Supporting Information for

Accelerating Ni(II) precatalyst initiation using reactive ligands and its impact on chain-growth polymerizations

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I. Materials

Flash chromatography was performed on SiliCycle silica gel (40-63 μm) and thin layer chromatography was performed on Merck TLC plates pre-coated with silica gel 60 F254. *i*-PrMgCl (2 M in THF) was purchased in 100 mL quantities from Aldrich. Bis(cyclooctadiene)nickel ($Ni(cod)_2$) and 1,2-bis(diphenylphosphino)ethane (dppe) were purchased from Strem. All other reagent grade materials and solvents were purchased from Aldrich, Acros, EMD, or Fisher and used without further purification unless otherwise noted. THF was dried and deoxygenated using an Innovative Technology (IT) solvent purification system composed of activated alumina, copper catalyst, and molecular sieves. *N*-Bromosuccinimide (NBS) was recrystallized from hot water and dried over P_2O_5. Compounds **1a-d**,[1] **2**,[2] **S1**,[3] **S2**,[4] **S3**,[1] **S4**,[4] **S5**,[5] **S6**,[1] **S7**,[5] **S8**,[1] **S9**,[5] **S10**,[1] **S11**,[6] were prepared from modified literature procedures.

II. General Experimental

NMR Spectroscopy: Unless otherwise noted, ^1H, ^{13}C, ^{19}F and ^{31}P NMR spectra for all compounds were acquired at rt in acetone-d_6 or $CDCl_3$ on a Varian vnmrs 700 operating at 700, 176, 660, and 283 MHz, Varian vnmrs 500 operating at 500, 126, 470, and 202 MHz or a Varian MR 400 operating at 400, 100, 376 and 162 MHz, respectively. For ^1H and ^{13}C spectra in deuterated solvents, the chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane (TMS) and referenced with residual solvent. ^{19}F NMR spectra were referenced to $CFCl_3$ and ^{31}P NMR spectra were referenced to H_3PO_4. For ^1H, ^{19}F and ^{31}P NMR spectra in non-deuterated THF, the chemical shift data are reported in units of δ (ppm) and referenced with the THF peak at 3.58 ppm in the ^1H NMR spectrum which is then applied to all nuclei. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), multiplet (m), broad resonance (br), and apparent triplet (at).

Mass Spectrometry: HRMS data were obtained on a Micromass AutoSpec Ultima Magnetic Sector mass spectrometer.

IR Spectroscopy: Samples were recorded using a Mettler Toledo ReactIR iC10 fitted with a Mercury Cadmium Telluride (MCT) detector, and AgX probe (9.5 mm x 1.5 mm) with a SiComp tip. The spectra were processed using icIR 4.0 software and raw absorbances were exported into Microsoft Excel or Sigma Plot 10 for analysis.

MALDI-TOF MS: MALDI-TOF mass spectra were recorded using Waters Tofspec-2E in reflectron mode at a unit mass resolution of 4000. The matrix, α-cyano-4-hydroxy-cinnamic acid (CHCA), was prepared at a concentration of 10 mg/mL in a solution of 50/50 (v/v) CH_3CN/EtOH. The instrument was mass calibrated with a mixture of peptides in the CHCA matrix. The polymer sample was dissolved in CH_2Cl_2 to obtain a ~1 mg/mL solution. A 3 μL aliquot of polymer solution was mixed with 3 μL of the matrix solution. This mixture (1 μL) was placed on the target plate and then air-dried.

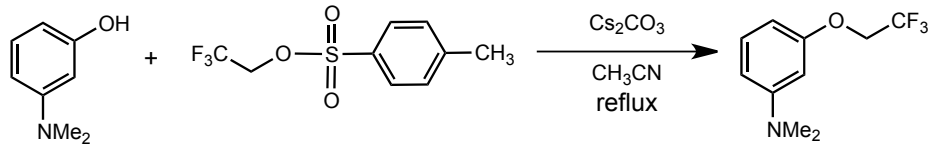
Gel-Permeation Chromatography: Polymer molecular weights were determined by

comparison with polystyrene standards (Varian, EasiCal PS-2 MW 580-377,400) on a Waters 1515 HPLC instrument equipped with Waters Styragel® (7.8 x 300 mm) THF HR 0.5, THF HR 1, and THF HR 4 type columns in sequence and analyzed with Waters 2487 dual absorbance detector (254 nm). Samples were dissolved in THF (with mild heating) and passed through a 0.2 μm PTFE filter prior to analysis.

Titrations of the Grignard Reagents: An accurately weighed sample of salicylaldehyde phenylhydrazone[7] (typically between 290-310 mg) was dissolved in 5.00 mL of THF. A 0.50 mL aliquot of this solution was stirred at rt while ArMgCl was added dropwise using a 500 μL syringe. The initial solution is yellow and turns bright orange at the end-point.

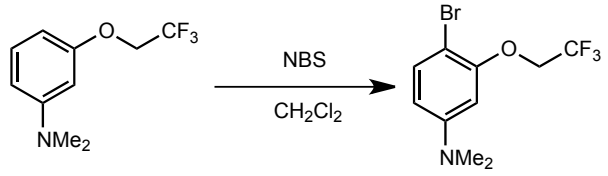
Statistical Analysis: Reported quantitative data represents the average of 2-3 experiments and the error bars represent the standard deviation in these measurements.

III. Synthetic Procedures



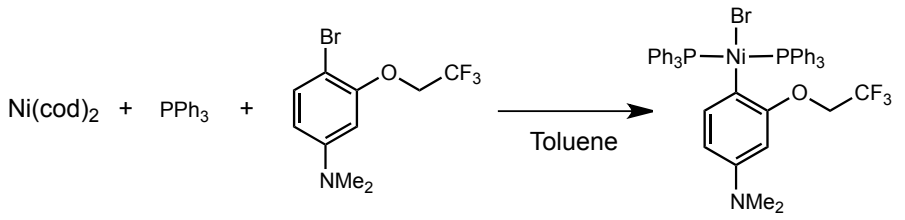
S1

S1. A 100 mL round-bottom flask was equipped with a stir bar. Sequentially, 3-(dimethylamino)phenol (756 mg, 5.51 mmol, 1.0 equiv), CH_3CN (40 mL), Cs_2CO_3 (3.81 g, 11.7 mmol, 2.0 equiv) and 2,2,2-trifluoroethyl tosylate (1.81 g, 7.12 mmol, 1.3 equiv) were added to the flask. The mixture was refluxed for 4 d. The reaction mixture was cooled and concentrated in vacuo. The resulting mixture was washed with brine (40 mL), extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layers were washed with water (2 x 30 mL) and brine (1 x 30 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting oil was purified with silica gel chromatography, using 10/90 (v/v) ethyl acetate/hexanes as the eluent to give 499 mg of **S1** as a clear liquid (41% yield). HRMS (EI): [M+] Calcd. for $C_{10}H_{12}F_3NO$, 219.0871; found, 219.0868. ^{19}F NMR (470 MHz, $CDCl_3$) δ -74.03 (t, $J_{H\text{-}F}$ = 8.2 Hz).



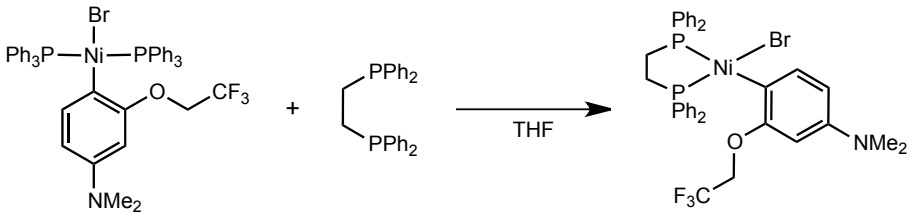
S1 **S2**

S2. A 10 mL oven-dried round-bottom flask was equipped with a stir bar. Sequentially, **S1** (210 mg, 0.96 mmol, 1.0 equiv), CH_2Cl_2 (3 mL), and NBS (180 mg, 0.99 mmol, 1.0 equiv) were added to the flask. The solution turned from clear to blue in 10 min. The solution was stirred at rt under N_2 overnight. The reaction was quenched with water (5 mL) and extracted with CH_2Cl_2 (3 x 10 mL). The combined organic layers were washed with water (2 x 20 mL) and brine (1 x 20 mL), then dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting oil was purified with prep HPLC, using 5/95 (v/v) ethyl acetate/hexanes as the eluent to give 114 mg of **S2** as a clear liquid (40% yield). HRMS (EI): [M+] Calcd. for $C_{10}H_{11}BrF_3NO$, 296.9976; found, 296.9975. ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.93 (t, $J_{H\text{-}F}$ = 8.2 Hz).



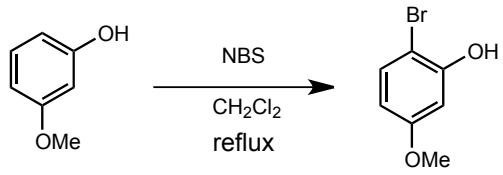
S2 **S3**

S3. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $Ni(cod)_2$ (70.1 mg, 0.255 mmol, 1.0 equiv), PPh_3 (135 mg, 0.515 mmol, 2.0 equiv), **S2** (83.7 mg, 0.281 mmol, 1.1 equiv), and toluene (2.5 mL) were added. The solution was stirred at rt overnight. The reaction was removed from the glovebox. Addition of hexanes (18 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL) and cold MeOH (5 mL). The resulting solid was recrystallized in THF/hexanes to give 85 mg of **S3** as a yellow solid (39% yield). ^{19}F NMR (470 MHz, CD_2Cl_2) δ -72.72.



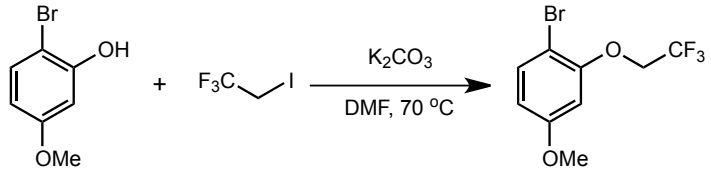
S3 **1a**

1a. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, **S3** (222 mg, 0.252 mmol, 1.0 equiv), dppe (112 mg, 0.281 mmol, 1.1 equiv), and THF (5 mL) were added. The solution was stirred at rt for 2 h. The deep red solution was concentrated in vacuo until ~2 mL of solution was left. Addition of hexanes (18 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL). The resulting solid was recrystallized in THF/hexanes to give 153 mg of **1a** as an orange solid (81% yield). ^{19}F NMR (376 MHz, acetone-d_6) δ -73.64 (t, $J_{H\text{-}F}$ = 9.5 Hz).



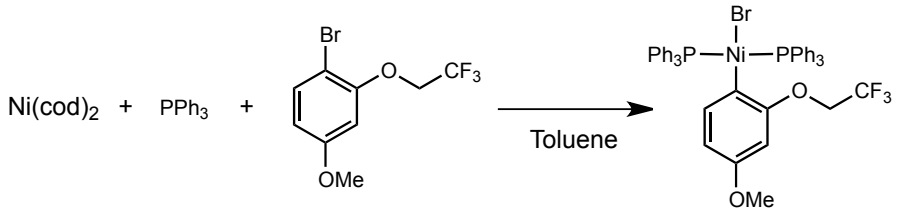
S4

S4. A 100 mL round-bottom flask was equipped with a stir bar. Sequentially, 3-methoxyphenol (1.3 mL, 12 mmol, 1.0 equiv), CH_2Cl_2 (36 mL), and NBS (2.15 g, 12.1 mmol, 1.0 equiv) were added to the flask. The flask was connected to condenser and the reaction was refluxed under N_2 for 2 d. The reaction was cooled to rt and quenched with water (40 mL). The organic layer was washed with water (1 x 40 mL) and brine (1 x 40 mL), then dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting oil was purified with silica gel chromatography, using 10/90 (v/v) ethyl acetate/hexanes as the eluent to give 1.167 g of **S4** as a clear liquid (48% yield). HRMS (EI): [M+] Calcd. for $C_{10}H_{11}BrF_3NO$, 201.9629; found, 201.9637.



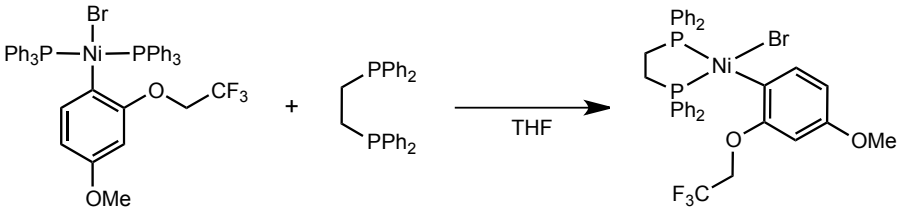
S4 **S5**

S5. A 35 mL bomb flask was equipped with a stir bar. Sequentially, **S4** (812 mg, 4.00 mmol, 1.0 equiv), DMF (12 mL), K_2CO_3 (1.66 g, 12.0 mmol, 3.0 equiv) and 2-iodo-1,1,1-trifluoroethane (1.6 mL, 16 mmol, 4.0 equiv) were added to the flask. The flask was capped and the reaction was heated to 70 °C for 6 d. Once cooled to rt, the reaction mixture was quenched with water (30 mL) and extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layers were washed with water (2 x 50 mL) and brine (1 x 50 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting oil was purified with silica gel chromatography, using 5/95 (v/v) ethyl acetate/hexanes as the eluent to give 865 mg of **S5** as a clear liquid (76% yield). HRMS (EI): [M+] Calcd. for $C_9H_8BrF_3O_2$, 283.9660; found, 283.9662. ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.87 (t, J_{H-F} = 8.3 Hz).



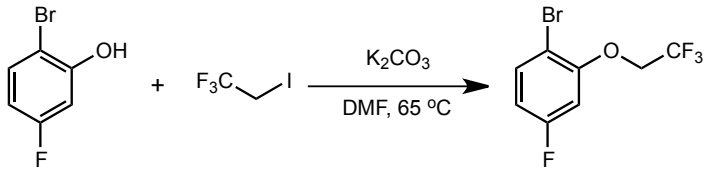
S5 **S6**

S6. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $Ni(cod)_2$ (281.5 mg, 1.023 mmol, 1.0 equiv), PPh_3 (537.5 mg, 2.049 mmol, 2.0 equiv), **S5** (314.0 mg, 1.102 mmol, 1.1 equiv), and toluene (10 mL) were added. The solution was stirred at rt for 2 h. The reaction was removed from the glovebox and transferred to a 100 mL round-bottom flask. The deep red solution was concentrated in vacuo until ~3 mL of solution was left. Addition of hexanes (50 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL) and cold MeOH (5 mL). The resulting solid was recrystallized in THF/hexanes to give 431.6 mg of **S6** as a yellow solid (50% yield). Elemental Analysis: Calcd for $C_{45}H_{38}BrF_3NiO_2P_2$, C, 62.24; H, 4.41; F, 6.56; Found C, 62.19; H, 4.47; F, 6.77. ^{19}F NMR (470 MHz, CD_2Cl_2) δ -72.66.



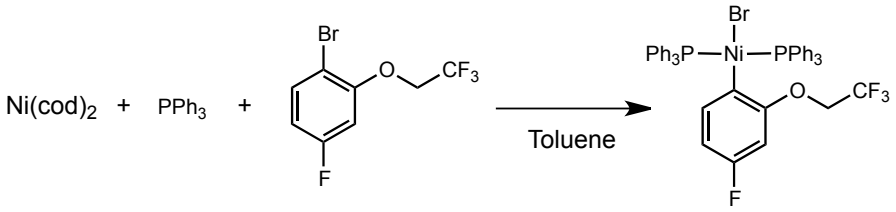
S6 **1b**

1b. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, **S6** (347.4 mg, 0.4001 mmol, 1.0 equiv), dppe (178.1 mg, 0.4470 mmol, 1.1 equiv), and THF (8 mL) were added. The solution was stirred at rt for 2 h. The deep red solution was concentrated in vacuo until ~2 mL of solution was left. Addition of hexanes (18 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL). The resulting solid was recrystallized in THF/hexanes to give 214.3 mg of **1b** as an orange solid (72% yield). Elemental Analysis: Calcd for $C_{35}H_{32}BrF_3NiO_2P_2$, C, 56.64; H, 4.35; F, 7.68; Found C, 56.75; H, 4.64; F, 7.41. ^{19}F NMR (470 MHz, acetone-d_6) δ -73.57 (t, $J_{H\text{-}F}$ = 6.7 Hz).



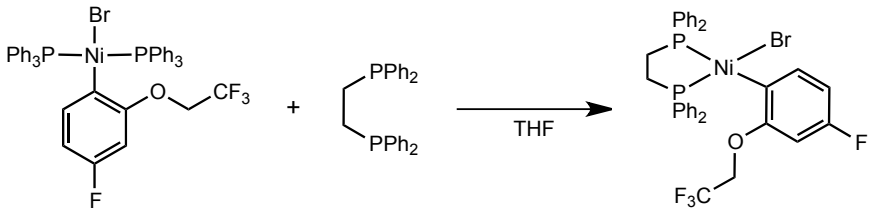
S7

S7. A 35 mL bomb flask was equipped with a stir bar. Sequentially, 2-bromo-5-fluorophenol (0.92 mL, 8.2 mmol, 1.0 equiv), DMF (18 mL), K_2CO_3 (3.40 g, 24.6 mmol, 3.0 equiv) and 2-iodo-1,1,1-trifluoroethane (3.2 mL, 33 mmol, 4.0 equiv) were added to the flask. The flask was capped and the reaction mixture was heated to 65 °C for 14 d. Once cooled to rt, the reaction mixture was quenched with water (40 mL) and extracted with CH_2Cl_2 (3 x 40 mL). The combined organic layers were washed with water (2 x 100 mL) and brine (1 x 100 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting oil was purified with silica gel chromatography, using 2/98 (v/v) ethyl acetate/hexanes as the eluent to give 1.67 g of **S7** as a clear liquid (75% yield). HRMS (EI): [M+] Calcd. for $C_8H_5BrF_4O$, 271.9460; found, 271.9456. ^{19}F NMR (470 MHz, $CDCl_3$) δ -74.24 (t, J_{H-F} = 8.3 Hz), -111.54 (q, J_{H-F} = 8.2 Hz).



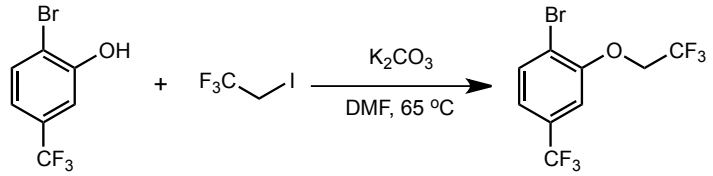
S7 **S8**

S8. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $Ni(cod)_2$ (276.2 mg, 1.004 mmol, 1.0 equiv), PPh_3 (525.3 mg, 2.003 mmol, 2.0 equiv), **S7** (410.8 mg, 1.505 mmol, 1.5 equiv), and toluene (10 mL) were added. The solution was stirred at rt for 3 h. The reaction was removed from the glovebox and transferred to a 100 mL round-bottom flask. Addition of hexanes (50 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL) and cold MeOH (5 mL). The resulting solid was dried in vacuo to give 663.6 mg of **S8** as a yellow solid (78% yield). Elemental Analysis: Calcd for $C_{44}H_{35}BrF_4NiOP_2$, C, 61.72; H, 4.12; F, 8.87; Found C, 61.99; H, 4.32; F, 8.97. ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.28 (t, J_{H-F} = 7.0 Hz), -123.50.



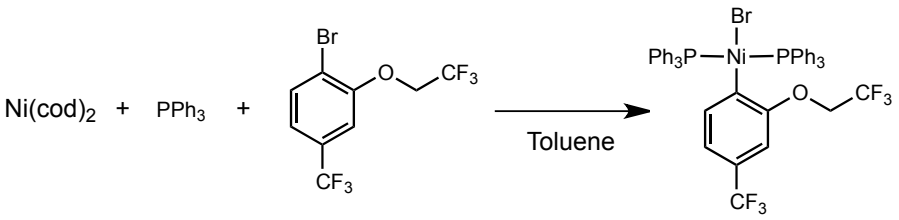
S8 **1c**

1c. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, **S8** (428.5 mg, 0.5004 mmol, 1.0 equiv), dppe (219.3 mg, 0.5504 mmol, 1.1 equiv), and THF (10 mL) were added. The solution was stirred at rt for 2 h. The deep red solution was concentrated in vacuo until ~1 mL of solution was left. Addition of hexanes (18 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL). The resulting solid was recrystallized in THF/hexanes to give 181.7 mg of **1c** as an orange solid (50% yield). Elemental Analysis: Calcd for $C_{34}H_{29}BrF_4NiOP_2$, C, 55.93; H, 4.00; F, 10.41; Found C, 56.04; H, 4.18; F, 10.16. ^{19}F NMR (470 MHz, acetone-d_6) δ -73.53 (t, $J_{H\text{-}F}$ = 8.2 Hz), -123.65 (q, $J_{H\text{-}F}$ = 8.6 Hz).



