_2)_3$terpy]RhMe(Cl)(I) **6'-iso** (in THF)

45	-0.000011000	-0.882330000	-0.080073000
53	-0.000049000	-3.634917000	-0.115282000
7	2.054032000	-0.533910000	-0.095208000
6	2.363663000	0.809253000	-0.080771000
6	3.697261000	1.265015000	-0.061865000
6	4.713702000	0.291947000	-0.059669000
6	4.416059000	-1.081820000	-0.074207000
6	3.049682000	-1.444665000	-0.092997000
7	-2.053994000	-0.533884000	-0.095180000
6	-2.363611000	0.809292000	-0.080736000
6	-3.697200000	1.265071000	-0.061856000
6	-4.713669000	0.292026000	-0.059691000
6	-4.416037000	-1.081744000	-0.074223000
6	-3.049665000	-1.444615000	-0.092981000
7	0.000029000	1.094114000	-0.091719000
6	1.195106000	1.735099000	-0.079585000
6	1.238413000	3.146770000	-0.063064000
6	-1.195043000	1.735117000	-0.079579000
6	-1.238325000	3.146787000	-0.063059000
6	0.000048000	3.819942000	-0.058206000
1	3.945770000	2.323903000	-0.047732000
1	5.196004000	-1.840804000	-0.070832000
1	2.743357000	-2.491030000	-0.103895000
1	2.170082000	3.708399000	-0.053208000
6	0.000089000	-0.926791000	-2.178279000
1	-3.945683000	2.323963000	-0.047724000
1	-5.195986000	-1.840723000	-0.070879000
1	-2.743369000	-2.490987000	-0.103857000
1	-2.169989000	3.708426000	-0.053210000
1	0.898943000	-1.456514000	-2.526863000

1	-0.899006000	-1.456021000	-2.526996000
1	0.000393000	0.106450000	-2.566549000
17	-0.000187000	-0.768211000	2.489618000
7	-6.135176000	0.735173000	-0.043492000
8	-7.012789000	-0.149578000	-0.042711000
8	-6.355944000	1.962889000	-0.033481000
7	0.000052000	5.308992000	-0.048417000
8	-1.106016000	5.884367000	-0.045801000
8	1.106136000	5.884354000	-0.045946000
7	6.135225000	0.735070000	-0.043430000
8	7.012819000	-0.149699000	-0.042501000
8	6.356013000	1.962785000	-0.033541000

[^{t}Bu$_3$terpy]RhI **7'** (in THF)

45	0.012144000	-1.261828000	-0.000105000
7	2.058474000	-0.884568000	-0.000073000
6	2.367989000	0.463956000	-0.000050000
6	3.700319000	0.925680000	0.000070000
6	4.792383000	0.018017000	0.000169000
6	4.448780000	-1.359059000	0.000115000
6	3.094145000	-1.755673000	-0.000003000
7	-2.037184000	-0.903968000	-0.000099000
6	-2.360046000	0.441025000	-0.000081000
6	-3.696627000	0.889483000	0.000034000
6	-4.779809000	-0.028980000	0.000139000
6	-4.422466000	-1.402452000	0.000086000
6	-3.063996000	-1.785499000	-0.000031000
7	0.004531000	0.692902000	-0.000130000
6	1.187085000	1.371488000	-0.000132000
6	1.206382000	2.785444000	-0.000190000
6	-1.187777000	1.361307000	-0.000150000
6	-1.217841000	2.770188000	-0.000209000
6	-0.007716000	3.520008000	-0.000226000
1	3.879948000	2.000490000	0.000103000
1	5.208281000	-2.139735000	0.000165000
1	2.820515000	-2.812155000	-0.000038000
1	2.162788000	3.303288000	-0.000218000
1	-3.886553000	1.962526000	0.000059000
1	-5.174034000	-2.190724000	0.000135000
1	-2.779399000	-2.839029000	-0.000070000
1	-2.179091000	3.283046000	-0.000251000
53	0.024653000	-4.015698000	-0.000175000
6	-0.052810000	5.064648000	-0.000239000
6	-0.807918000	5.551989000	-1.272790000
6	-0.807610000	5.551952000	1.272521000
6	1.365010000	5.693374000	-0.000402000
1	-0.284149000	5.232915000	-2.190065000
1	-1.837220000	5.160309000	-1.316908000
1	-0.866479000	6.653972000	-1.275779000
1	-0.283555000	5.232933000	2.189651000
1	-0.866266000	6.653930000	1.275513000

1	-1.836859000	5.160165000	1.316934000
1	1.275858000	6.791792000	-0.000408000
1	1.942250000	5.406655000	0.894755000
1	1.942053000	5.406615000	-0.895675000
6	6.245733000	0.536398000	0.000337000
6	6.475983000	1.405275000	-1.272178000
6	6.475667000	1.405368000	1.272837000
6	7.276119000	-0.621976000	0.000513000
1	6.331286000	0.809603000	-2.189636000
1	5.788952000	2.266331000	-1.314565000
1	7.507669000	1.797147000	-1.275923000
1	6.330733000	0.809769000	2.190306000
1	7.507357000	1.797227000	1.276811000
1	5.788640000	2.266440000	1.314993000
1	8.296013000	-0.203630000	0.000663000
1	7.176324000	-1.258945000	0.895276000
1	7.176607000	-1.258979000	-0.894257000
6	-6.238444000	0.474458000	0.000343000
6	-6.477304000	1.340858000	1.272980000
6	-6.477635000	1.341048000	-1.272105000
6	-7.256835000	-0.694488000	0.000392000
1	-6.326521000	0.746580000	2.190358000
1	-5.799019000	2.208790000	1.315455000
1	-7.512878000	1.722324000	1.276876000
1	-6.327075000	0.746910000	-2.189610000
1	-7.513214000	1.722500000	-1.275683000
1	-5.799376000	2.208998000	-1.314614000
1	-8.280962000	-0.286650000	0.000548000
1	-7.150636000	-1.330309000	-0.894435000
1	-7.150411000	-1.330425000	0.895109000