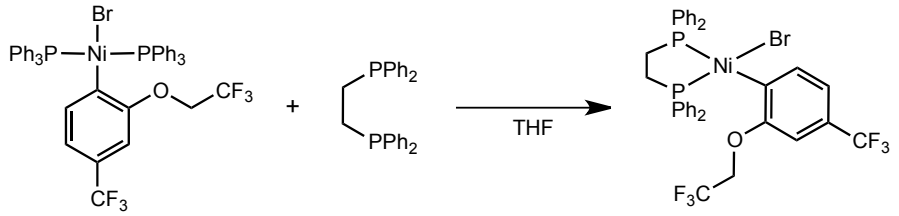
S9

S9. A 35 mL bomb flask was equipped with a stir bar. Sequentially, 2-bromo-5-trifluoromethylphenol (1.98 g, 8.22 mmol, 1.0 equiv), DMF (18 mL), K_2CO_3 (3.40 g, 24.6 mmol, 3.0 equiv) and 2-iodo-1,1,1-trifluoroethane (3.2 mL, 33 mmol, 4.0 equiv) were added to the flask. The flask was capped and the reaction mixture was heated to 65 °C for 14 d. Once cooled to rt, the reaction mixture was quenched with water (40 mL) and extracted with CH_2Cl_2 (3 x 40 mL). The combined organic layers were washed with water (2 x 100 mL) and brine (1 x 100 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting oil was purified with silica gel chromatography, using 2/98 (v/v) ethyl acetate/hexanes as the eluent to give 1.39 g of **S9** as a clear liquid (53% yield). HRMS (EI): [M+] Calcd. for $C_9H_5BrF_6O$, 321.9428; found, 321.9428. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.80, -73.82 (t, $J_{H\text{-}F}$ = 8.2 Hz).



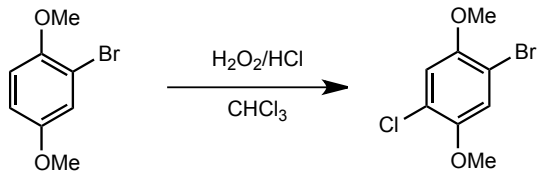
S9 **S10**

S10. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $Ni(cod)_2$ (140.1 mg, 0.5093 mmol, 1.0 equiv), PPh_3 (262.9 mg, 1.002 mmol, 2.0 equiv), **S9** (194.1 mg, 0.6008 mmol, 1.2 equiv), and toluene (5 mL) were added. The solution was stirred at rt for 3 h. The reaction was removed from the glovebox and transferred to a 100 mL round-bottom flask. The deep red solution was concentrated in vacuo until ~2 mL of solution was left. Addition of hexanes (40 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL) and cold MeOH (5 mL). The resulting solid was dried in vacuo to give 226.1 mg of **S10** as a yellow solid (50% yield). Elemental Analysis: Calcd for $C_{45}H_{35}BrF_6NiOP_2$, C, 59.64; H, 3.89; F, 12.58; Found C, 59.94; H, 3.91; F, 12.29. ^{19}F NMR (470 MHz, $CDCl_3$) δ -61.82, -72.18 (t, $J_{H\text{-}F}$ = 8.4 Hz).



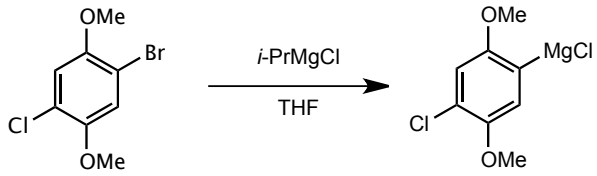
S10 **1d**

1d. A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, **S10** (383.1 mg, 0.4227 mmol, 1.0 equiv), dppe (186.2 mg, 0.4673 mmol, 1.1 equiv), and THF (10 mL) were added. The solution was stirred at rt for 2 h. The deep red solution was concentrated in vacuo until ~1 mL of solution was left. Addition of hexanes (18 mL) led to a yellow orange precipitate. The solid was filtered and washed with hexanes (20 mL). The resulting solid was recrystallized in THF/hexanes to give 241.9 mg of **1d** as an orange solid (74% yield). Elemental Analysis: Calcd for $C_{35}H_{29}BrF_6NiOP_2$, C, 53.88; H, 3.75; F, 14.61; Found C, 54.40; H, 4.01; F, 14.21. ^{19}F NMR (470 MHz, acetone-d_6) δ –61.93, -73.51.



S11

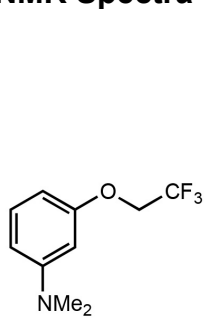
S11. A 100 mL round-bottom flask was equipped with a stir bar. Sequentially, 2-bromo-1,4-dimethoxybenzene (1.90 g, 8.75 mmol, 1.0 equiv) and $CHCl_3$ (7.5 mL) were added to the flask. Then, HCl (6 mL, 12 M) was added slowly. While stirring the reaction mixture vigorously, 30% H_2O_2 in H_2O (3.75 mL, 36.3 mmol, 4.0 equiv) was added via syringe pump over 45 min. The solution was stirred at rt overnight. The reaction mixture was extracted with $CHCl_3$ (3 x 25 mL). The combined organic layers were washed with 5% $NaHCO_3$ solution (1 x 50 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo. The resulting solid was purified with silica gel chromatography, using 50/50 (v/v) hexanes/CH_2Cl_2 as the eluent to give 1.495 g of **S11** as a off-white solid (68% yield). HRMS (EI): [M+] Calcd. for $C_8H_8BrClO_2$, 249.9396; found, 249.9403.



S11 **2**

2. All actions were performed in a glovebox under N_2 atmosphere. A 20 mL vial was equipped with a stir bar. Sequentially, **S11** (240 mg, 0.955 mmol, 1.0 equiv), THF (1.0 mL), and *i*-PrMgCl (0.43 mL, 0.86 mmol, 0.9 equiv) were added to the flask. The reaction mixture was stirred at rt for 8 h.

IV. NMR Spectra



S1

Figure S1. ^{1}H and ^{13}C NMR spectra of **S1**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.17 (t, J = 8.3 Hz, 1H), 6.44 (dd, J = 8.3, 2.3 Hz, 1H), 6.32 (t, J = 2.4 Hz, 1H), 6.27 (dd, J = 8.0, 2.4 Hz, 1H), 4.34 (q, $J_{H\text{-}F}$ = 8.1 Hz, 2H), 2.95 (s, 6H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 158.76, 152.20, 130.06, 123.65 (q, $J_{C\text{-}F}$ = 277.9 Hz), 107.30, 101.71, 100.19, 65.97 (q, $J_{C\text{-}F}$ = 35.7 Hz), 40.59.

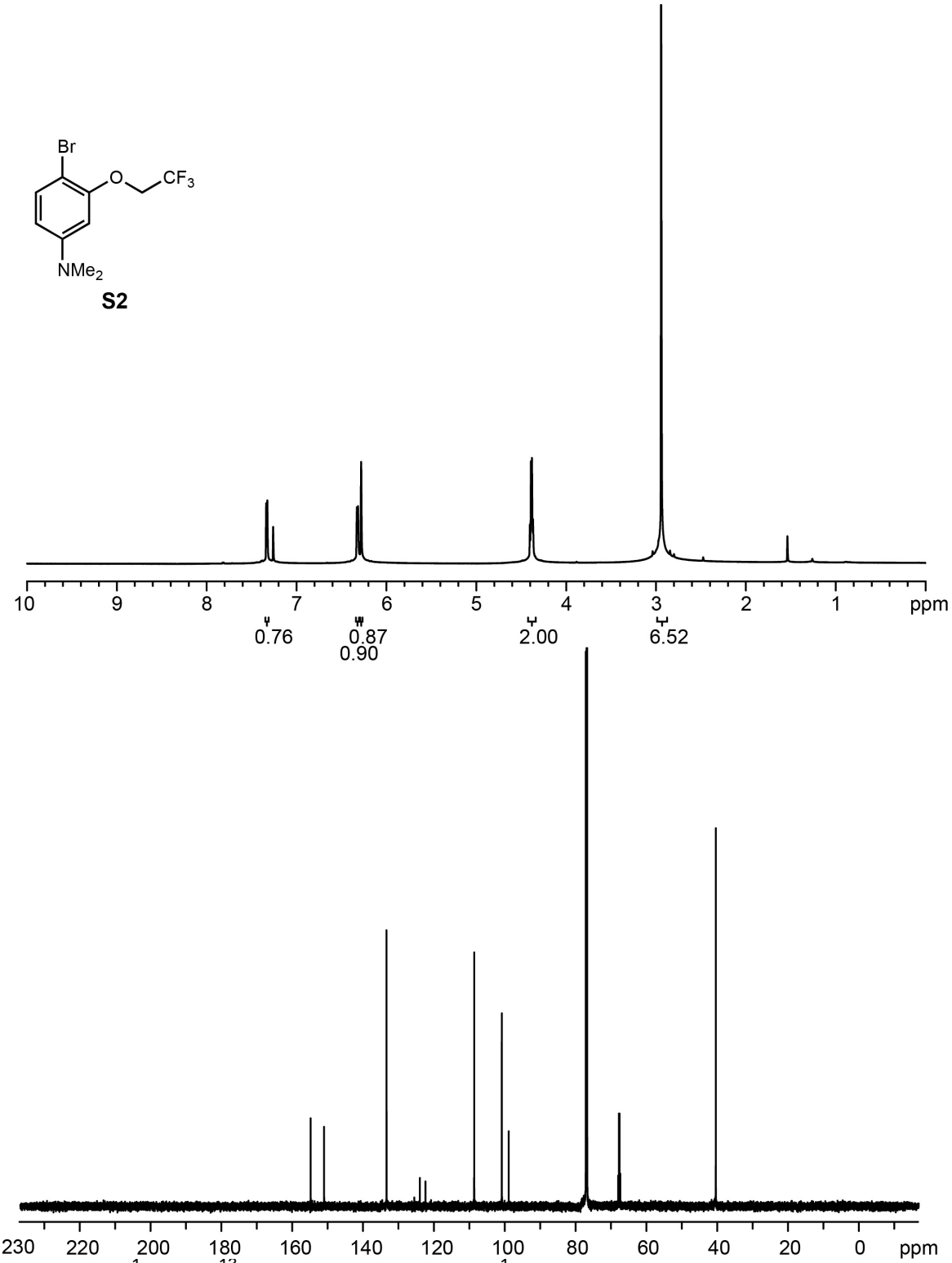


Figure S2. ^{1}H and ^{13}C NMR spectra of **S2**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.33 (d, J = 8.6 Hz, 1H), 6.32 (d, J = 8.5 Hz, 1H), 6.28 (s, 1H), 4.39 (q, $J_{H\text{-}F}$ = 8.0 Hz, 2H), 2.94 (s, 6H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 155.05, 151.27, 133.63, 123.42 (q, $J_{C\text{-}F}$ = 278.3 Hz), 108.87, 101.08, 99.13, 67.93 (q, $J_{C\text{-}F}$ = 35.4 Hz), 40.66.

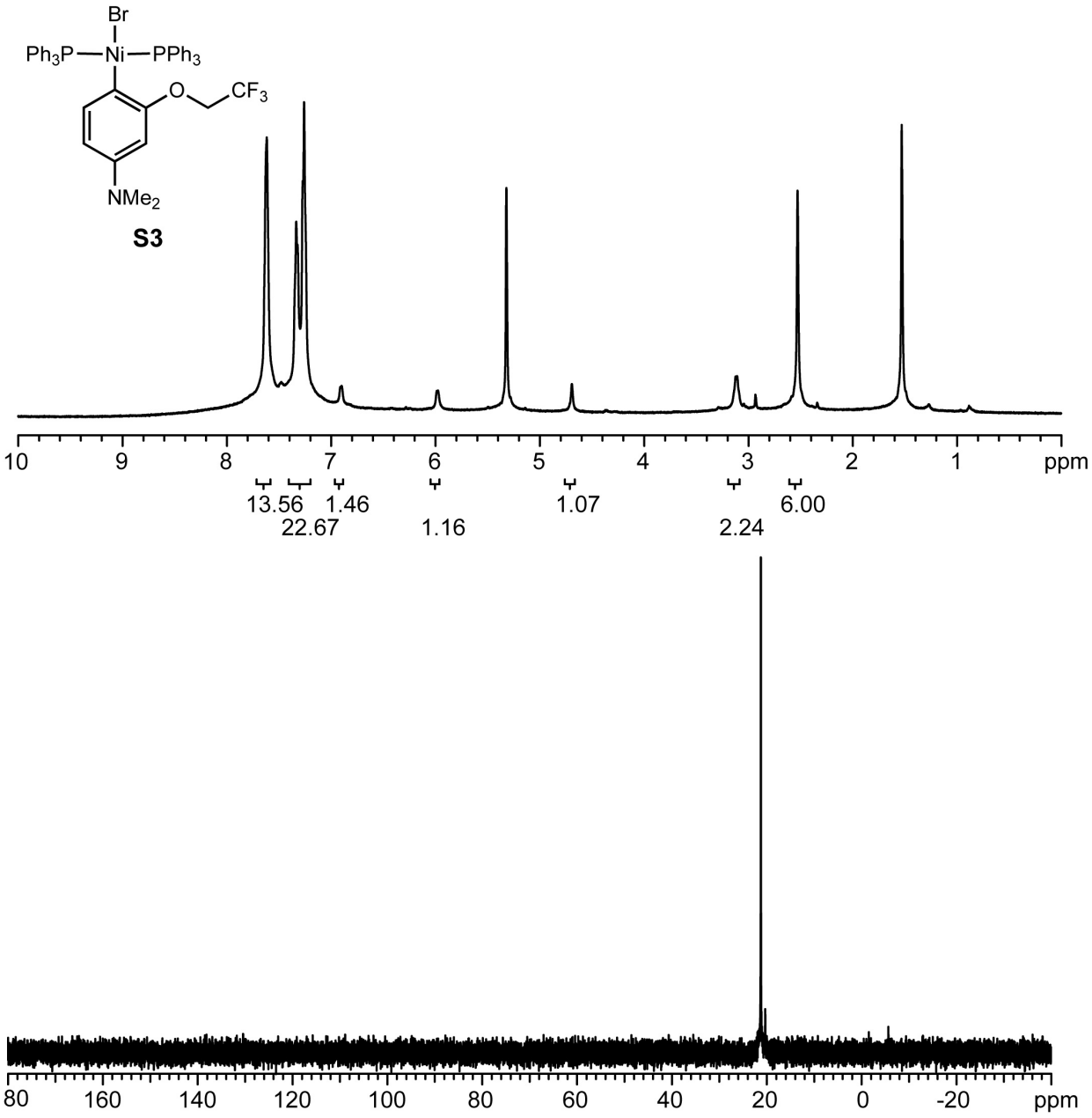


Figure S3. ^{1}H and ^{31}P NMR spectra of **S3**. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.62 (bs, 12H), 7.34-7.26 (m, 18H), 6.90 (d, *J* = 5.9 Hz, 1H), 5.97 (t, *J* = 5.9 Hz, 1H), 4.69 (s, 1H), 3.11 (q, *J* = 7.2 Hz, 2H), 2.53 (s, 6H). ^{31}P NMR (202 MHz, CD_2Cl_2) δ 21.22.

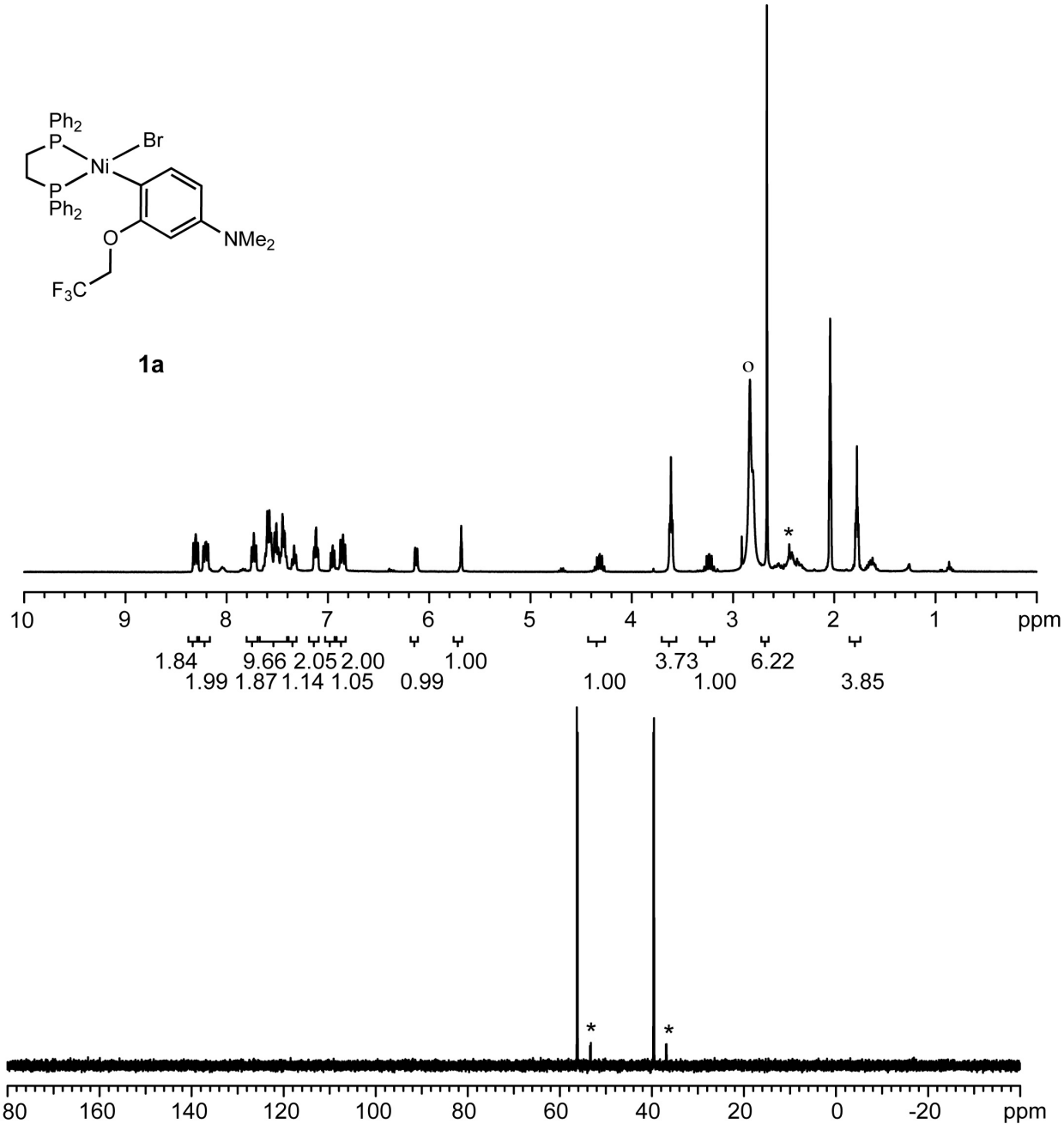


Figure S4. ^{1}H and ^{31}P NMR spectra of **1a**. ^{1}H NMR (400 MHz, acetone-d_6) δ 8.31 (at, J = 8.8 Hz, 2H), 8.23-8.18 (m, 2H), 7.73 (at, J = 8.5 Hz, 2H), 7.62-7.41 (m, 9H), 7.33 (at, J = 7.0 Hz, 1H), 7.14-7.10 (m, 2H), 6.95 (at, J = 6.8 Hz, 1H), 6.88-6.83 (m, 2H), 6.12 (d, J = 8.3 Hz, 1H), 5.68 (s, 1H), 4.32 (m, 1H), 3.61 (t, J = 6.0 Hz, 3H), 3.24 (m, 1H), 2.67 (s, 6H), 1.79-1.76 (m, 4H). residual °H_2O and *impurity. ^{31}P NMR (162 MHz, acetone-d_6) δ 56.21 (d, J = 26.5 Hz), 39.60 (d, J = 26.5 Hz).

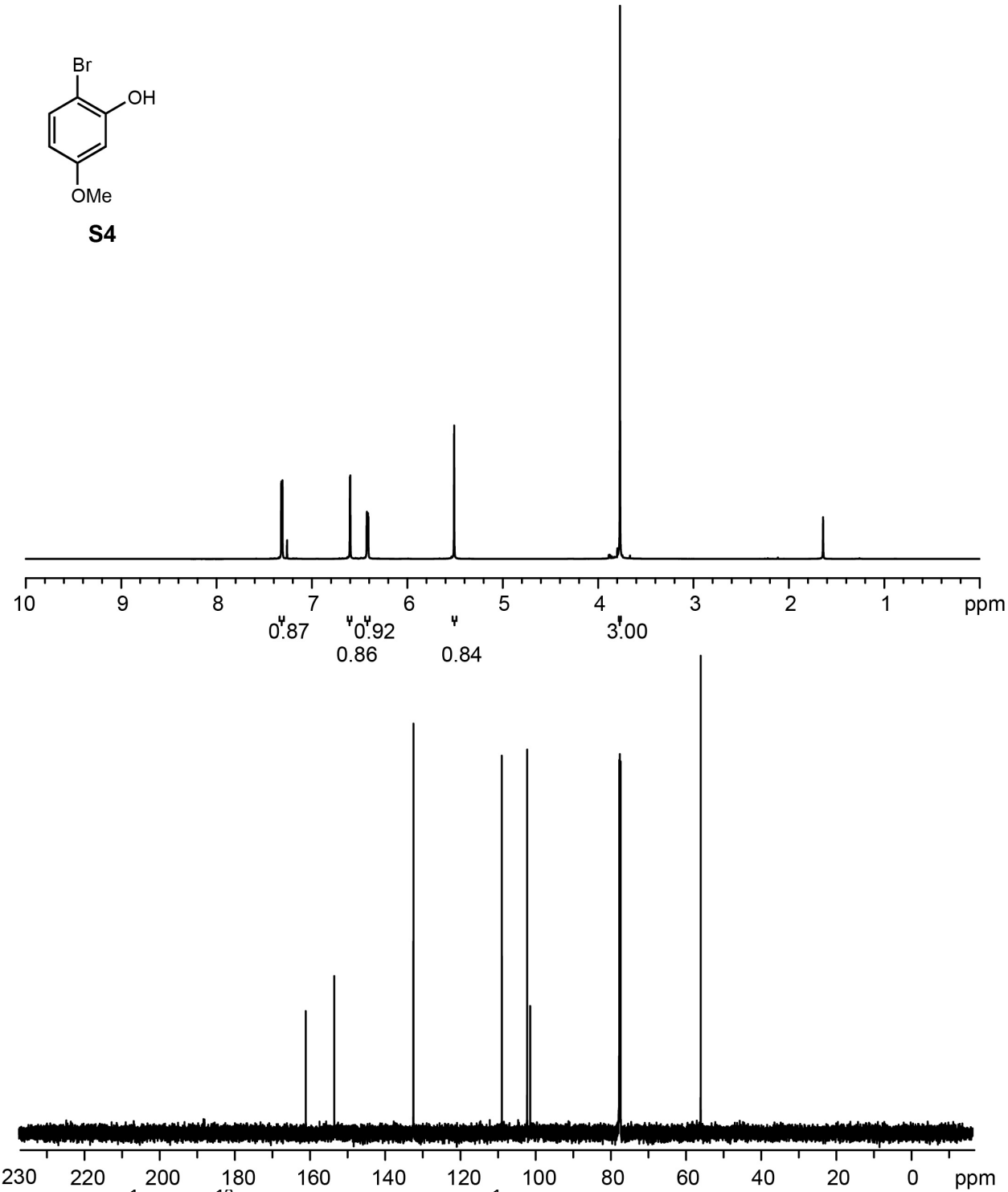


Figure S5. ^{1}H and ^{13}C NMR spectra of **S4**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.8 Hz, 1H), 6.60 (d, *J* = 2.9 Hz, 1H), 6.42 (dd, *J* = 8.8, 2.9 Hz, 1H), 5.51 (s, 1H), 3.77 (s, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 160.73, 153.14, 132.09, 108.57, 101.82, 101.02, 55.67.

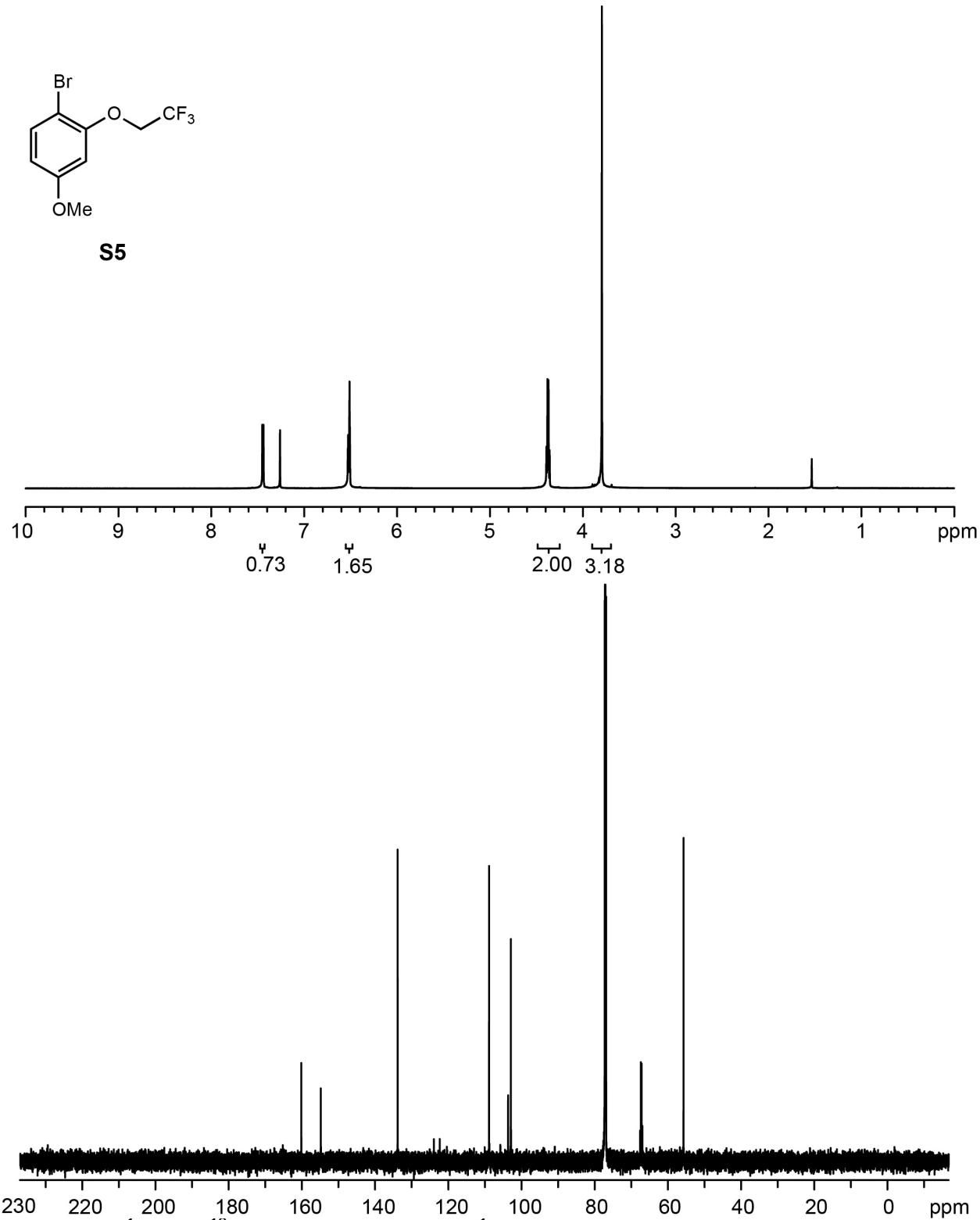


Figure S6. ^{1}H and ^{13}C NMR spectra of **S5**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.44 (d, J = 8.5 Hz, 1H), 6.53 (m, 2H), 4.37 (q, J_{H-F} = 8.1 Hz, 2H), 3.79 (s, 1H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 160.26, 154.92, 133.93, 123.23 (q, J_{C-F} = 278.5 Hz), 108.97, 103.76, 103.01, 67.39 (q, J_{C-F} = 35.9 Hz), 55.82.

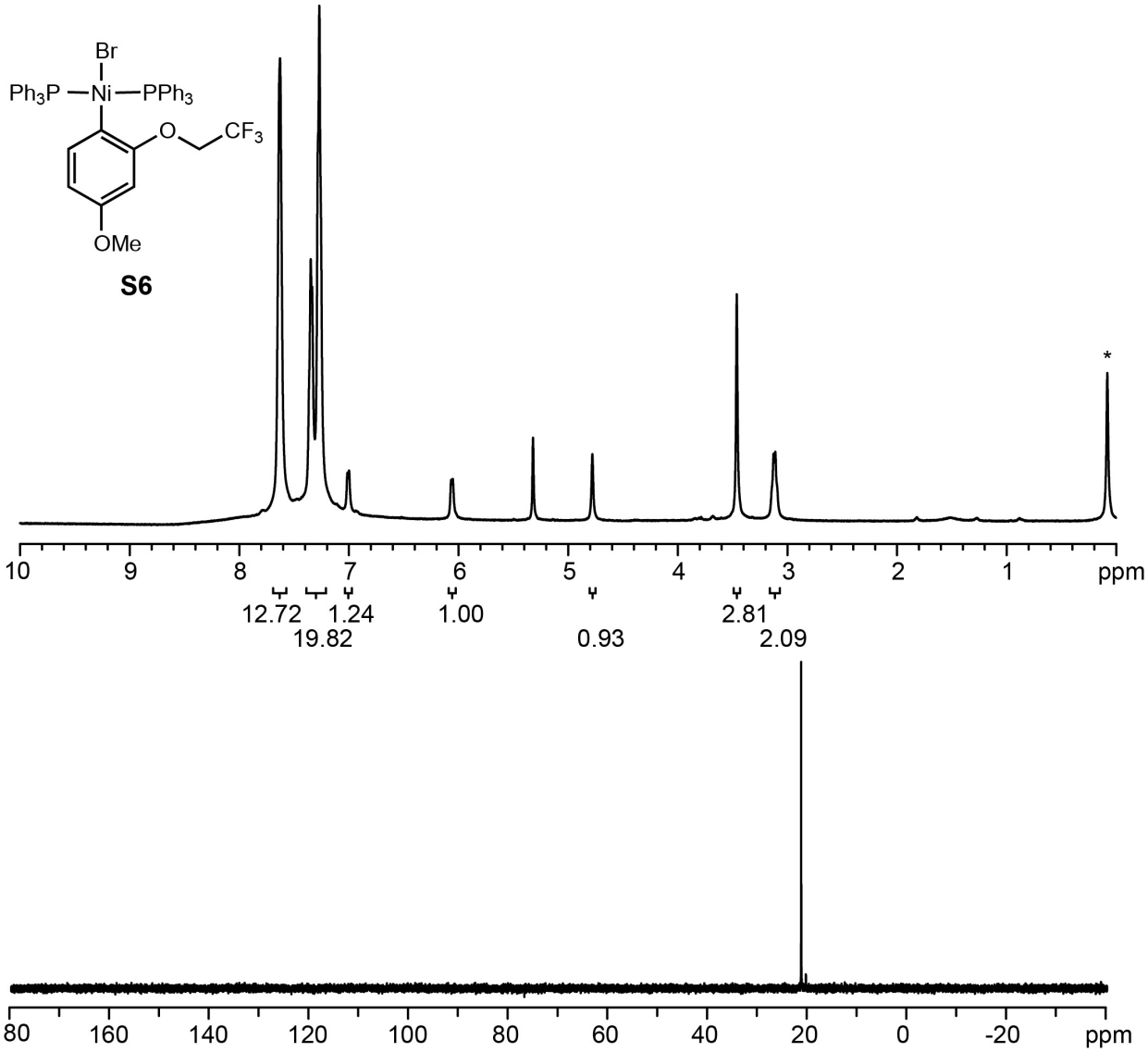


Figure S7. ^{1}H and ^{31}P NMR spectra of **S6**. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.63 (bs, 12H), 7.36-7.26 (m, 18H), 7.01 (d, J = 7.7 Hz, 1H), 6.06 (at, J = 7.7 Hz, 1H), 4.78 (s, 1H) 3.46 (s, 3H), 3.12 (q, $J_{H\text{-}F}$ = 8.4 Hz, 2H). *residual grease. ^{31}P NMR (202 MHz, CD_2Cl_2) δ 21.43.

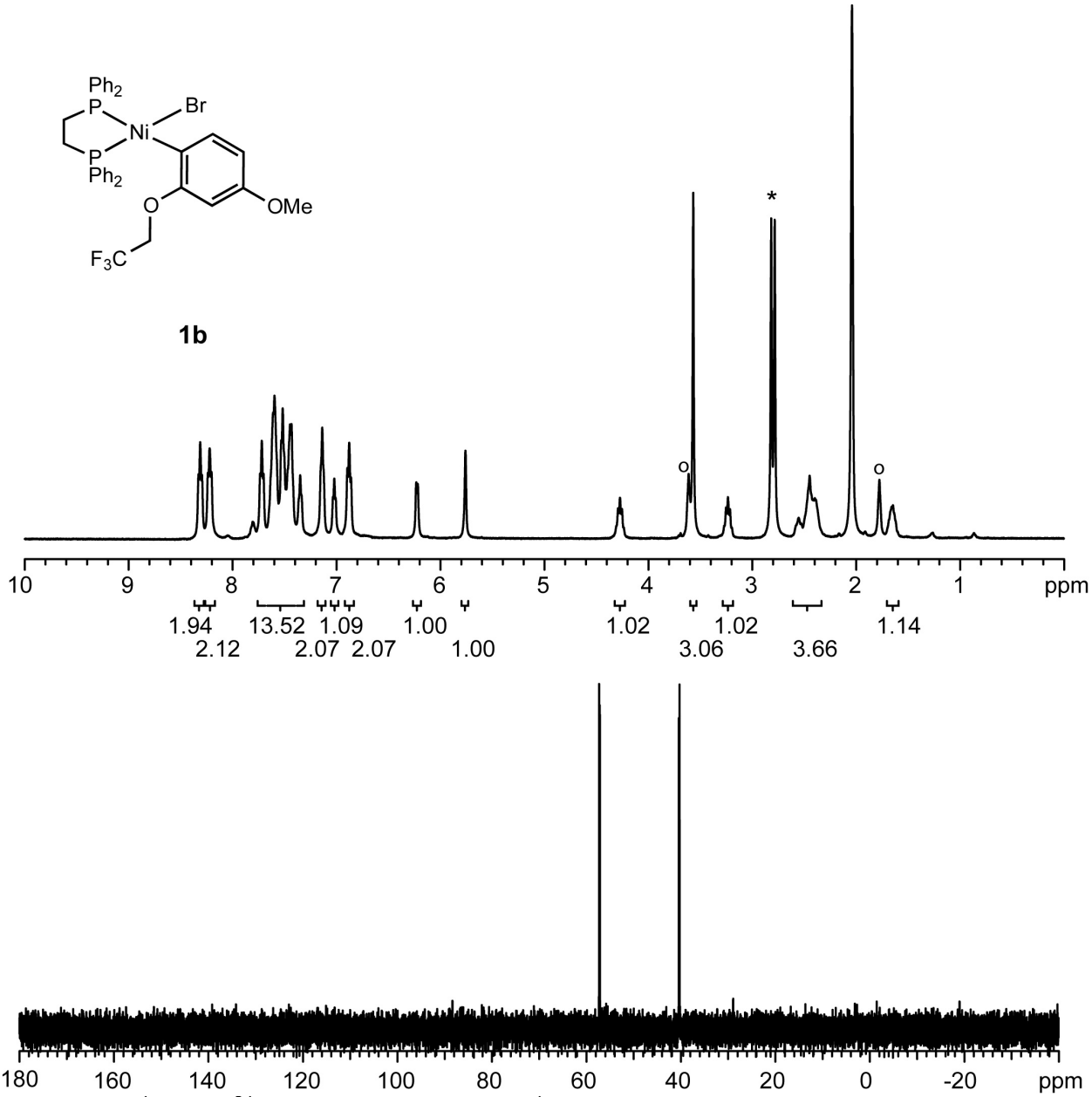


Figure S8. ^{1}H and ^{31}P NMR spectra of **1b**. ^{1}H NMR (500 MHz, acetone-d_6) δ 8.31 (at, J = 8.6 Hz, 2H), 8.22 (at, J = 8.6 Hz, 2H), 7.72-7.35 (m, 13H), 7.15-7.12 (m, 2H), 7.02 (at, J = 6.3 Hz, 1H), 6.88 (at, J = 9.0 Hz, 2H), 6.23 (d, J = 7.0 Hz, 1H), 5.76 (s, 1H), 4.27 (m, 1H), 3.57 (s, 3H), 3.23 (m, 1H), 2.55-2.40 (m, 3H), 1.78 (s, 1H), 1.62 (m, 1H). residual *H_2O and °THF. ^{31}P NMR (200 MHz, acetone-d_6) δ 57.23 (d, J = 28.9 Hz), 40.34 (d, J = 28.9 Hz).

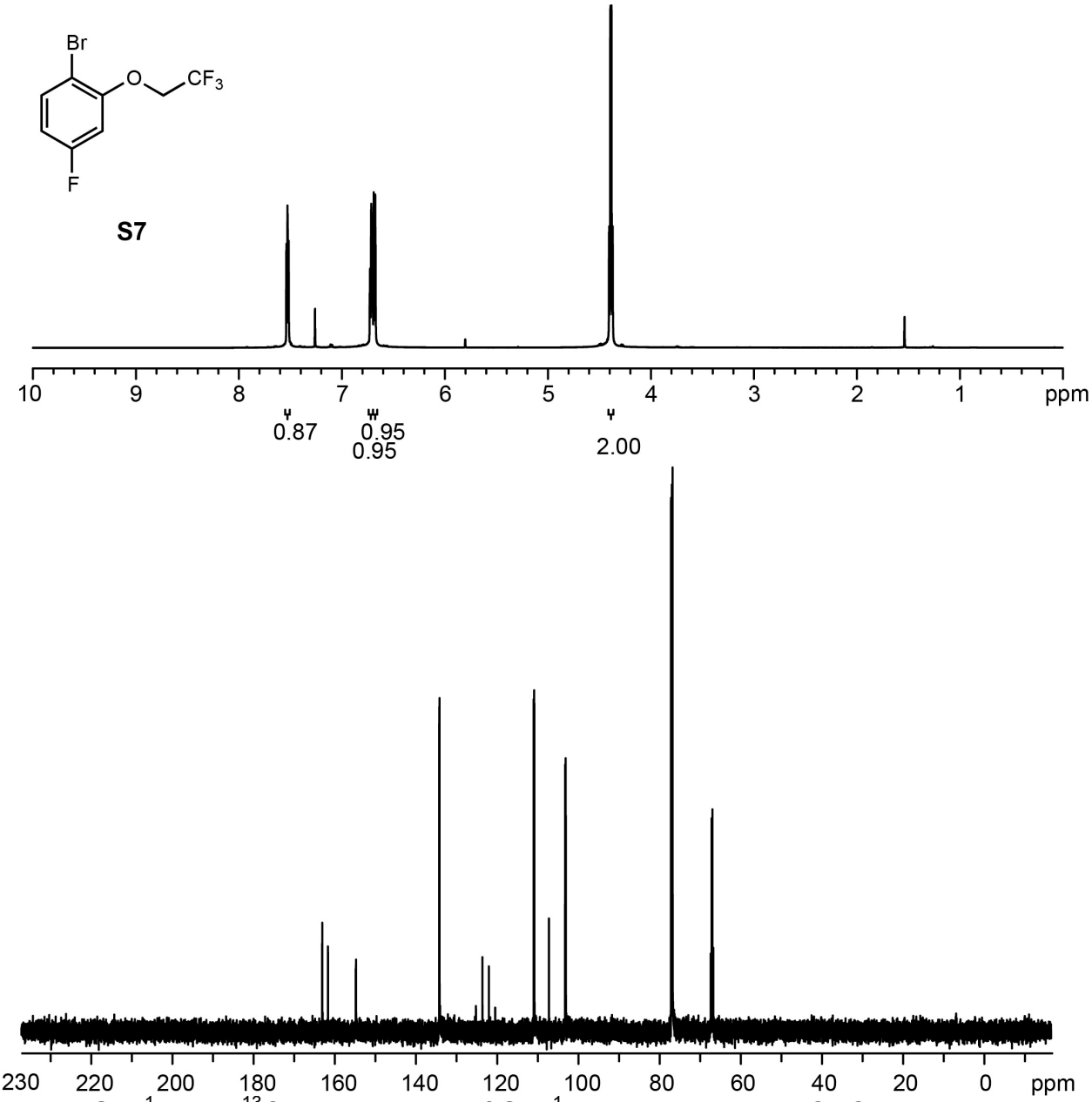


Figure S9. ^{1}H and ^{13}C NMR spectra of **S7**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.53 (at, J = 7.4 Hz, 1H), 6.71 (at, J = 8.1 Hz, 1H), 6.68 (d, J = 9.8 Hz, 1H), 4.39 (q, J_{H-F} = 8.1 Hz, 2H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 162.55 (d, J_{C-F} = 248.0 Hz), 154.96 (d, J_{C-F} = 9.5 Hz), 134.41 (d, J_{C-F} = 9.7 Hz), 123.02 (q, J_{C-F} = 278.6 Hz), 111.11 (d, J_{C-F} = 21.9 Hz), 107.42, 103.37 (d, J_{C-F} = 26.5 Hz), 67.27 (q, J_{C-F} = 36.0 Hz).