[^{t}Bu$_3$terpy]RhMe(I)$_2$ **8'** (in THF)

45	0.010401000	-1.044627000	-0.400732000
53	0.021715000	-3.818160000	-0.637055000
7	2.066794000	-0.669217000	-0.405681000
6	2.366950000	0.674734000	-0.335337000
6	3.697177000	1.134437000	-0.315921000
6	4.786982000	0.222851000	-0.368056000
6	4.443673000	-1.150399000	-0.442813000
6	3.087755000	-1.546505000	-0.459691000
7	-2.049184000	-0.688848000	-0.408025000
6	-2.363422000	0.651680000	-0.338098000
6	-3.698451000	1.097089000	-0.318232000
6	-4.778563000	0.174018000	-0.369924000
6	-4.420711000	-1.195434000	-0.446008000
6	-3.060850000	-1.576973000	-0.462862000
7	0.001892000	0.931776000	-0.306068000
6	1.185634000	1.586452000	-0.275752000
6	1.206984000	2.997296000	-0.186463000
6	-1.191580000	1.576379000	-0.278246000
6	-1.223529000	2.982642000	-0.191817000

6	-0.010385000	3.725445000	-0.135814000
1	3.880635000	2.206591000	-0.258199000
1	5.202001000	-1.930406000	-0.486705000
1	2.808026000	-2.599647000	-0.514651000
1	2.161534000	3.515876000	-0.150746000
6	0.011007000	-0.936177000	-2.485784000
1	-3.893030000	2.167271000	-0.259744000
1	-5.170582000	-1.983500000	-0.490339000
1	-2.769682000	-2.626964000	-0.518057000
1	-2.182915000	3.496472000	-0.162007000
1	0.915297000	-1.432740000	-2.869441000
1	-0.885445000	-1.445453000	-2.871088000
1	0.003850000	0.122488000	-2.798528000
53	0.012155000	-1.070985000	2.582559000
6	-0.054768000	5.265464000	-0.021857000
6	-0.821411000	5.651572000	1.278904000
6	1.362844000	5.891418000	0.038005000
6	-0.801240000	5.843886000	-1.261064000
1	-1.854373000	5.267541000	1.280600000
1	-0.310139000	5.255905000	2.172595000
1	-0.870521000	6.750002000	1.367451000
1	1.948429000	5.676371000	-0.871675000
1	1.271748000	6.986167000	0.121490000
1	1.931152000	5.537569000	0.914359000
1	-0.858673000	6.942523000	-1.179985000
1	-0.270586000	5.595402000	-2.195950000
1	-1.830594000	5.458608000	-1.340824000
6	6.240340000	0.738599000	-0.342163000
6	6.468153000	1.667996000	-1.571860000
6	6.467963000	1.544793000	0.971728000
6	7.269247000	-0.419719000	-0.397154000
1	6.324440000	1.117682000	-2.517340000
1	5.781075000	2.530133000	-1.571453000
1	7.499384000	2.059748000	-1.555761000
1	6.315633000	0.907471000	1.859059000
1	7.501998000	1.928725000	0.996895000
1	5.787075000	2.407758000	1.051728000
1	8.288853000	-0.001884000	-0.374454000
1	7.167954000	-1.099533000	0.465238000
1	7.171961000	-1.011677000	-1.322513000
6	-6.237605000	0.673342000	-0.339749000
6	-6.472602000	1.465677000	0.981341000
6	-6.477134000	1.610623000	-1.561079000
6	-7.253664000	-0.495876000	-0.403839000
1	-6.313950000	0.821958000	1.862917000
1	-5.799355000	2.333882000	1.068557000
1	-7.510144000	1.839786000	1.010249000
1	-6.326593000	1.070677000	-2.511449000
1	-7.513189000	1.989204000	-1.541523000
1	-5.801146000	2.481389000	-1.552900000
1	-8.277817000	-0.089406000	-0.379322000

1	-7.148744000	-1.080402000	-1.333101000
1	-7.145957000	-1.180495000	0.453949000

$[(NO_2)_3terpy]RhMe(Cl)_2$ **9'** (in THF)