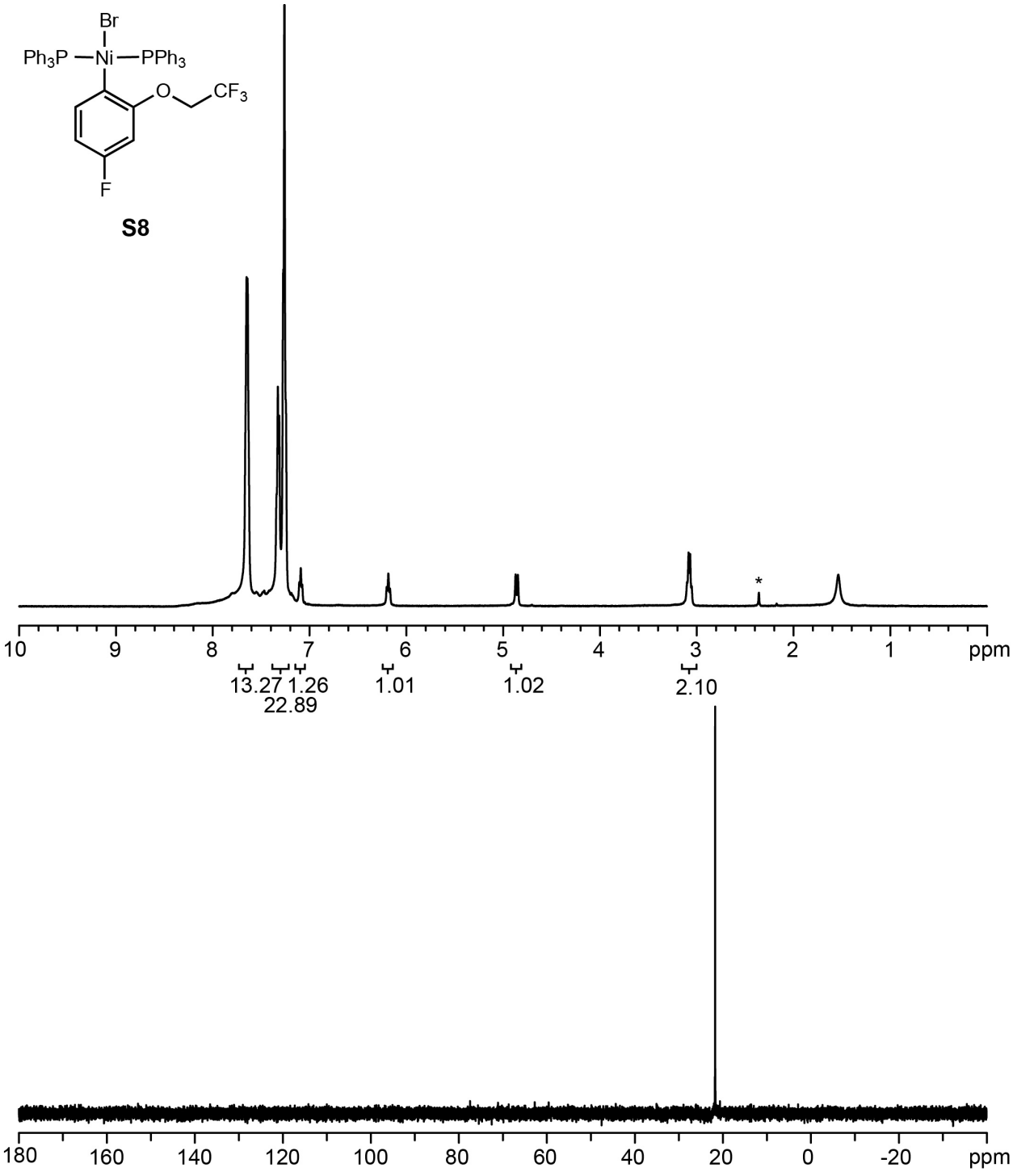
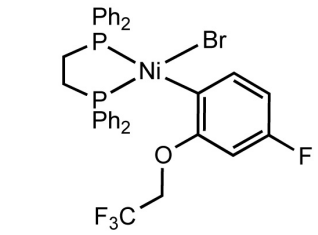


Figure S10. ^{1}H and ^{31}P NMR spectra of **S8**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (bs, 12H), 7.34-7.24 (m, 18H), 7.09 (at, *J* = 7.8 Hz, 1H), 6.19 (at, *J* = 8.7 Hz, 1H), 4.86 (d, *J* = 11.9 Hz, 1H), 3.08 (q, J_{H-F} = 8.4 Hz, 2H). *residual toluene. ^{31}P NMR (202 MHz, $CDCl_3$) δ 21.76.



1c

Figure S11. ^{1}H and ^{31}P NMR spectra of **1c**. ^{1}H NMR (500 MHz, acetone-d_6) δ 8.33 (at, J = 8.9 Hz, 2H), 8.25 (at, J = 8.3 Hz, 2H), 7.72-7.39 (m, 13H), 7.20-7.12 (m, 3H), 6.93 (at, J = 9.1 Hz, 2H), 6.36 (at, J = 7.7 Hz, 1H), 5.94 (d, J = 12.3 Hz, 1H), 4.30 (m, 1H), 3.32 (m, 1 H), 2.59-2.43 (m, 3H), 1.79-1.66 (m, 1H). residual *H_2O and °THF. ^{31}P NMR (200 MHz, acetone-d_6) δ 58.46 (d, J = 30.5 Hz), 41.26 (d, J = 30.5 Hz).

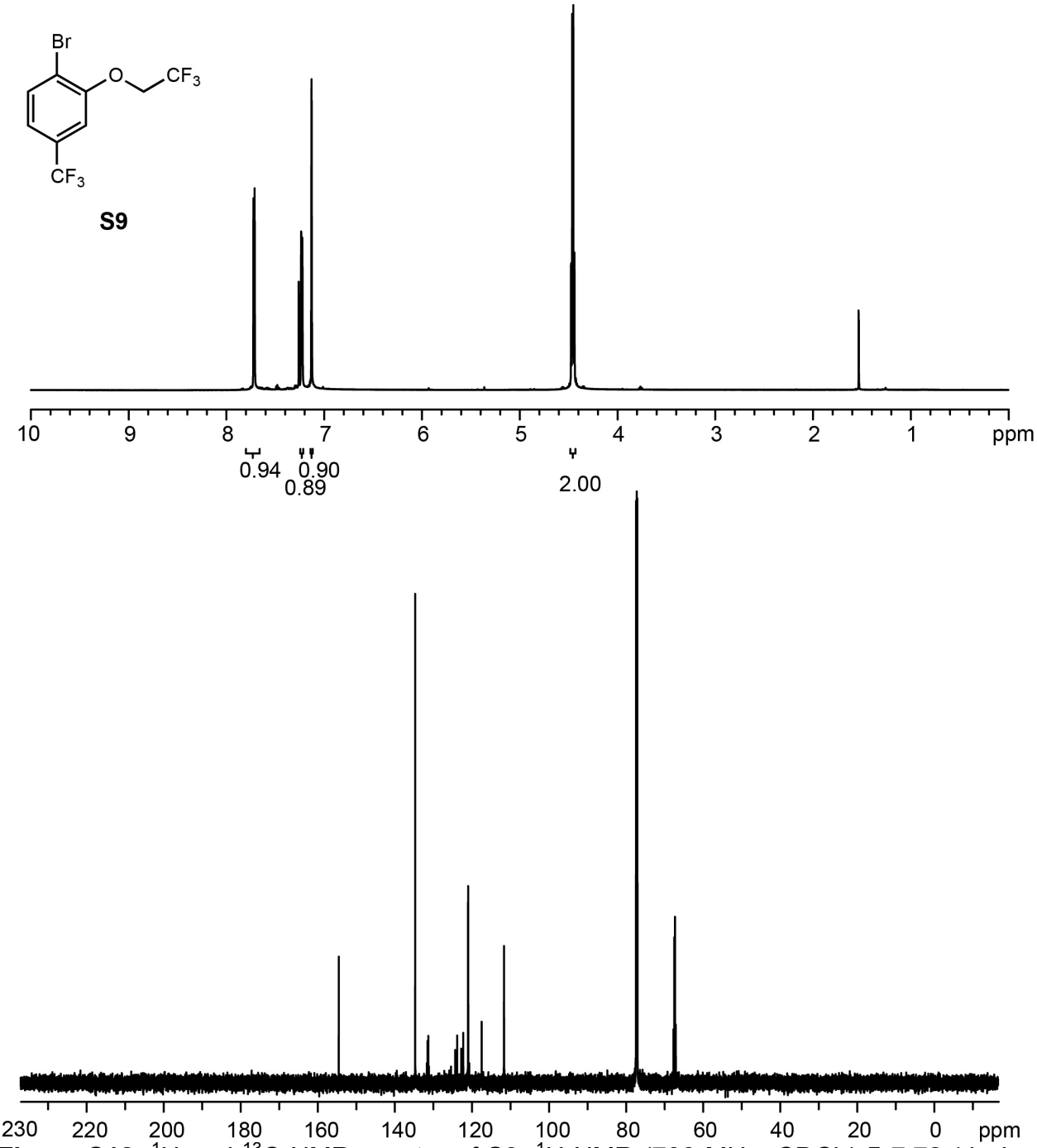


Figure S12. ^{1}H and ^{13}C NMR spectra of **S9**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.72 (d, J = 8.3 Hz, 1H), 7.23 (d, J = 8.2 Hz, 1H), 7.13 (s, 1H), 4.46 (q, $J_{H\text{-}F}$ = 7.8 Hz, 2H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 154.48, 134.66, 131.34 (q, $J_{C\text{-}F}$ = 33.2 Hz), 123.48 (q, $J_{C\text{-}F}$ = 272.5 Hz), 122.97 (q, $J_{C\text{-}F}$ = 277.8 Hz), 120.91 (q, $J_{C\text{-}F}$ = 4.1 Hz), 117.39, 111.59 (q, $J_{C\text{-}F}$ = 3.38 Hz), 67.33 (q, $J_{C\text{-}F}$ = 36.6 Hz).

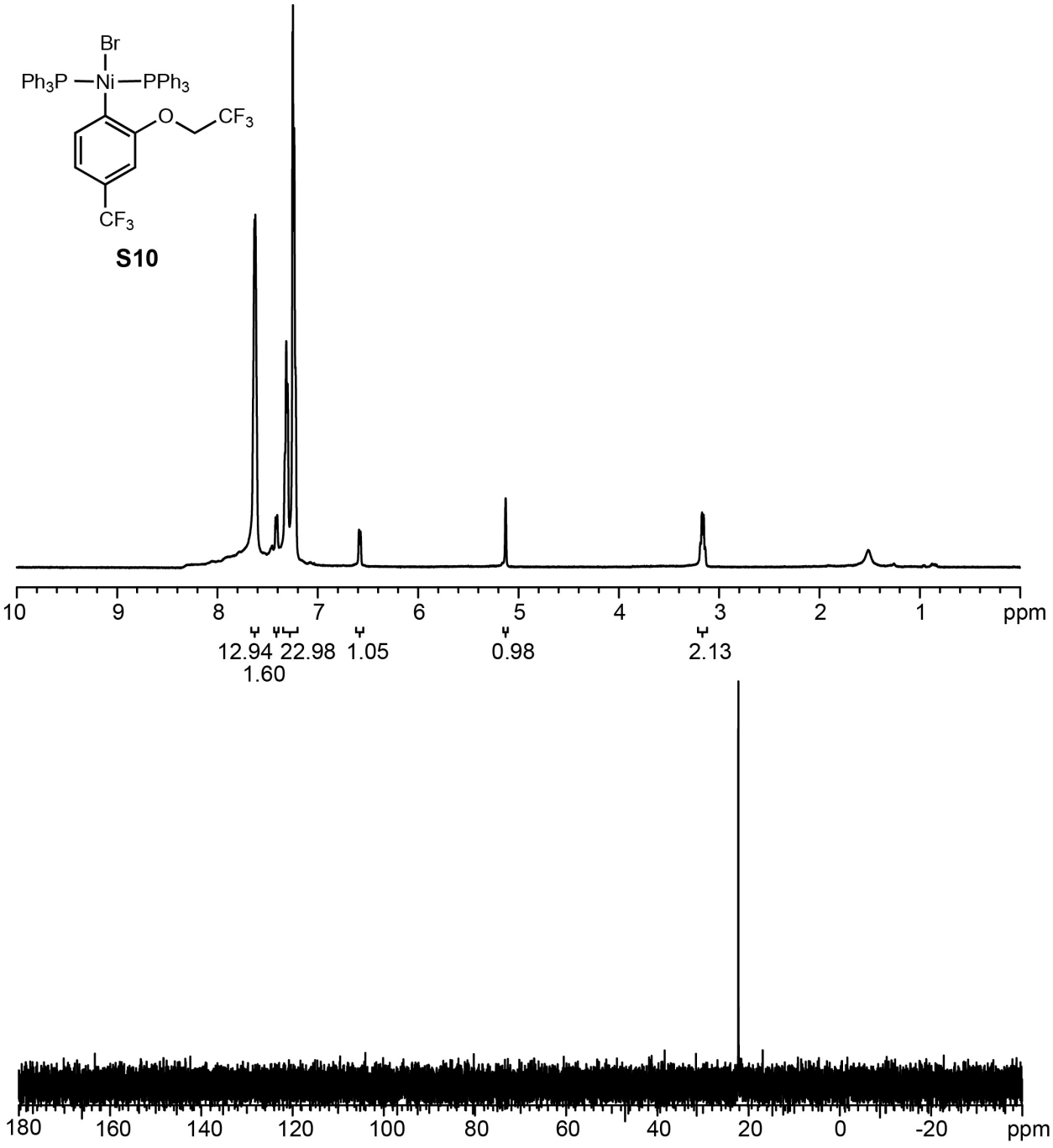


Figure S13. ^{1}H and ^{31}P NMR spectra of **S10**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (bs, 12H), 7.41 (d, J = 7.3 Hz, 1H), 7.33-7.22 (m, 18H), 6.58 (d, J = 6.7 Hz, 1H), 5.13 (s, 1H), 3.16 (q, $J_{H\text{-}F}$ = 8.2 Hz, 2H). ^{31}P NMR (202 MHz, $CDCl_3$) δ 22.23.

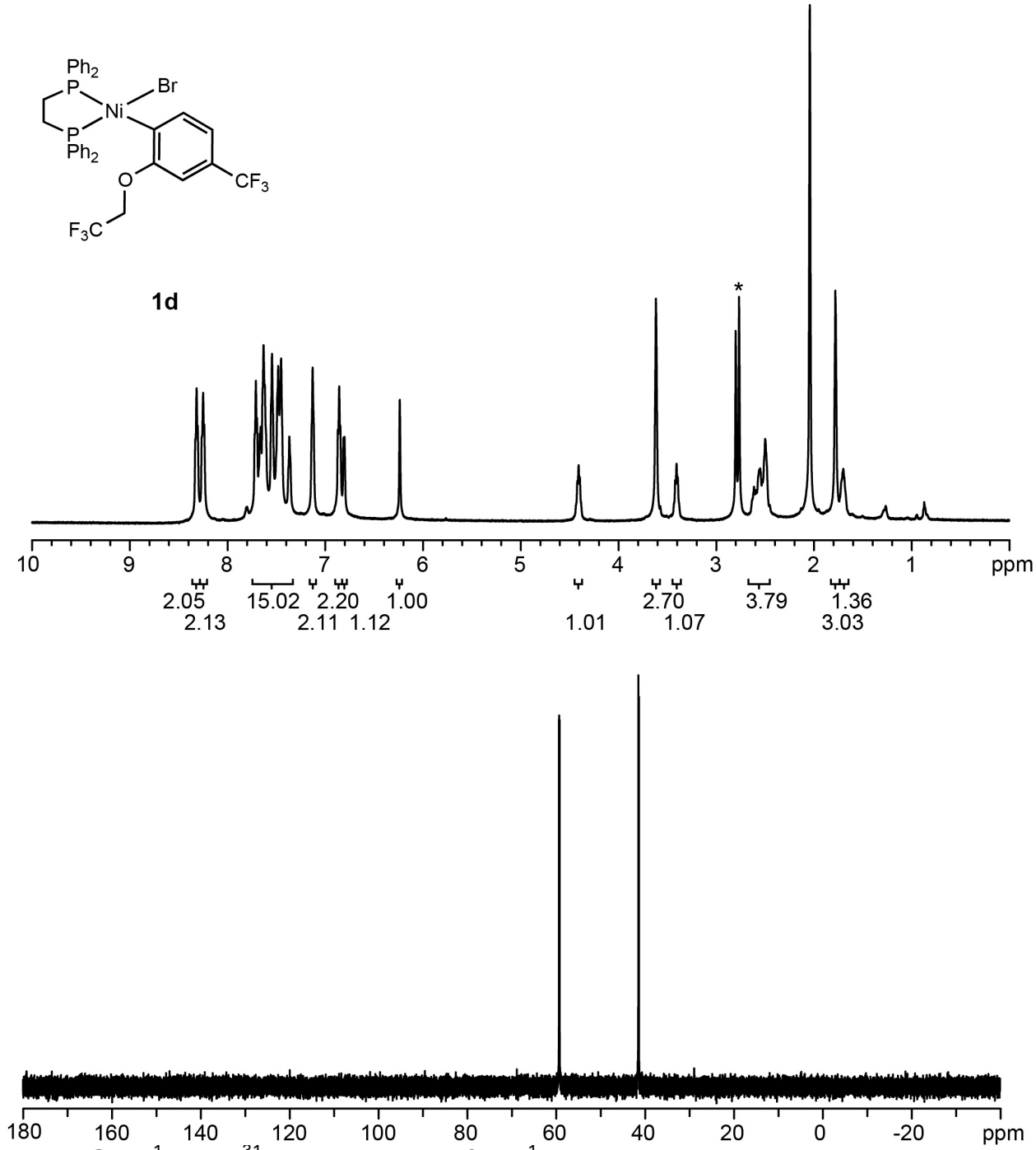


Figure S14. ^{1}H and ^{31}P NMR spectra of **1d**. ^{1}H NMR (500 MHz, acetone-d_6) δ 8.32 (at, J = 7.6 Hz, 2H), 8.25 (at, J = 7.6 Hz, 2H), 7.71-7.37 (m, 15H), 7.13 (s, 2H), 6.86 (at, J = 8.0 Hz, 2H), 6.81 (d, J = 6.9 Hz, 1H), 6.24 (s, 1H), 4.41 (m, 1H), 3.62 (s, 3H), 3.41 (m, 1H), 2.61-2.50 (m, 4H), 1.78-1.70 (m, 4H). *residual H_2O. ^{31}P NMR (200 MHz, acetone-d_6) δ 59.25 (d, J = 32.7 Hz), 41.40 (d, J = 32.7 Hz).

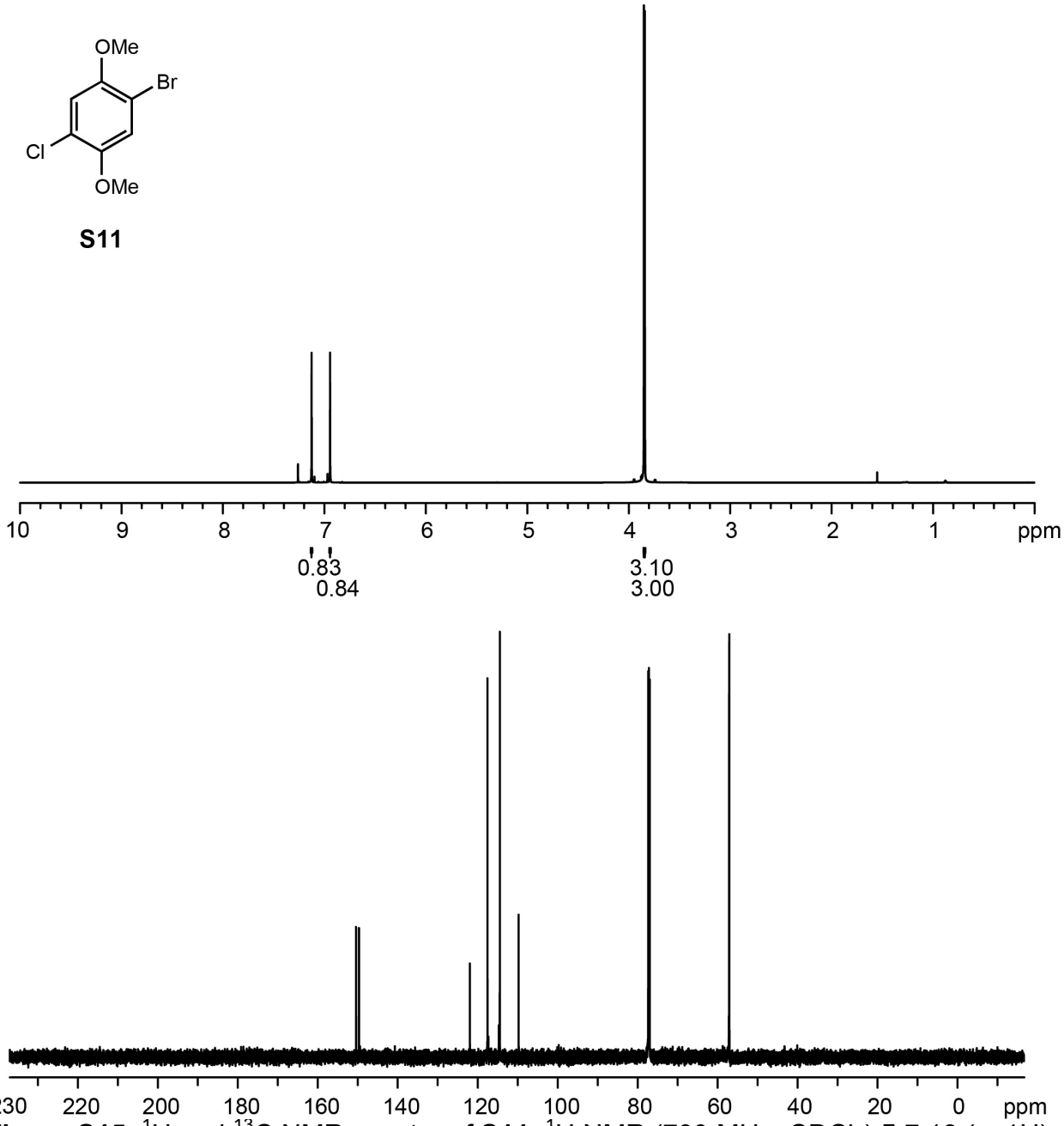


Figure S15. ^{1}H and ^{13}C NMR spectra of **S11**. ^{1}H NMR (700 MHz, $CDCl_3$) δ 7.13 (s, 1H), 6.94 (s, 1H), 3.85 (s, 3H), 3.84 (s, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 150.41, 149.67, 121.94, 117.54, 114.46, 109.75, 57.11, 57.06.

V. Initiation Rate Studies

*GRIM reaction of monomer **2***

After 8 h of GRIM reaction of monomer **2** (see Synthetic Procedure), an aliquot (~0.5 mL) was quenched with 12M HCl (0.5 mL) and then extracted with CH_2Cl_2 (2 x 1.5 mL), dried over $MgSO_4$, filtered, and then concentrated. The sample was redissolved in 1 mL CH_2Cl_2 and analyzed by GC-MS.

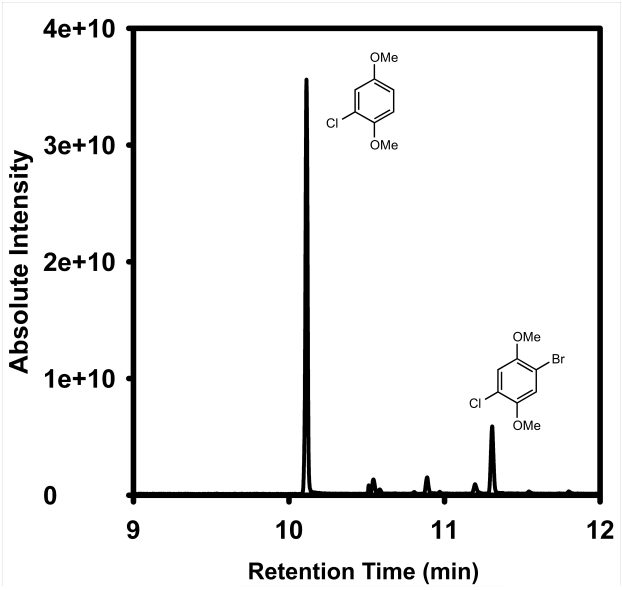


Figure S16. GC trace of quenched monomer **2**.

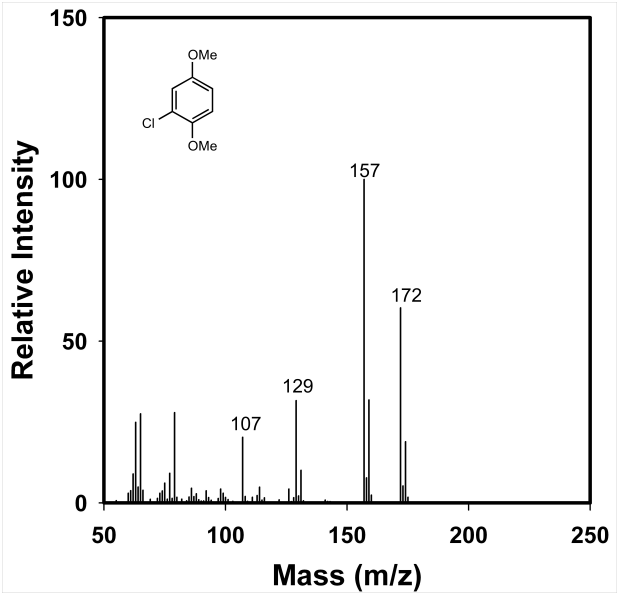


Figure S17. GC-MS trace of peak at 10.11 min for quenched monomer **2**.

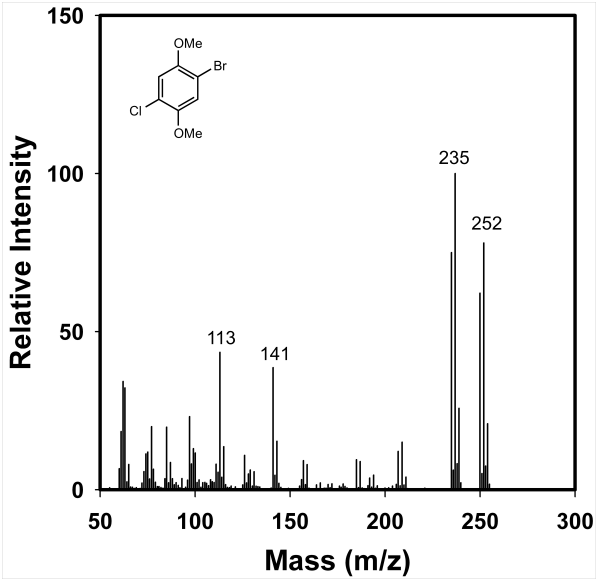
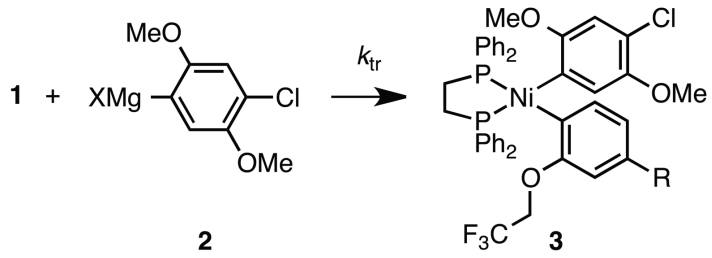


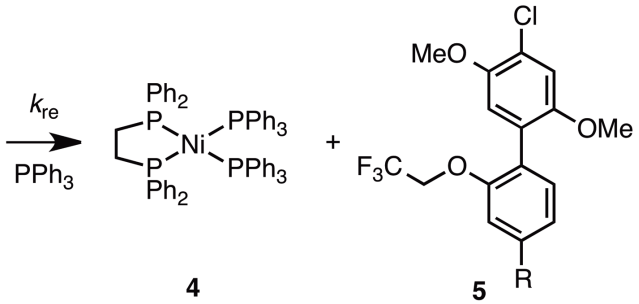
Figure S18. GC-MS trace of peak at 11.31 min for unreacted **S11**.

Representative Procedure for Performing NMR Spectroscopic Initiation Rate Studies:
In a glovebox under N_2 atmosphere, in a 4 mL vial, a nickel stock solution was prepared by dissolving **1b** (19.7 mg, 0.0265 mmol, 1.0 equiv) and PPh_3 (14.9 mg, 0.0568 mmol, 2.1 equiv) in THF (1.0 mL). Then, trifluoromethyl benzene (26 µL, 0.34 M in THF, 0.33 equiv) was added as an internal standard. An NMR tube was charged with this solution (0.8 mL), sealed with a septum, and removed from the glovebox. The tube was cooled to 0 °C in the NMR spectrometer for ~40 min. Immediately prior to acquiring kinetic data, **2** (0.2 mL, 0.2 M in THF, 2.0 equiv, kept at 0 °C) was injected into the tube. The tube was rapidly inverted once and then inserted into the spectrometer at 0 °C. Each ^{19}F NMR spectrum was taken with the following parameters using Varian vnmr 500; acquisition time = 1.5 s, relaxation time = 3.0 s, scan size = 4, and pre-acquisition delay = 120 s.

Representative Procedure for Performing Igor Pro Analysis:
The integrated peak value of **3b** was converted to concentration using an internal standard. The concentration was fit to the equations below using Igor Pro v6.22A. 'CollumKinetic 5000' was used as the master procedure file and the analysis was performed using the same procedure reported in 'Fitting to Differential equations in Igor Pro' provided by the Collum group.[8] The reductive elimination constant is calculated to significant digits that encompass one standard deviation.



2 **3**



4 **5** (1)

$$\frac{d[\mathbf{3}]}{dt} = -k_{re}[\mathbf{3}] \quad (2)$$

Control experiment

Initiation rate studies were performed with varying [PPh_3] to determine its effect on the rate of reductive elimination (temp = 0 °C, [**1b**] = 0.02 M, and [**2**] = 0.04 M).

Table S1. Rate data for catalyst **1b** with varying [PPh_3].

[PPh_3] (M)	k_{re} (s^{-1} x 10^{-3})
0.04	0.671 ± 0.006
0.08	0.69 ± 0.07
0.16	0.72 ± 0.09

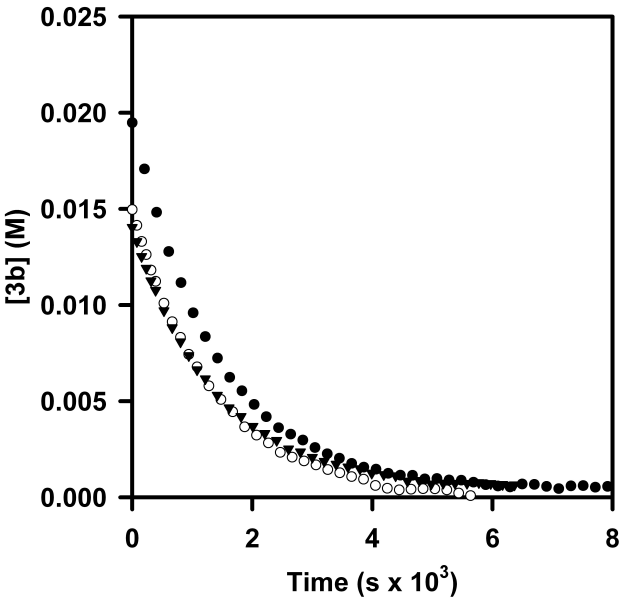


Figure S19. Plot of concentration versus time for catalyst **3b** generated *in situ* from catalyst **1b** with varying [PPh_3], (0.04 M (●), 0.08 M (○), 0.16 M(▼)).

Initiation rate studies were performed with varying [**2**] to determine its effect on the rate of reductive elimination (temp = 0 °C, [**1b**] = 0.02 M, and [PPh_3] = 0.04 M).

Table S2. Rate data for catalyst **1b** with varying [**2**].

[**2**] (M)	k_{re} (s^{-1} x 10^{-3})
0.04	0.671 ± 0.006
0.08	0.73 ± 0.01
0.16	0.73 ± 0.10

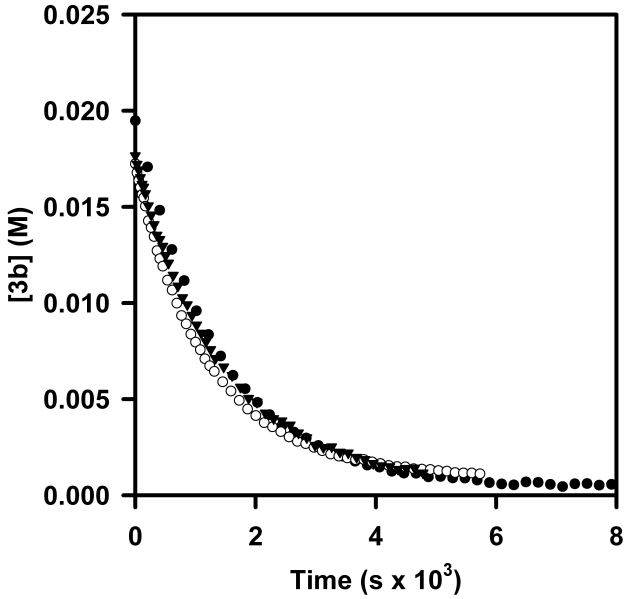


Figure S20. Plot of concentration versus time for catalyst **3b** generated *in situ* from catalyst **1b** with varying [**2**], (0.04 M (●), 0.08 M (○), 0.16 M(▼)).

The catalyst initiation was observed using ^{19}F and ^{31}P NMR spectroscopy to support the peak assignments.

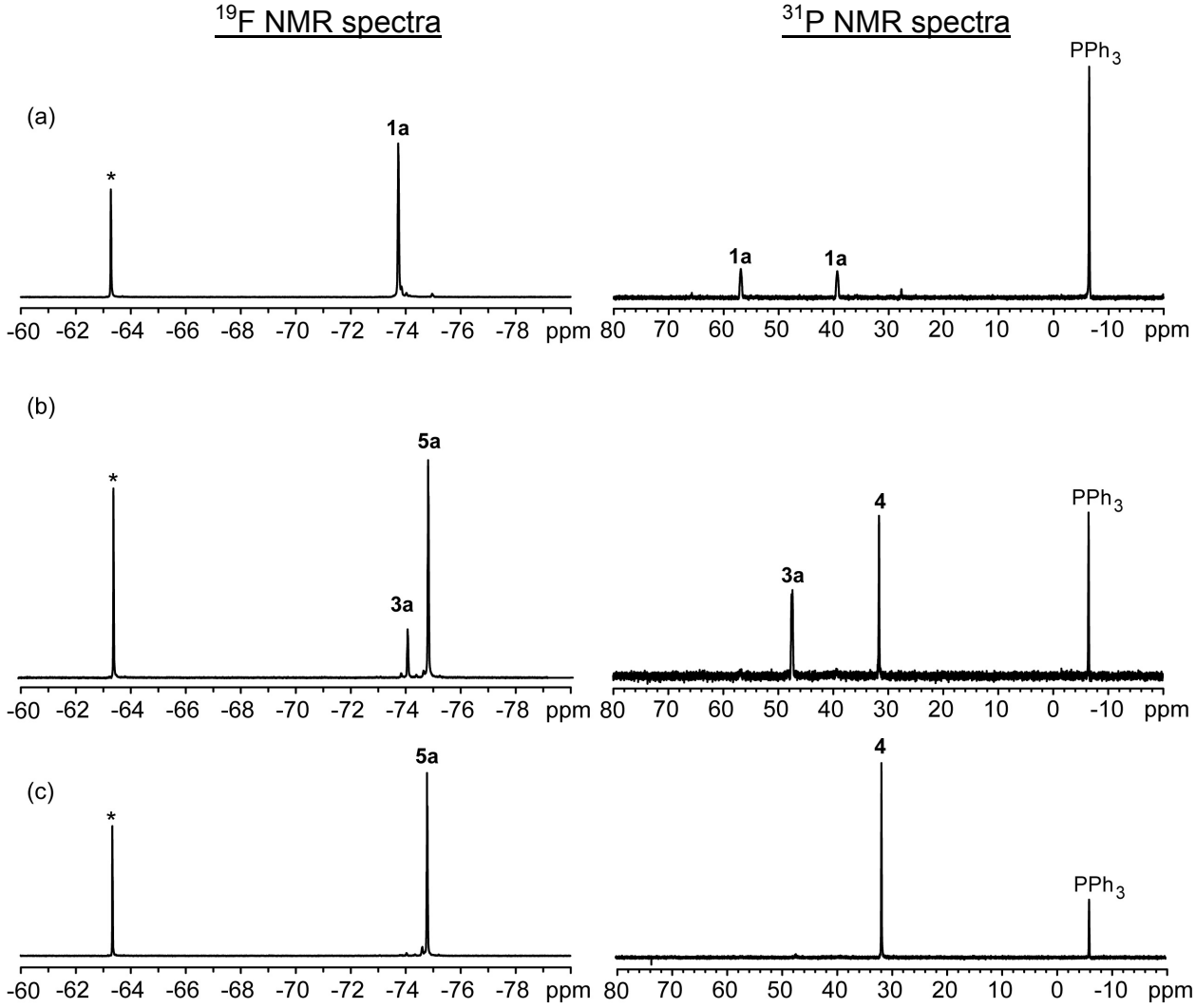


Figure S21. Representative ^{19}F and ^{31}P NMR spectra of initiation rate study for catalyst **1a** at the (a) beginning, (b) middle, and (c) end of the reaction. *Represents the internal standard, trifluoromethyl benzene.