45	0.000006000	-1.346448000	-0.118340000
17	0.000014000	-3.758435000	-0.216510000
7	2.042524000	-1.014542000	-0.123477000
6	2.363344000	0.324935000	-0.087858000
6	3.702716000	0.762355000	-0.060737000
6	4.704738000	-0.226651000	-0.072068000
6	4.391049000	-1.597360000	-0.105784000
6	3.020168000	-1.942684000	-0.131427000
7	-2.042514000	-1.014559000	-0.123396000
6	-2.363341000	0.324918000	-0.087803000
6	-3.702717000	0.762329000	-0.060674000
6	-4.704734000	-0.226683000	-0.071975000
6	-4.391035000	-1.597390000	-0.105672000
6	-3.020153000	-1.942706000	-0.131322000
7	0.000002000	0.616807000	-0.093550000
6	1.197317000	1.256625000	-0.073633000
6	1.239504000	2.667645000	-0.038982000
6	-1.197319000	1.256618000	-0.073602000
6	-1.239517000	2.667636000	-0.038963000
6	-0.000012000	3.340144000	-0.025989000
1	3.967057000	1.817165000	-0.030604000
1	5.163109000	-2.364352000	-0.111524000
1	2.690641000	-2.982178000	-0.156018000
1	2.170842000	3.229926000	-0.022571000
6	-0.000060000	-1.374552000	-2.209874000
1	-3.967064000	1.817138000	-0.030559000
1	-5.163091000	-2.364387000	-0.111386000
1	-2.690620000	-2.982199000	-0.155894000
1	-2.170862000	3.229913000	-0.022546000
1	0.899300000	-1.909861000	-2.548875000
1	-0.899322000	-1.910065000	-2.548809000
1	-0.000190000	-0.344901000	-2.606889000
17	0.000077000	-1.304713000	2.460858000
7	-6.132142000	0.196970000	-0.048174000
8	-6.998156000	-0.699207000	-0.059066000
8	-6.369676000	1.421357000	-0.020905000
7	-0.000041000	4.828518000	-0.000569000
8	-1.106049000	5.404331000	0.007013000
8	1.105918000	5.404410000	0.007433000
7	6.132143000	0.197011000	-0.048276000
8	6.998159000	-0.699165000	-0.059017000
8	6.369666000	1.421395000	-0.020788000

$[(NO_2)_3terpy]RhMe(Cl)(TFA)$ **10'** (in THF)

45	0.073638000	-0.626393000	-0.055937000
8	0.742528000	-2.612560000	0.009621000

7	2.032866000	0.020748000	-0.071433000
6	2.142344000	1.391704000	-0.084303000
6	3.398799000	2.030151000	-0.056828000
6	4.538728000	1.204676000	-0.018681000
6	4.438371000	-0.198421000	-0.006372000
6	3.136899000	-0.750013000	-0.033352000
7	-2.024223000	-0.604596000	-0.075265000
6	-2.534300000	0.674874000	-0.079078000
6	-3.920606000	0.925378000	-0.041802000
6	-4.776257000	-0.191420000	0.000780000
6	-4.272450000	-1.502905000	0.005217000
6	-2.866105000	-1.657724000	-0.037017000
7	-0.241561000	1.305655000	-0.116135000
6	0.845102000	2.124641000	-0.113893000
6	0.673584000	3.525210000	-0.128604000
6	-1.519102000	1.763896000	-0.112702000
6	-1.772992000	3.153281000	-0.127675000
6	-0.651573000	4.005829000	-0.138942000
1	3.500432000	3.113608000	-0.059417000
1	5.318807000	-0.837249000	0.026044000
1	2.964673000	-1.826503000	-0.016450000
1	1.511961000	4.218143000	-0.131219000
6	0.079756000	-0.798169000	-2.137433000
1	-4.326770000	1.934581000	-0.040858000
1	-4.927919000	-2.371134000	0.037076000
1	-2.394952000	-2.641031000	-0.061367000
1	-2.779631000	3.565375000	-0.128578000
1	-0.240717000	0.142851000	-2.613830000
1	1.099208000	-1.056109000	-2.463170000
1	-0.614954000	-1.610136000	-2.399994000
8	-0.981754000	-3.980728000	-0.652294000
6	0.176555000	-3.728053000	-0.286645000
6	1.192892000	-4.928194000	-0.123191000
9	0.667116000	-6.105453000	-0.535035000
9	2.331840000	-4.718567000	-0.845500000
9	1.566288000	-5.080930000	1.178088000
17	0.049060000	-0.550736000	2.498599000
7	5.884995000	1.841524000	0.012283000
8	5.932707000	3.088052000	0.014760000
8	6.876875000	1.087484000	0.032685000
7	-0.875359000	5.477778000	-0.159085000
8	-2.055227000	5.880329000	-0.161085000
8	0.131981000	6.212228000	-0.174001000
7	-6.248477000	0.031397000	0.040020000
8	-6.981482000	-0.975400000	0.082403000
8	-6.653205000	1.211393000	0.026062000

[$(NO_2)_3$terpy]RhMe(Cl)(TFA) **10'-iso** (in THF)

45	0.041466000	-1.029451000	-0.976471000
17	0.046697000	-3.332474000	-1.682068000
7	2.086219000	-0.704149000	-0.883924000

6	2.403448000	0.576150000	-0.486222000
6	3.741711000	0.985811000	-0.319449000
6	4.744620000	0.030370000	-0.573133000
6	4.434169000	-1.280725000	-0.975510000
6	3.064002000	-1.601380000	-1.118183000
7	-2.002064000	-0.706188000	-0.894973000
6	-2.322316000	0.585500000	-0.542172000
6	-3.660706000	1.006785000	-0.424635000
6	-4.662685000	0.048437000	-0.671628000
6	-4.349641000	-1.276141000	-1.023707000
6	-2.978039000	-1.605730000	-1.126344000
7	0.039536000	0.863314000	-0.440187000
6	1.234815000	1.474979000	-0.247395000
6	1.275494000	2.831422000	0.142604000
6	-1.157632000	1.481501000	-0.286776000
6	-1.202597000	2.840631000	0.088360000
6	0.034993000	3.483018000	0.299032000
1	4.004511000	1.993846000	-0.004908000
1	5.207470000	-2.021669000	-1.168689000
1	2.736159000	-2.596019000	-1.423277000
1	2.206219000	3.367097000	0.315896000
6	0.012602000	-0.484021000	-2.986663000
1	-3.925389000	2.024793000	-0.146403000
1	-5.121638000	-2.019794000	-1.211410000
1	-2.647836000	-2.609307000	-1.397577000
1	-2.135688000	3.383472000	0.221865000
1	-0.071219000	0.611252000	-3.091638000
1	0.943477000	-0.834110000	-3.458430000
1	-0.849001000	-0.972274000	-3.466357000
8	0.192171000	-1.765153000	1.143683000
6	-0.409519000	-1.226224000	2.135909000
8	-1.168613000	-0.238787000	2.185217000
6	-0.087419000	-1.979821000	3.491250000
9	1.247395000	-1.925828000	3.779542000
9	-0.427397000	-3.298730000	3.426637000
9	-0.744035000	-1.450948000	4.555020000
7	-6.090651000	0.456007000	-0.554774000
8	-6.328255000	1.644317000	-0.259162000
8	-6.956475000	-0.416253000	-0.761701000
7	0.032093000	4.916836000	0.701824000
8	-1.074039000	5.480833000	0.814255000
8	1.136168000	5.461544000	0.899462000
7	6.171520000	0.426789000	-0.409065000
8	6.405884000	1.598917000	-0.052904000
8	7.038291000	-0.438167000	-0.639827000

[terpy]RhI (in THF)

45	0.000025000	-0.244285000	0.000045000
7	-2.049740000	0.116151000	0.000035000
6	-2.365624000	1.462281000	-0.000019000
6	-3.705704000	1.916828000	0.000013000

6	-4.757664000	0.976071000	0.000012000
6	-4.430377000	-0.399968000	0.000017000
6	-3.069747000	-0.778246000	0.000053000
7	2.049674000	0.116548000	0.000062000
6	2.365320000	1.462736000	-0.000004000
6	3.705315000	1.917533000	0.000006000
6	4.757455000	0.976979000	-0.000010000
6	4.430416000	-0.399121000	0.000016000
6	3.069859000	-0.777652000	0.000078000
7	-0.000173000	1.710452000	0.000014000
6	-1.194043000	2.378209000	-0.000021000
6	-1.224239000	3.792098000	-0.000056000
6	1.193567000	2.378443000	-0.000004000
6	1.223487000	3.792339000	-0.000051000
6	-0.000446000	4.502032000	-0.000080000
1	-3.920819000	2.985882000	0.000018000
1	-5.797895000	1.308484000	0.000001000
1	-5.201033000	-1.172452000	-0.000006000
1	-2.772985000	-1.828256000	0.000090000
1	-2.172584000	4.330293000	-0.000063000
1	3.920222000	2.986629000	-0.000015000
1	5.797625000	1.309583000	-0.000058000
1	5.201210000	-1.171468000	-0.000015000
1	2.773303000	-1.827719000	0.000118000
1	2.171727000	4.330723000	-0.000049000
1	-0.000553000	5.593547000	-0.000098000
53	0.000318000	-2.993544000	-0.000046000

[terpy]RhMe(I)$_2$ (in THF)

45	0.000075000	-0.201413000	-0.454000000
53	0.000155000	-2.975478000	-0.581644000
7	2.060830000	0.156878000	-0.471933000
6	2.366671000	1.500567000	-0.475674000
6	3.704448000	1.954260000	-0.470445000
6	4.753763000	1.008760000	-0.463394000
6	4.428487000	-0.365250000	-0.462367000
6	3.066318000	-0.744265000	-0.467368000
7	-2.060673000	0.156822000	-0.472154000
6	-2.366572000	1.500495000	-0.475984000
6	-3.704371000	1.954126000	-0.470933000
6	-4.753641000	1.008575000	-0.464005000
6	-4.428301000	-0.365420000	-0.462893000
6	-3.066114000	-0.744370000	-0.467689000
7	0.000044000	1.780058000	-0.461326000
6	1.194593000	2.423094000	-0.479141000
6	1.227122000	3.837426000	-0.497819000
6	-1.194525000	2.423055000	-0.479295000
6	-1.227101000	3.837385000	-0.498003000
6	-0.000001000	4.540217000	-0.504795000
1	3.923101000	3.022145000	-0.468369000
1	5.794089000	1.340163000	-0.457428000

1	5.198753000	-1.137517000	-0.455560000
1	2.763800000	-1.792288000	-0.465194000
1	2.172766000	4.379012000	-0.507596000
6	0.000298000	-0.188832000	-2.545403000
1	-3.923077000	3.022001000	-0.468914000
1	-5.793984000	1.339927000	-0.458206000
1	-5.198532000	-1.137723000	-0.456173000
1	-2.763548000	-1.792379000	-0.465442000
1	-2.172766000	4.378933000	-0.507949000
1	0.900184000	-0.709438000	-2.906004000
1	-0.899958000	-0.708699000	-2.906157000
1	-0.000016000	5.631627000	-0.518456000
1	0.000742000	0.854389000	-2.906100000
53	-0.000397000	-0.114368000	2.512336000