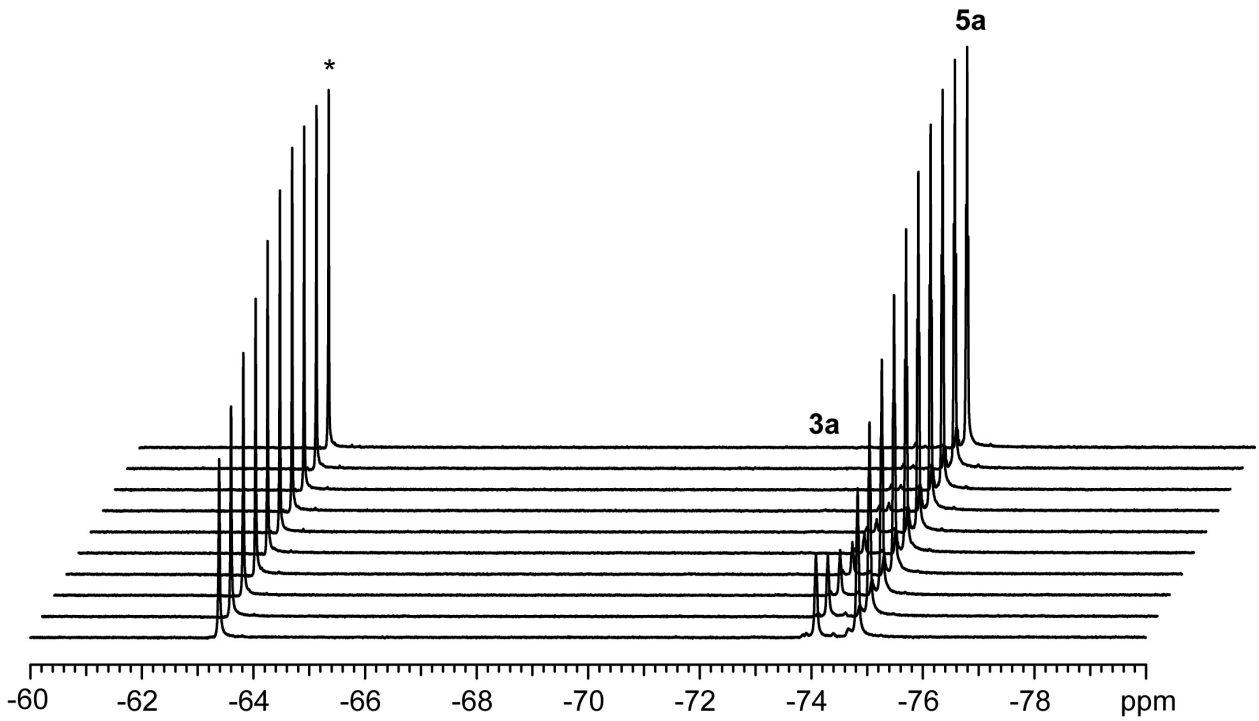


Figure S22. Representative ^{19}F NMR spectral array for catalyst **1a**. *Represents internal standard, trifluoromethyl benzene.

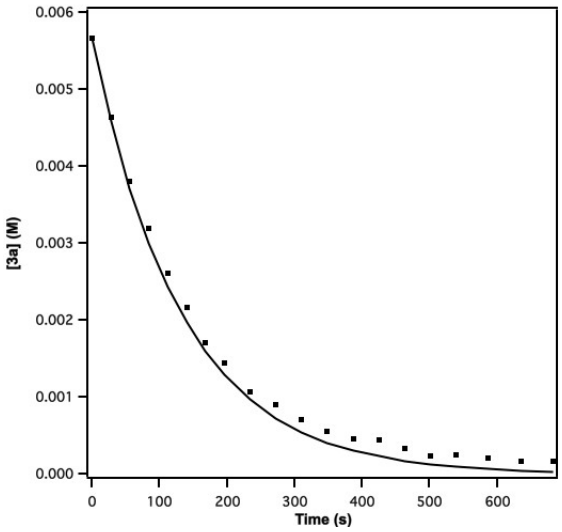


Figure S23. Plot of concentration versus time for data in Figure S22.

Table S3. Rate data for catalyst **1a**.

Trial	k_{re} (s^{-1} x 10^{-3})
1	6.84
2	6.92
Average	6.88 ± 0.06

The catalyst initiation was observed using ^{19}F and ^{31}P NMR spectroscopy to support the peak assignments.

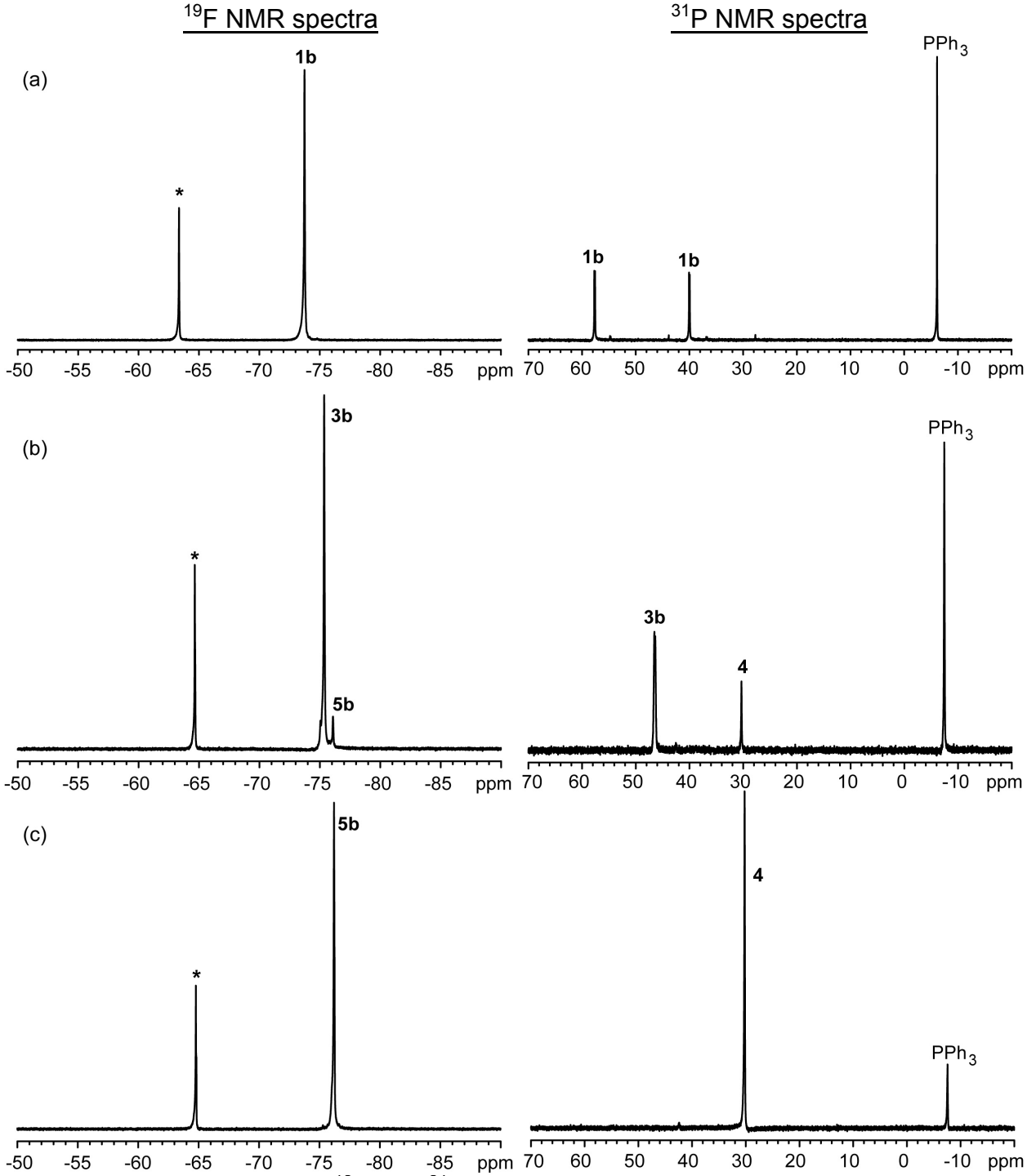


Figure S24. Representative ^{19}F and ^{31}P NMR spectra of initiation rate study for catalyst **1b** at the (a) beginning, (b) middle, and (c) end of the reaction. *Represents the internal standard, trifluoromethyl benzene.

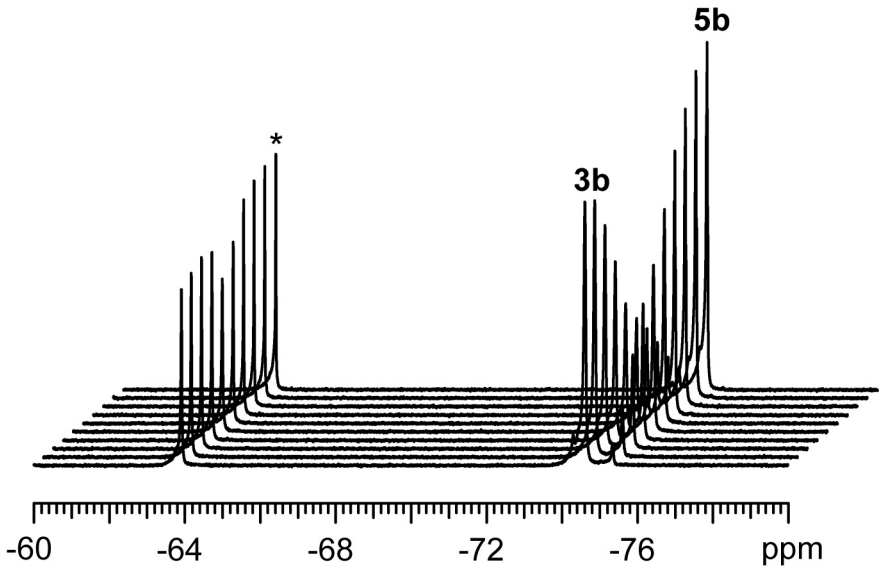


Figure S25. Representative ^{19}F NMR spectral array for catalyst **1b**. *Represents internal standard, trifluoromethyl benzene.

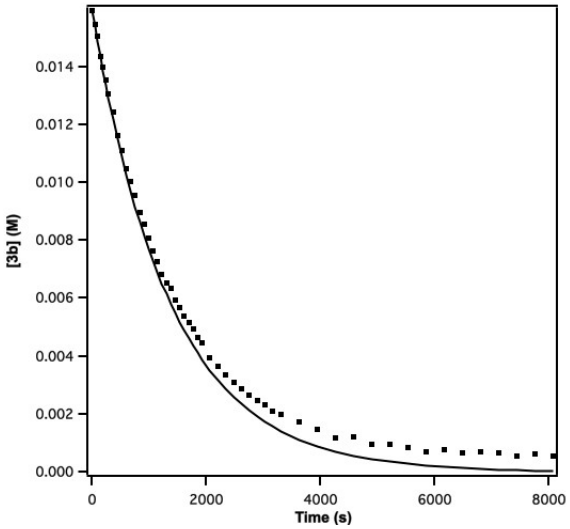


Figure S26. Plot of concentration versus time for data in Figure S25.

Table S4. Rate data for catalyst **1b**.

Trial	k_{re} (s^{-1} x 10^{-3})
1	0.666
2	0.675
Average	0.671 ± 0.006

The catalyst initiation was observed using ^{19}F and ^{31}P NMR spectroscopy to support the peak assignments.

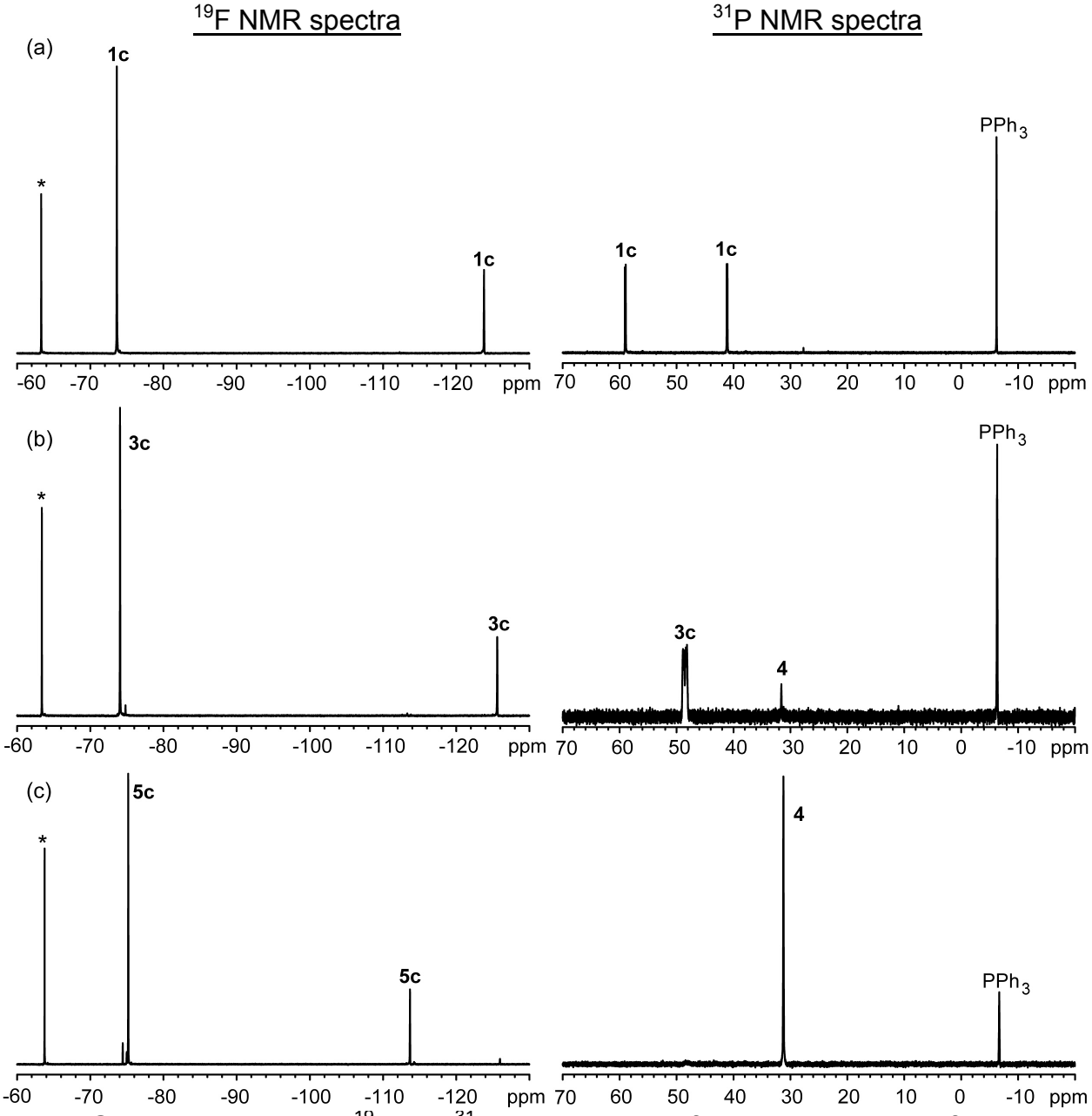


Figure S27. Representative ^{19}F and ^{31}P NMR spectra of initiation rate study for catalyst **1c** at the (a) beginning, (b) middle, and (c) end of the reaction. *Represents the internal standard, trifluoromethyl benzene.

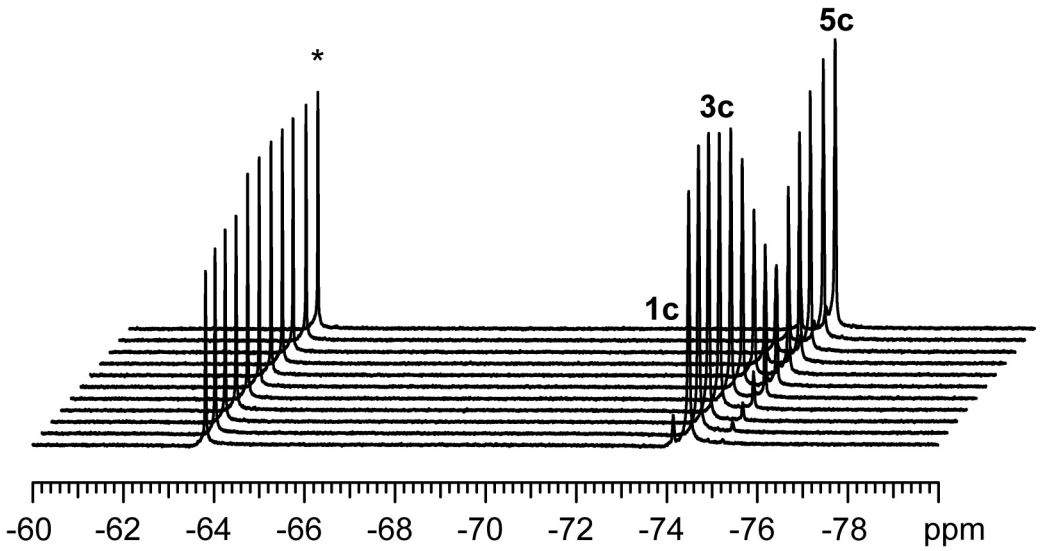


Figure S28. Representative ^{19}F NMR spectral array for catalyst **1c**. *Represents internal standard, trifluoromethyl benzene.

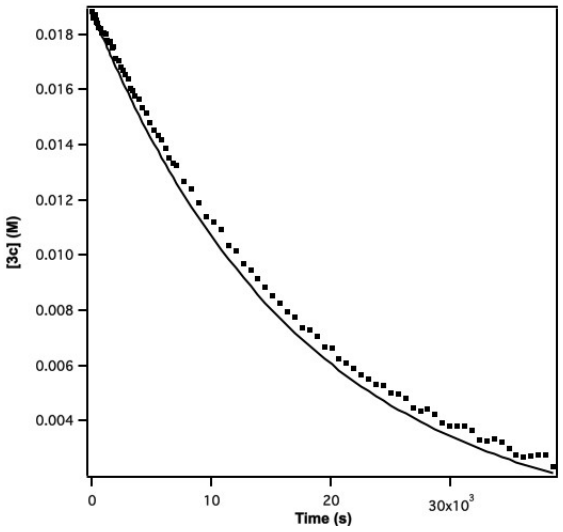


Figure S29. Plot of concentration versus time for data in Figure S28.

Table S5. Rate data for catalyst **1c**.

Trial	k_{re} (s^{-1} x 10^{-3})
1	0.0519
2	0.0521
Average	0.0520 ± 0.0001

The catalyst initiation was observed using ^{19}F and ^{31}P NMR spectroscopy to support the peak assignments.

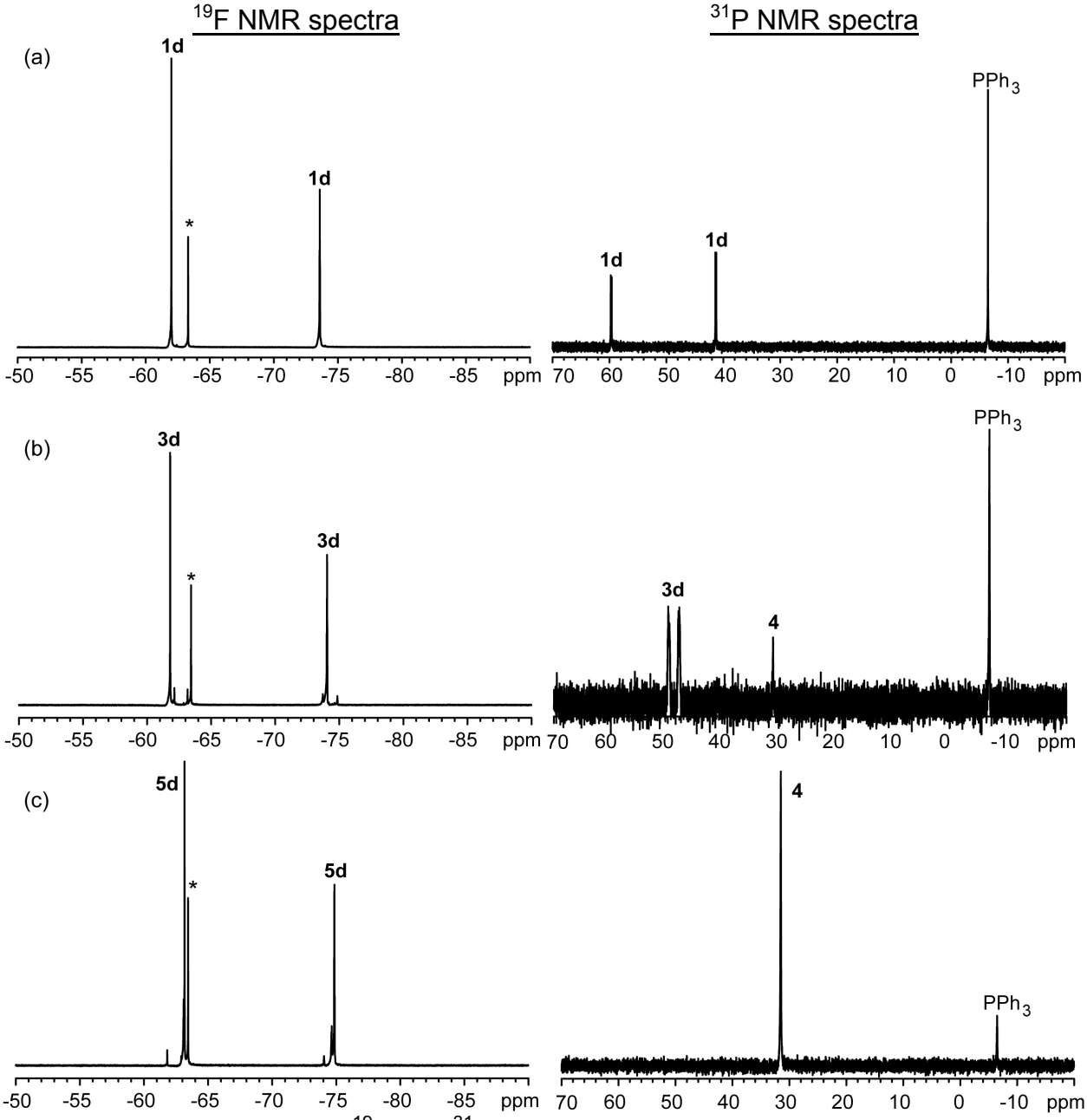


Figure S30. Representative ^{19}F and ^{31}P NMR spectra of initiation rate study for catalyst **1d** at the (a) beginning, (b) middle, and (c) end of the reaction. *Represents the internal standard, trifluoromethyl benzene.