CH_3Cl (in CH_3NO_2)

6	-1.158645000	-0.000091000	0.000001000
1	-1.493446000	0.569050000	-0.876357000
1	-1.493476000	0.474908000	0.930679000
1	-1.493394000	-1.043529000	-0.054339000
17	0.672481000	0.000007000	0.000001000

$[(NO_2)_3terpy]RhCl$ **2'** (in CH_3NO_2)

45	0.000015000	-1.488642000	0.000141000
7	-2.034238000	-1.155119000	-0.000132000
6	-2.363791000	0.188333000	-0.000020000
6	-3.704001000	0.627653000	-0.000035000
6	-4.710942000	-0.355508000	-0.000058000
6	-4.395683000	-1.730480000	-0.000115000
6	-3.029106000	-2.076462000	-0.000170000
7	2.034256000	-1.155047000	0.000178000
6	2.363814000	0.188375000	-0.000027000
6	3.704008000	0.627709000	0.000067000
6	4.710950000	-0.355455000	-0.000044000
6	4.395704000	-1.730459000	-0.000052000
6	3.029117000	-2.076410000	0.000153000
7	-0.000002000	0.442659000	0.000272000
6	-1.199230000	1.111112000	0.000361000
6	-1.237643000	2.517439000	0.000362000
6	1.199213000	1.111143000	0.000223000
6	1.237596000	2.517491000	0.000157000
6	-0.000044000	3.201926000	0.000195000
1	-3.961355000	1.684673000	0.000157000
1	-5.167664000	-2.497390000	0.000023000
1	-2.709527000	-3.119188000	-0.000205000
1	-2.172411000	3.074121000	0.000431000
1	3.961303000	1.684721000	0.000055000
1	5.167628000	-2.497352000	-0.000120000
1	2.709427000	-3.119082000	0.000185000
1	2.172322000	3.074210000	-0.000070000

17	0.000067000	-3.891621000	-0.000236000
7	-6.130300000	0.068508000	-0.000027000
8	-7.003264000	-0.825014000	-0.000178000
8	-6.373482000	1.294441000	-0.000034000
7	-0.000067000	4.672276000	-0.000051000
8	-1.106307000	5.259905000	-0.000451000
8	1.106156000	5.259939000	-0.000142000
7	6.130304000	0.068565000	-0.000144000
8	7.003260000	-0.824957000	-0.000217000
8	6.373514000	1.294488000	-0.000158000

$[(NO_2)_3terpy]RhMe(Cl)_2$ **9'** (in CH_3NO_2)

45	-0.000059000	-1.349144000	-0.106664000
17	-0.000033000	-3.769471000	-0.192836000
7	2.045215000	-1.014922000	-0.119573000
6	2.363898000	0.325033000	-0.085492000
6	3.702421000	0.765545000	-0.069125000
6	4.706075000	-0.221328000	-0.092628000
6	4.395484000	-1.592487000	-0.129042000
6	3.025217000	-1.940355000	-0.141722000
7	-2.045260000	-1.014923000	-0.119401000
6	-2.363964000	0.325041000	-0.085338000
6	-3.702491000	0.765528000	-0.068950000
6	-4.706138000	-0.221354000	-0.092453000
6	-4.395528000	-1.592509000	-0.128860000
6	-3.025259000	-1.940365000	-0.141526000
7	-0.000038000	0.615019000	-0.083770000
6	1.197009000	1.254891000	-0.065264000
6	1.239367000	2.665765000	-0.029461000
6	-1.197078000	1.254905000	-0.065209000
6	-1.239426000	2.665779000	-0.029376000
6	-0.000025000	3.337668000	-0.014756000
1	3.963318000	1.821133000	-0.040546000
1	5.168077000	-2.358580000	-0.147049000
1	2.700548000	-2.981122000	-0.169390000
1	2.171386000	3.226575000	-0.014390000
6	-0.000543000	-1.375097000	-2.195581000
1	-3.963398000	1.821113000	-0.040393000
1	-5.168106000	-2.358617000	-0.146865000
1	-2.700579000	-2.981129000	-0.169188000
1	-2.171440000	3.226594000	-0.014207000
1	0.900822000	-1.907975000	-2.533146000
1	-0.900505000	-1.910651000	-2.532632000
1	-0.002165000	-0.345254000	-2.589651000
17	0.000788000	-1.313546000	2.491281000
7	-6.132578000	0.204488000	-0.079423000
8	-7.001029000	-0.689586000	-0.104209000
8	-6.369947000	1.428663000	-0.045051000
7	-0.000011000	4.825805000	0.014235000
8	-1.105499000	5.402803000	0.024897000
8	1.105477000	5.402797000	0.024513000

7	6.132517000	0.204528000	-0.079570000
8	7.000975000	-0.689558000	-0.103613000
8	6.369877000	1.428724000	-0.045913000

$[(NO_2)_3terpy]RhMe(Cl)]^+$ **11'** (in CH_3NO_2)