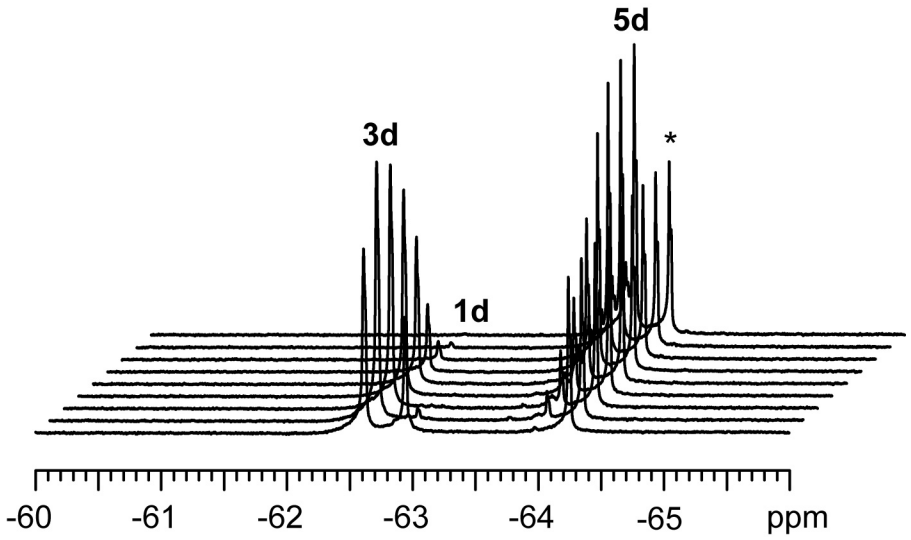


Figure S31. Representative ^{19}F NMR spectral array for catalyst **1d**. *Represents internal standard, trifluoromethyl benzene.

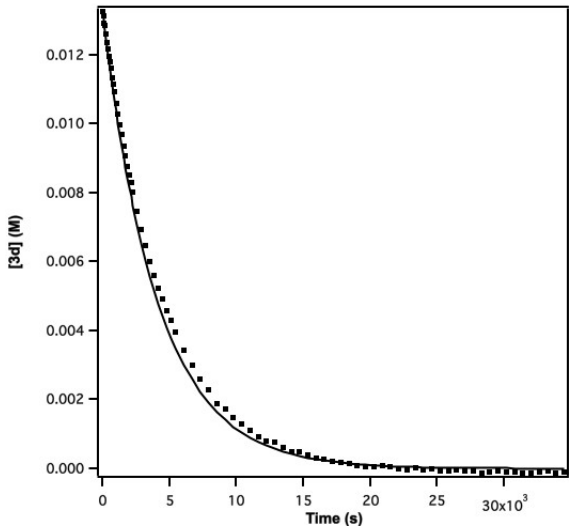


Figure S32. Plot of concentration versus time for data in Figure S31.

Table S6. Rate data for catalyst **1d**.

Trial	k_{re} (s^{-1} x 10^{-3})
1	0.2233
2	0.220
Average	0.222 ± 0.002

VI. Polymerization

Representative Procedure for M_n and PDI versus Conversion Studies utilizing React IR:
The IR probe was inserted through an O-ring sealed 14/20 ground glass adapter (custom-made) into an oven-dried 50 mL 2-neck flask equipped with a stir bar. The other neck was fitted with a three-way adapter fitted with a septum for injections/aliquot sampling and an N_2 line. The oven-dried flask was cooled under vacuum. The flask was then filled with N_2 and evacuated again for a total of three cycles. The flask was charged with THF (6.5 mL) and cooled to 0 °C over 15 min. After recording a background spectrum, monomer **6** (2.5 mL, 0.41 M in THF, 1.0 equiv) was added by syringe and allowed to equilibrate for at least 10 min at 0 °C before proceeding. The catalyst solution (1.0 mL, 0.015 M in THF, 0.015 equiv) was then injected and spectra were recorded every 30 s over the entire reaction. To account for mixing and temperature equilibration, spectra recorded in the first 60 s of the reaction were discarded. Aliquots (~0.5 mL) were taken through the three way adapter via syringe and immediately quenched with 12 M HCl (~1 mL). Each aliquot was then extracted with CH_2Cl_2 (2 x 1.5 mL) (with mild heating if polymer had precipitated), dried over $MgSO_4$, filtered, and then concentrated. The samples were dissolved in THF (with heating), and passed through a 0.2 μm PTFE filter for GPC analysis.

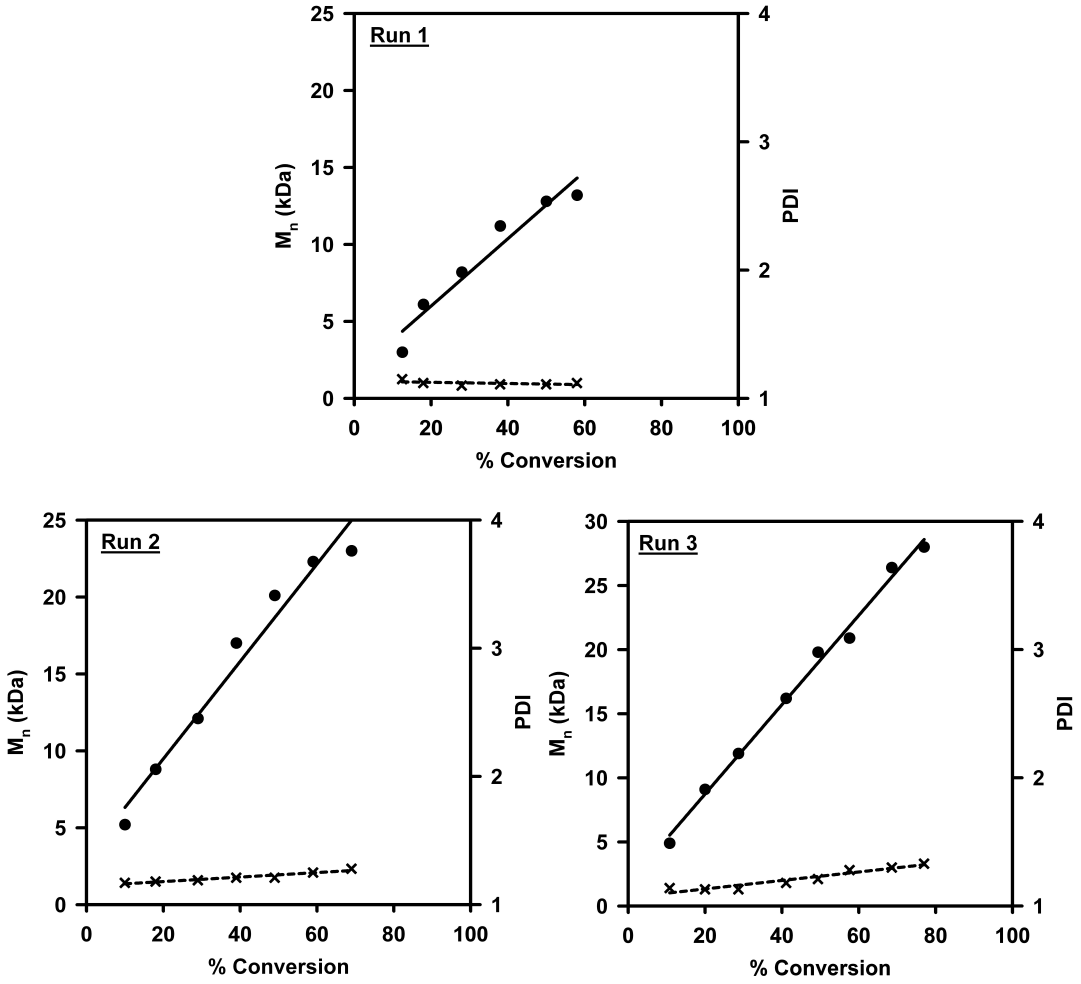


Figure S33. Plot of Mn (●) and PDI (**x**) versus conversion for **1a** (temp = 0 °C, [**1a**] = 0.0015 M, [**6**] = 0.10 M (Run 1), 0.10 M (Run 2), 0.01 M (Run 3)).

Table S7. Data for the plot in Figure S33, Run 1.

% Conversion	M_n (kDa)	PDI
13	3.0	1.15
19	6.1	1.12
28	8.2	1.10
38	11.2	1.11
50	12.8	1.11
58	13.2	1.12

Table S8. Data for the plot in Figure S33, Run 2.

% Conversion	M_n (kDa)	PDI
10	5.2	1.17
18	8.8	1.18
29	12.1	1.19
39	17.0	1.21
49	20.1	1.21
59	22.3	1.25
69	23.0	1.28

Table S9. Data for the plot in Figure S33, Run 3.

% Conversion	M_n (kDa)	PDI
11	4.9	1.14
20	9.1	1.13
29	11.9	1.13
41	16.2	1.18
49	19.8	1.21
58	20.9	1.28
69	26.4	1.30
77	28.0	1.33

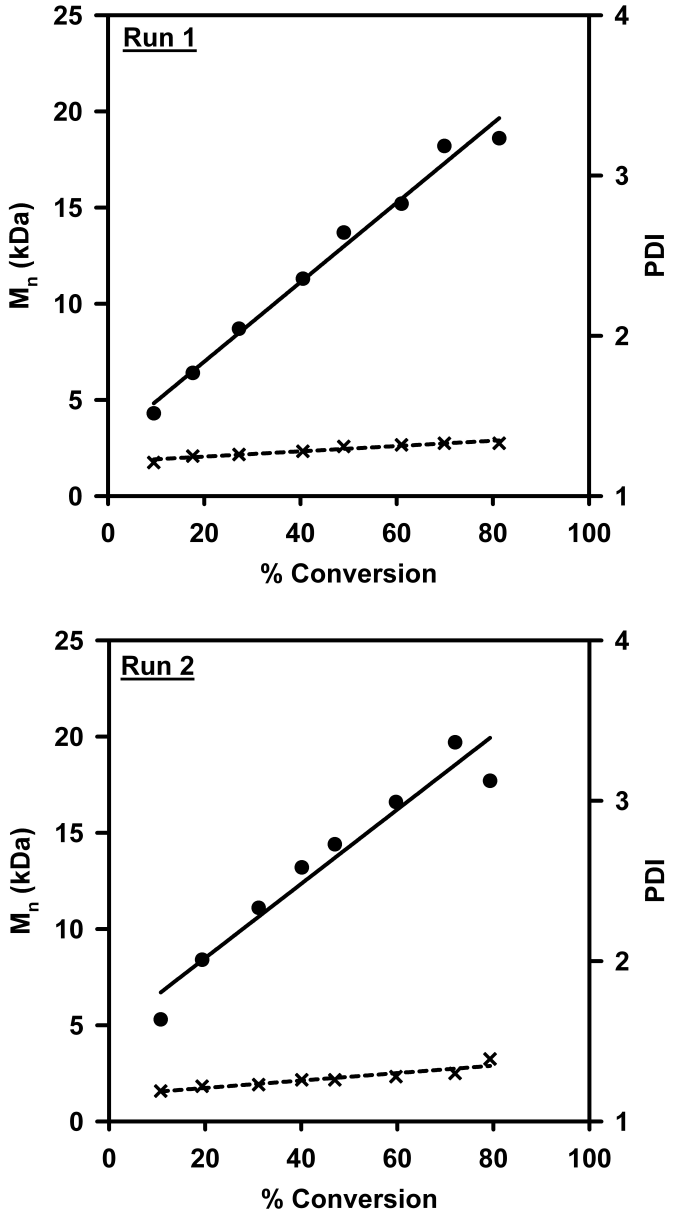


Figure S34. Plot of Mn (●) and PDI (**x**) versus conversion for **1b** (temp = 0 °C, [**1b**] = 0.0015 M, [**6**] = 0.10 M (Run 1), 0.10 M (Run 2)).

Table S10. Data for the plot in Figure S34, Run 1.

% Conversion	M_n (kDa)	PDI
10	4.3	1.21
18	6.4	1.25
27	8.7	1.26
41	11.3	1.28
49	13.7	1.31
61	15.2	1.32
70	18.2	1.33
81	18.6	1.33

Table S11. Data for the plot in Figure S34, Run 2.

% Conversion	M_n (kDa)	PDI
11	5.3	1.19
19	8.4	1.22
31	11.1	1.23
40	13.2	1.26
47	14.4	1.26
60	16.6	1.28
72	19.7	1.30
79	17.7	1.39

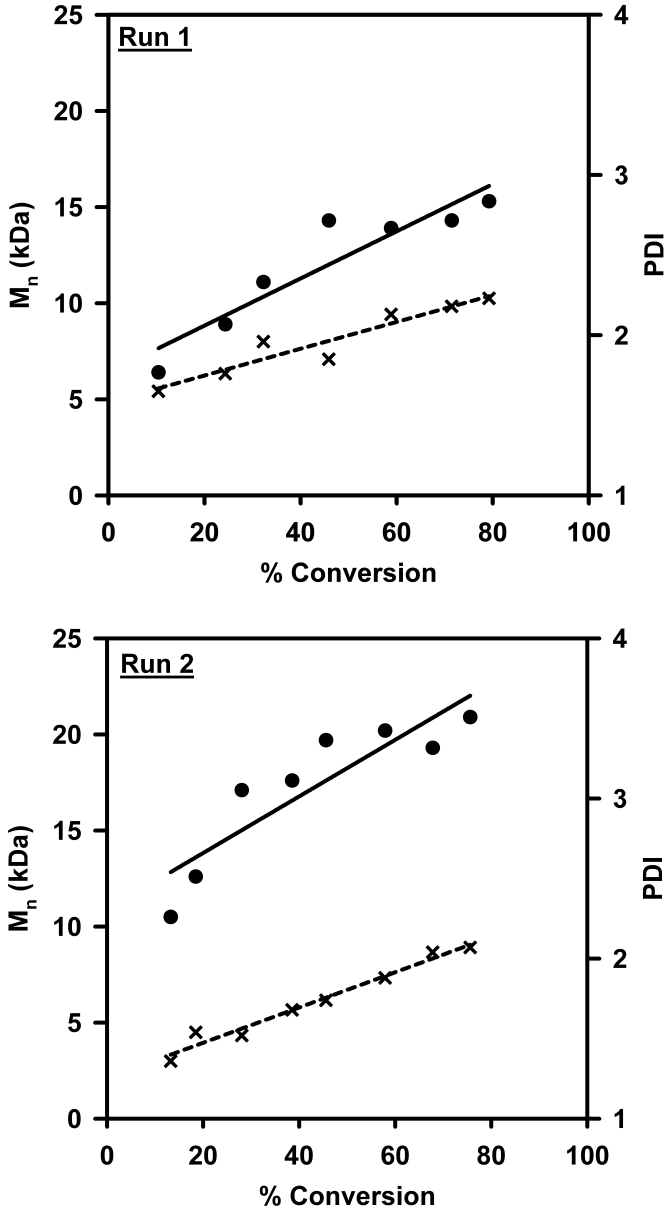


Figure S35. Plot of M_n (●) and PDI (**x**) versus conversion for **1c** (temp = 0 °C, [**1c**] = 0.0015 M, [**6**] = 0.10 M (Run 1), 0.10 M (Run 2)).

Table S12. Data for the plot in Figure S35, Run 1.

% Conversion	M_n (kDa)	PDI
10	6.4	1.65
24	8.9	1.76
32	11.1	1.96
46	14.3	1.85
59	13.9	2.13
71	14.3	2.18
79	15.3	2.23

Table S13. Data for the plot in Figure S35, Run 2.

% Conversion	M_n (kDa)	PDI
13	10.5	1.36
18	12.6	1.54
28	17.1	1.52
39	17.6	1.68
46	19.7	1.74
59	20.2	1.88
68	19.3	2.04
76	20.9	2.07

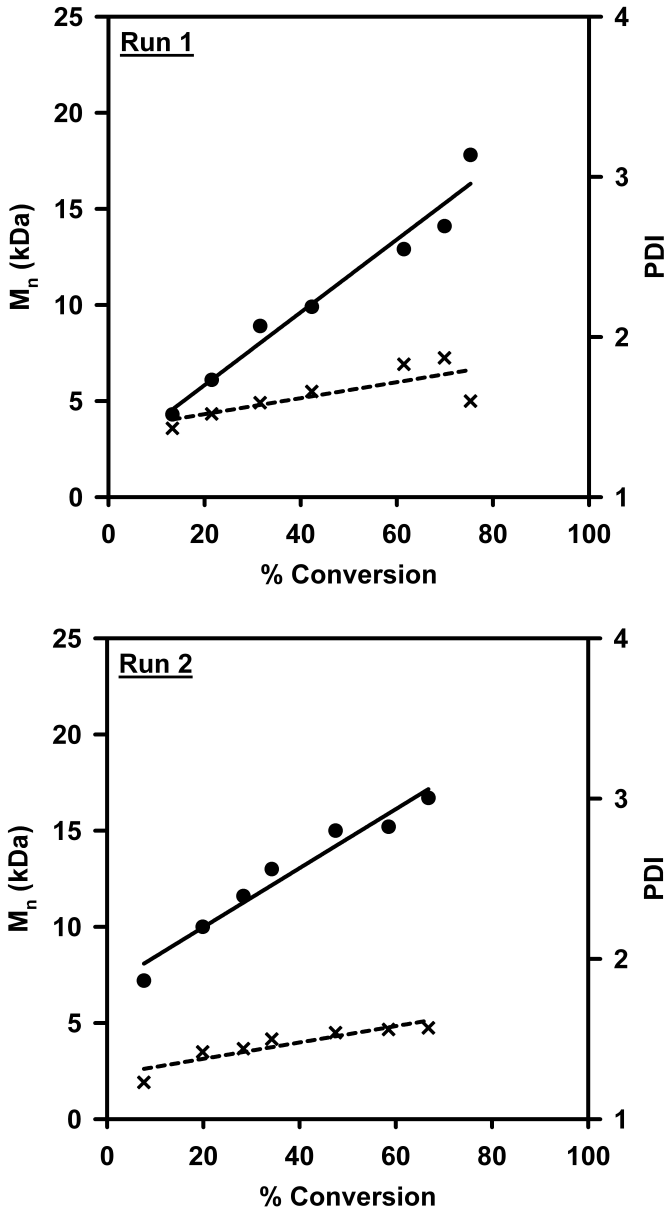


Figure S36. Plot of Mn (●) and PDI (**x**) versus conversion for **1d** (temp = 0 °C, [**1d**] = 0.0015 M, [**6**] = 0.10 M (Run 1), 0.10 M (Run 2)).

Table S14. Data for the plot in Figure S36, Run 1.

% Conversion	M_n (kDa)	PDI
13	4.3	1.43
21	6.1	1.52
32	8.9	1.59
42	9.9	1.66
61	12.9	1.83
70	14.1	1.87
75	17.8	1.60

Table S15. Data for the plot in Figure S36, Run 2.