45	0.000091000	-1.446328000	-0.046563000
17	-0.001227000	-3.820637000	-0.247375000
7	-2.053043000	-1.105122000	-0.065154000
6	-2.367578000	0.237582000	-0.047802000
6	-3.704015000	0.681724000	-0.065797000
6	-4.709951000	-0.303135000	-0.105976000
6	-4.405044000	-1.674680000	-0.127022000
6	-3.035460000	-2.027910000	-0.102302000
7	2.052412000	-1.104657000	-0.065807000
6	2.366767000	0.238064000	-0.047175000
6	3.703145000	0.682339000	-0.065125000
6	4.709168000	-0.302353000	-0.106606000
6	4.404388000	-1.673927000	-0.128976000
6	3.034911000	-2.027345000	-0.104118000
7	-0.000435000	0.526669000	-0.025519000
6	-1.198034000	1.166541000	-0.023195000
6	-1.240318000	2.577900000	-0.006846000
6	1.196987000	1.166856000	-0.022276000
6	1.239036000	2.578215000	-0.005948000
6	-0.000704000	3.248689000	0.004181000
1	-3.962868000	1.738157000	-0.052457000
1	-5.179723000	-2.438215000	-0.158880000
1	-2.716267000	-3.070646000	-0.113188000
1	-2.171986000	3.139575000	-0.001845000
6	0.011459000	-1.523592000	2.014758000
1	3.961861000	1.738792000	-0.050855000
1	5.179136000	-2.437345000	-0.161915000
1	2.715798000	-3.070091000	-0.115866000
1	2.170600000	3.140061000	-0.000531000
1	-0.929114000	-2.000338000	2.321863000
1	0.877507000	-2.135891000	2.299527000
1	0.092246000	-0.505547000	2.421322000
7	6.135962000	0.129282000	-0.126846000
8	7.004759000	-0.762424000	-0.174940000
8	6.367296000	1.353920000	-0.094314000
7	-0.000890000	4.739285000	0.025246000
8	-1.106803000	5.313763000	0.033051000
8	1.104877000	5.314035000	0.033931000
7	-6.136818000	0.128357000	-0.125983000
8	-7.005570000	-0.763498000	-0.171935000
8	-6.368218000	1.353029000	-0.095378000

TS-A1 (in CH_3NO_2)

45	0.000000000	-1.278502000	0.007325000
17	0.000004000	-3.669540000	-0.710382000

7	2.036123000	-0.939557000	-0.064788000
6	2.362966000	0.405453000	-0.065237000
6	3.705680000	0.842273000	-0.040647000
6	4.710134000	-0.140494000	-0.016508000
6	4.393916000	-1.517980000	-0.008820000
6	3.029585000	-1.863031000	-0.029032000
7	-2.036124000	-0.939558000	-0.064795000
6	-2.362967000	0.405452000	-0.065241000
6	-3.705682000	0.842271000	-0.040650000
6	-4.710135000	-0.140497000	-0.016512000
6	-4.393917000	-1.517982000	-0.008826000
6	-3.029585000	-1.863033000	-0.029040000
7	-0.000001000	0.661057000	-0.108784000
6	1.202743000	1.326144000	-0.081297000
6	1.239172000	2.731775000	-0.066998000
6	-1.202746000	1.326144000	-0.081299000
6	-1.239174000	2.731774000	-0.067000000
6	-0.000001000	3.416633000	-0.066595000
1	3.963756000	1.899081000	-0.039455000
1	5.165427000	-2.284818000	0.012185000
1	2.713420000	-2.906183000	-0.021072000
1	2.173143000	3.289614000	-0.055878000
6	0.000023000	-2.217156000	-2.502809000
1	-3.963759000	1.899079000	-0.039456000
1	-5.165427000	-2.284822000	0.012178000
1	-2.713419000	-2.906184000	-0.021082000
1	-2.173146000	3.289613000	-0.055883000
1	-0.000039000	-3.134675000	-3.088431000
1	-0.927792000	-1.646797000	-2.555937000
1	0.927915000	-1.646921000	-2.555932000
7	-6.128226000	0.282420000	0.002151000
8	-7.000296000	-0.612488000	0.023207000
8	-6.373882000	1.508389000	-0.004537000
7	-0.000002000	4.883677000	-0.058506000
8	1.106965000	5.472824000	-0.055427000
8	-1.106969000	5.472824000	-0.055430000
7	6.128225000	0.282423000	0.002152000
8	7.000295000	-0.612484000	0.023210000
8	6.373880000	1.508393000	-0.004540000
17	-0.000006000	-1.986563000	2.465343000

TS-A2^{+} (in CH_3NO_2)

45	0.000487000	-1.403847000	-0.112797000
17	0.001212000	-3.782354000	-0.051066000
7	-2.048128000	-1.060635000	-0.129580000
6	-2.365918000	0.282256000	-0.069139000
6	-3.701810000	0.732187000	-0.075881000
6	-4.713886000	-0.242738000	-0.156156000
6	-4.410686000	-1.614957000	-0.227478000
6	-3.044504000	-1.971908000	-0.208887000

7	2.047456000	-1.060010000	-0.126952000
6	2.365425000	0.282965000	-0.065642000
6	3.701198000	0.733088000	-0.073327000
6	4.713494000	-0.241445000	-0.155640000
6	4.410347000	-1.613614000	-0.228098000
6	3.044241000	-1.970769000	-0.208749000
7	0.000004000	0.549174000	-0.037493000
6	-1.196675000	1.203480000	-0.008250000
6	-1.238148000	2.611003000	0.068064000
6	1.196199000	1.204010000	-0.005377000
6	1.237003000	2.611574000	0.071174000
6	-0.000752000	3.287260000	0.108949000
1	-3.953572000	1.789321000	-0.026258000
1	-5.186943000	-2.374650000	-0.293141000
1	-2.740335000	-3.017590000	-0.258150000
1	-2.171647000	3.168749000	0.097090000
6	0.003267000	-2.857940000	2.061275000
1	3.952657000	1.790287000	-0.023367000
1	5.186571000	-2.373187000	-0.295581000
1	2.740560000	-3.016615000	-0.259940000
1	2.170226000	3.169658000	0.102500000
1	-0.212968000	-3.877421000	2.376847000
1	1.025217000	-2.522800000	2.242889000
1	-0.795079000	-2.144042000	2.270337000
7	6.134411000	0.195110000	-0.168659000
8	7.008829000	-0.689815000	-0.258282000
8	6.364879000	1.418993000	-0.089125000
7	-0.001209000	4.767629000	0.193808000
8	-1.107156000	5.346180000	0.225625000
8	1.104373000	5.346688000	0.228770000
7	-6.135027000	0.193490000	-0.167577000
8	-7.009328000	-0.691750000	-0.254920000
8	-6.365663000	1.417380000	-0.088953000

TS-B1 (in CH_3NO_2)

45	0.000935000	-1.194695000	-0.421984000
17	-0.001302000	-3.657740000	-0.531789000
7	-2.031760000	-0.877299000	-0.270452000
6	-2.360666000	0.459538000	-0.124744000
6	-3.702432000	0.896274000	-0.096620000
6	-4.708438000	-0.079459000	-0.219123000
6	-4.389483000	-1.448908000	-0.370022000
6	-3.025163000	-1.793085000	-0.394414000
7	2.034621000	-0.880362000	-0.267362000
6	2.365071000	0.455890000	-0.120273000
6	3.707392000	0.890719000	-0.089153000
6	4.712264000	-0.086368000	-0.210372000
6	4.391747000	-1.455203000	-0.363084000
6	3.026940000	-1.797442000	-0.390263000
7	0.002303000	0.717822000	-0.064538000
6	-1.199307000	1.375717000	-0.008735000

6	-1.236105000	2.774230000	0.143186000
6	1.204875000	1.373772000	-0.006212000
6	1.243586000	2.772204000	0.145986000
6	0.004168000	3.451547000	0.221483000
1	-3.960884000	1.947260000	0.014400000
1	-5.161173000	-2.210202000	-0.463829000
1	-2.700364000	-2.827507000	-0.512737000
1	-2.169120000	3.330512000	0.199554000
6	-0.016319000	-1.639359000	2.186095000
1	3.967121000	1.941238000	0.023256000
1	5.162563000	-2.217505000	-0.455894000
1	2.700841000	-2.831362000	-0.509528000
1	2.177348000	3.327003000	0.204478000
1	-0.097752000	-0.571024000	2.357604000
1	-0.906248000	-2.226194000	1.990971000
1	0.958095000	-2.088897000	2.033834000
17	0.008312000	-0.967716000	-3.036614000
17	-0.029787000	-2.112764000	4.434888000
7	6.127827000	0.332152000	-0.177636000
8	7.000852000	-0.556889000	-0.289233000
8	6.377576000	1.551021000	-0.040945000
7	0.005165000	4.912149000	0.383489000
8	1.112217000	5.496241000	0.449777000
8	-1.101061000	5.498248000	0.445747000
7	-6.123414000	0.341100000	-0.190002000
8	-6.997480000	-0.546811000	-0.302655000
8	-6.371766000	1.560482000	-0.055185000

TS-B2^{+} (in CH_3NO_2)

45	-0.004398000	-1.264497000	-0.537632000
17	-0.000660000	-3.598514000	-1.110710000
7	-2.049684000	-0.930394000	-0.503225000
6	-2.374642000	0.394775000	-0.290785000
6	-3.714275000	0.832020000	-0.239947000
6	-4.719097000	-0.138542000	-0.413054000
6	-4.406698000	-1.494197000	-0.630052000
6	-3.038065000	-1.839063000	-0.667165000
7	2.038582000	-0.920655000	-0.511019000
6	2.358079000	0.406604000	-0.303143000
6	3.695773000	0.850775000	-0.260305000
6	4.704565000	-0.115092000	-0.435968000
6	4.397716000	-1.472920000	-0.647548000
6	3.030733000	-1.824655000	-0.677196000
7	-0.008781000	0.659905000	-0.227069000
6	-1.208145000	1.308282000	-0.134944000
6	-1.251119000	2.701050000	0.077356000
6	1.187618000	1.314671000	-0.142291000
6	1.224540000	2.707840000	0.068814000
6	-0.014679000	3.374529000	0.179077000
1	-3.974617000	1.875363000	-0.074884000
1	-5.179037000	-2.248752000	-0.764825000

1	-2.715974000	-2.867709000	-0.833334000
1	-2.185642000	3.251090000	0.162579000
6	0.045110000	-1.748494000	1.910922000
1	3.951676000	1.895851000	-0.099258000
1	5.173084000	-2.224031000	-0.784147000
1	2.713284000	-2.855255000	-0.839675000
1	2.156689000	3.262857000	0.147514000
1	0.710568000	-2.571789000	1.675661000
1	0.449580000	-0.769096000	2.143401000
1	-1.028978000	-1.896566000	1.888737000
17	0.093940000	-2.325350000	4.178984000
7	-6.142771000	0.284332000	-0.365841000
8	-7.012719000	-0.597742000	-0.513389000
8	-6.382623000	1.495538000	-0.181931000
7	-0.017900000	4.837174000	0.406333000
8	1.086552000	5.415254000	0.489954000
8	-1.124936000	5.408500000	0.501466000
7	6.126242000	0.315079000	-0.397768000
8	6.999856000	-0.563076000	-0.547150000
8	6.361023000	1.528088000	-0.219137000

TS-C1 (in CH_3NO_2)

45	0.000004000	-0.236510000	-1.345094000
17	-0.000001000	-2.231083000	-2.797524000
7	-2.032729000	-0.064315000	-1.038864000
6	-2.363143000	0.954258000	-0.159859000
6	-3.706491000	1.294840000	0.109481000
6	-4.711089000	0.561105000	-0.547170000
6	-4.389293000	-0.477288000	-1.453863000
6	-3.025323000	-0.744903000	-1.667134000
7	2.032738000	-0.064332000	-1.038855000
6	2.363156000	0.954240000	-0.159851000
6	3.706507000	1.294814000	0.109491000
6	4.711101000	0.561070000	-0.547156000
6	4.389299000	-0.477322000	-1.453847000
6	3.025328000	-0.744927000	-1.667122000
7	0.000007000	1.131911000	0.038532000
6	-1.203626000	1.641341000	0.458154000
6	-1.240528000	2.701440000	1.381676000
6	1.203643000	1.641331000	0.458158000
6	1.240550000	2.701428000	1.381683000
6	0.000012000	3.212997000	1.835870000
1	-3.968324000	2.095239000	0.798370000
1	-5.159684000	-1.049806000	-1.966208000
1	-2.697461000	-1.527252000	-2.352638000
1	-2.173546000	3.125001000	1.746439000
6	-0.000012000	-2.086246000	0.635961000
1	3.968343000	2.095214000	0.798377000
1	5.159688000	-1.049847000	-1.966190000
1	2.697462000	-1.527274000	-2.352626000
1	2.173569000	3.124979000	1.746452000

1	-0.000024000	-1.279154000	1.362744000
1	-0.934192000	-2.396524000	0.180538000
1	0.934182000	-2.396520000	0.180564000
17	0.000015000	1.323002000	-3.385256000
53	-0.000033000	-3.945706000	2.418942000
7	6.124775000	0.885366000	-0.281710000
8	6.998495000	0.217857000	-0.880100000
8	6.376423000	1.808980000	0.526022000
7	0.000015000	4.310445000	2.807970000
8	1.107194000	4.752378000	3.199877000
8	-1.107161000	4.752390000	3.199869000
7	-6.124761000	0.885408000	-0.281725000
8	-6.998485000	0.217904000	-0.880117000
8	-6.376405000	1.809022000	0.526009000

TS-C2^{+} (in CH_3NO_2)

45	-0.020715000	-0.389609000	-1.420364000
17	-0.003492000	-2.231387000	-2.959287000
7	-2.067359000	-0.130537000	-1.228245000
6	-2.401936000	0.945049000	-0.428824000
6	-3.744840000	1.297879000	-0.181820000
6	-4.742965000	0.507539000	-0.782367000
6	-4.420858000	-0.593023000	-1.599942000
6	-3.050080000	-0.870207000	-1.791728000
7	2.018271000	-0.062829000	-1.261419000
6	2.329832000	1.023674000	-0.467499000
6	3.664416000	1.415752000	-0.235143000
6	4.678827000	0.653397000	-0.844347000
6	4.380184000	-0.457658000	-1.656696000
6	3.016134000	-0.774647000	-1.833973000
7	-0.037827000	1.180963000	-0.267853000
6	-1.241436000	1.693664000	0.129151000
6	-1.292959000	2.819401000	0.975130000
6	1.154087000	1.736018000	0.106623000
6	1.182109000	2.865035000	0.949403000
6	-0.061049000	3.382842000	1.373118000
1	-4.012930000	2.147181000	0.443199000
1	-5.187873000	-1.207542000	-2.066955000
1	-2.720988000	-1.704227000	-2.412551000
1	-2.230906000	3.248945000	1.319704000
6	0.062136000	-1.964554000	0.597957000
1	3.914304000	2.272518000	0.387122000
1	5.159874000	-1.050982000	-2.130085000
1	2.704982000	-1.619269000	-2.449591000
1	2.110797000	3.329415000	1.273446000
1	0.744692000	-2.563834000	0.004300000
1	0.442095000	-1.160364000	1.218929000
1	-1.008768000	-2.097630000	0.485613000
53	0.152863000	-3.646311000	2.599410000
7	-6.169191000	0.847648000	-0.544278000
8	-7.033056000	0.130414000	-1.088655000

8	-6.418230000	1.829660000	0.185398000
7	-0.073713000	4.562475000	2.265598000
8	1.026576000	5.052664000	2.598482000
8	-1.184034000	5.000289000	2.636125000
7	6.096946000	1.034139000	-0.620194000
8	6.975577000	0.341503000	-1.172751000
8	6.325041000	2.023262000	0.106762000

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