% Conversion	M_n (kDa)	PDI
8	7.2	1.23
20	10.0	1.42
28	11.6	1.44
34	13.0	1.50
47	15.0	1.54
59	15.2	1.56
67	16.7	1.57

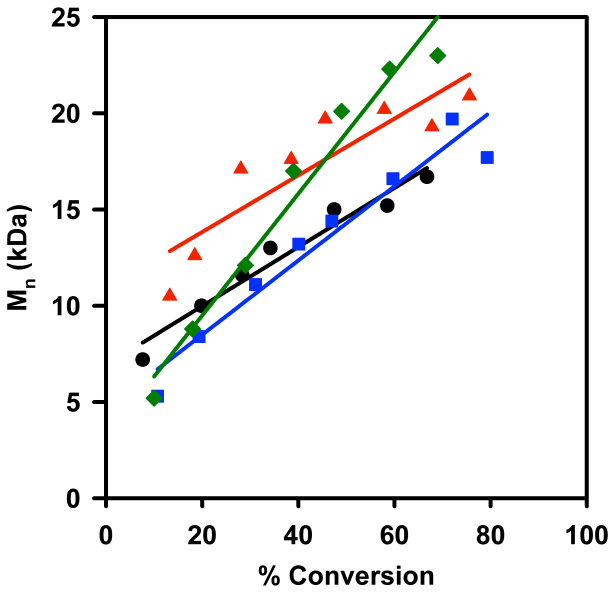


Figure S37. Representative plot of M_n versus conversion for all four catalysts. Samples within ±4% of target conversion were included (**1a**(◆); **1b**(■); **1c**(▲); **1d**(●)).

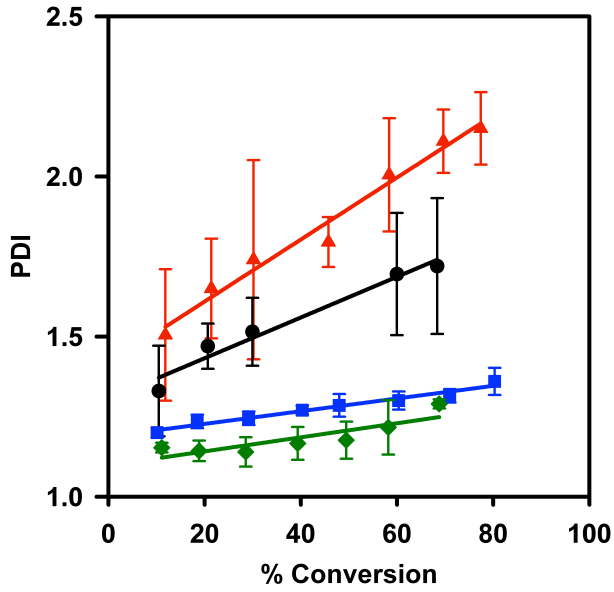


Figure S38. Plot of average PDI versus conversion for all four catalysts with error bars. Samples within ±4% of target conversion were included (**1a**(◆); **1b**(■); **1c**(▲); **1d**(●)).

Comparison of propagation and simulated Ni initiator consumption

The React IR was used to determine [**6**] over time. The data for [**1a**-**d**] was simulated based on rate constant and initiation concentration where $[Ni]_0$ = 0.0015 M using equation (3).

$$[Ni] = [Ni]_0 e^{-k_{re\,(initiation)}t} \quad (3)$$

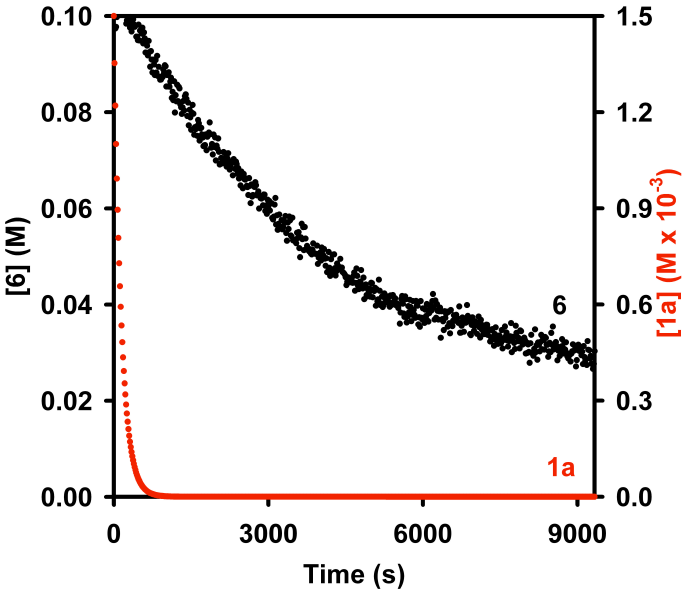


Figure S39. Plot of [**6**] (●) and simulated [**1a**] (●) versus time.

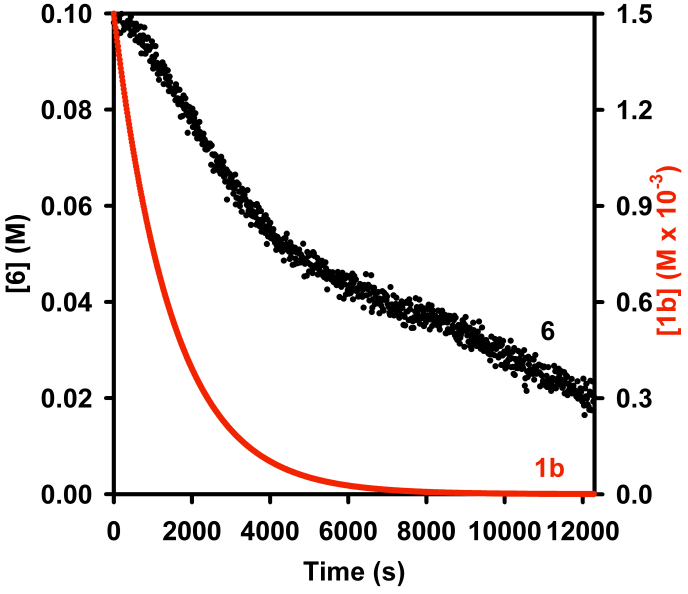


Figure S40. Plot of [**6**] (●) and simulated [**1b**] (●) versus time.

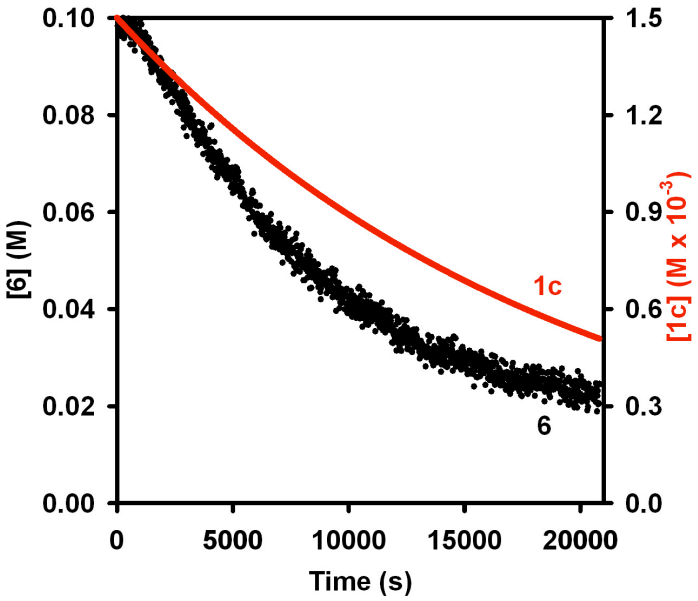


Figure S41. Plot of [**6**] (●) and simulated [**1c**] (●) versus time.

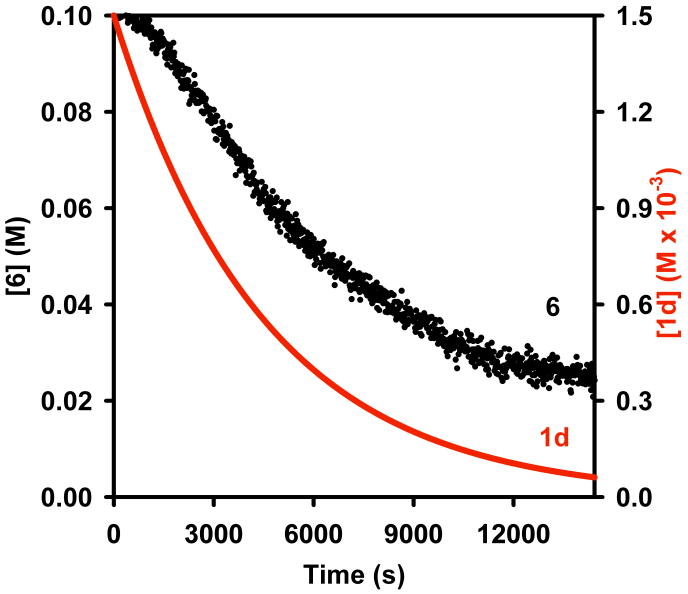


Figure S42. Plot of [**6**] (●) and simulated [**1d**] (●) versus time.

Representative Procedure for Preparation of Oligomers for MALDI-TOF MS Studies:
All actions were performed in a glovebox under N_2 atmosphere. A 20 mL vial was equipped with a stir bar. Sequentially, **1b** (12 mg, 0.016 mmol, 1 equiv), THF (4.8 mL), and **6** (0.20 mL, 0.46 M, 7 equiv) were added to the flask. After 1.5 h, the reaction was removed from the glovebox and poured into HCl (3 mL, 12 M) and then extracted with CH_2Cl_2 (3 x 5 mL). The combined organic layers were dried over $MgSO_4$ and filtered. The filtrate was concentrated in vacuo. The resulting solid was washed with MeOH (20 mL) to give **P6** as an off-white solid: M_n: 2.1 kDa, PDI: 1.23 (GPC). For the MS sample a small amount of polymer was dissolved in $CHCl_3$ and first filtered through a pipet column of basic, acidic, and neutral alumina to remove residual Ni and the solution was concentrated in vacuo. The general procedure was followed for MALDI-TOF MS sample preparation (see General Experimental pS2).

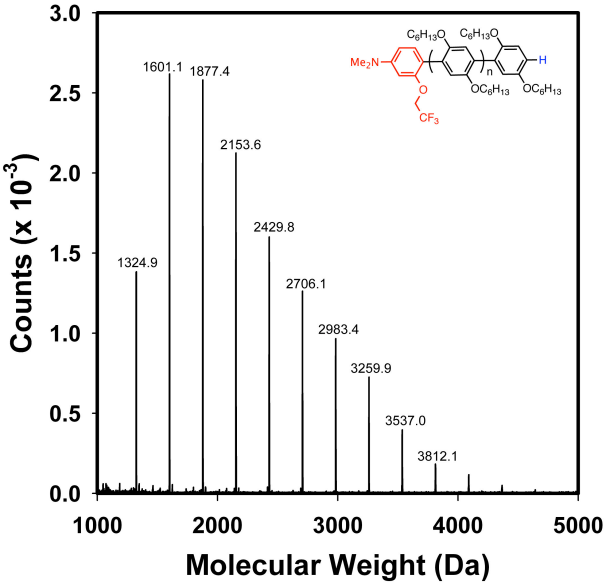


Figure S43. MALDI-TOF MS spectrum of **P6a** initiated with **1a**.

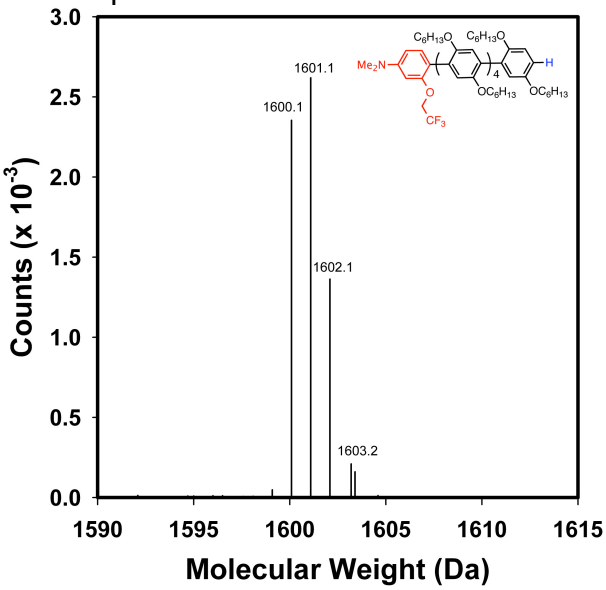


Figure S44. Expanded view of Figure S43.

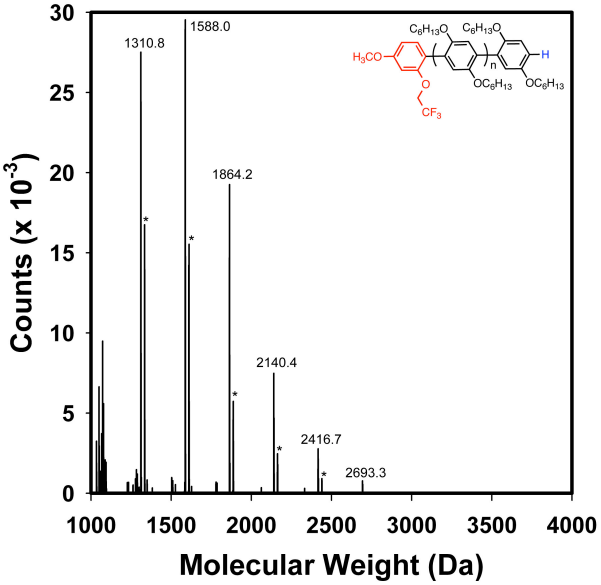


Figure S45. MALDI-TOF MS spectrum of **P6b** initiated with **1b**. *Represents $[M + Na]^+$.

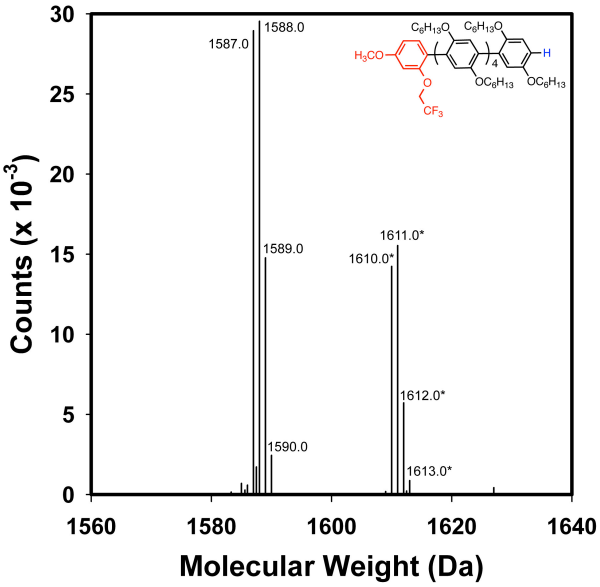


Figure S46. Expanded view of Figure S45. *Represents $[M + Na]^+$.

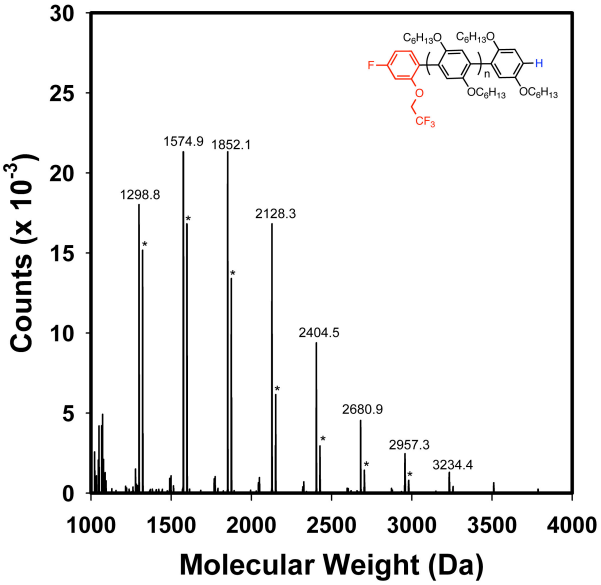


Figure S47. MALDI-TOF MS spectrum of **P6c** initiated with **1c**. *Represents $[M + Na]^+$.

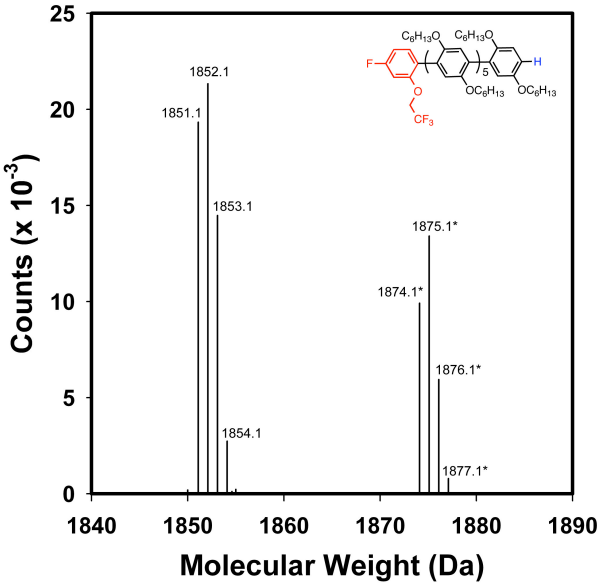


Figure S48. Expanded view of Figure S47. *Represents $[M + Na]^+$.

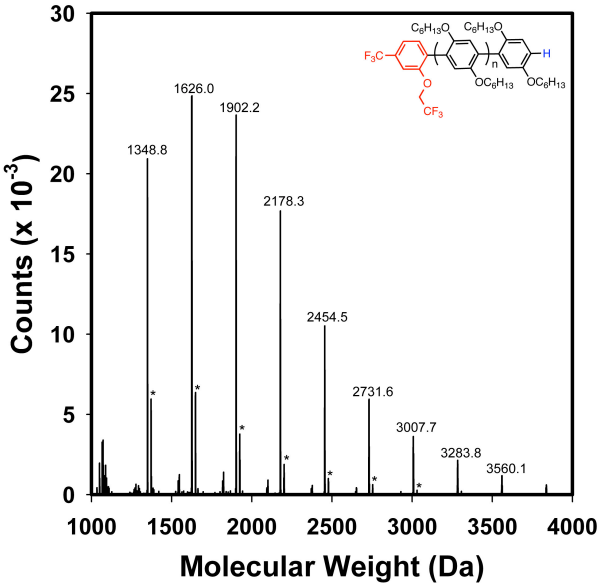


Figure S49. MALDI-TOF MS spectrum of **P6d** initiated with **1d**. *Represents $[M + Na]^+$.

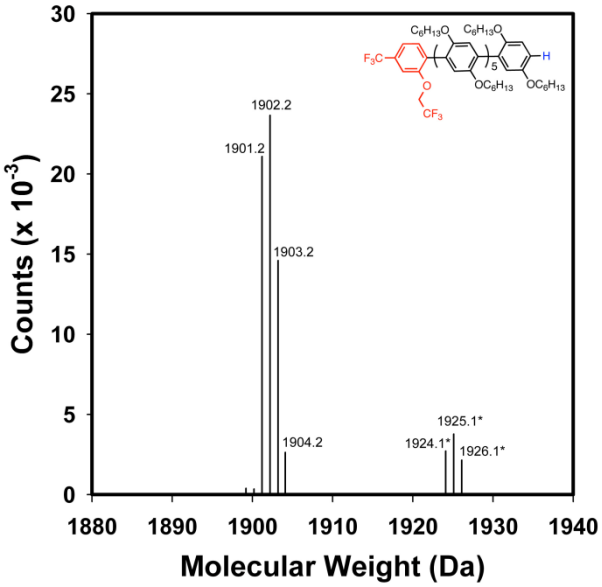


Figure S50. Expanded view of Figure S49. *Represents $[M + Na]^+$.

VII. Computational Studies

Transition states (TSs) on the spin-singlet potential energy surface were optimized for the reductive elimination from **3** for 20 substituents (see Table S16). For selected substituted systems, we also examined the triplet electronic state, which is at least 30 kcal mol^{-1} higher in energy than the singlet. For R = H, we performed a systematic search of conformations of **3** to identify the low-lying rotamers of the aryl substituents and phosphine substituents. The resulting lowest-lying conformation is depicted in Fig. S50, for both **3** and the corresponding TS. Reactants (**3**) and TSs for each of the 20 substituents were then optimized based on this low-lying conformation. Free energy barriers were computed based on the quasi-harmonic-oscillator/rigid-rotor approximation, at a temperature of 273 K. For all reported TSs, there was a single imaginary frequency with an imaginary mode indicative of the forming C–C bond and breaking C–Ni bonds. Optimized Cartesian coordinates for all 20 reactants and TSs are listed at the end of this file.

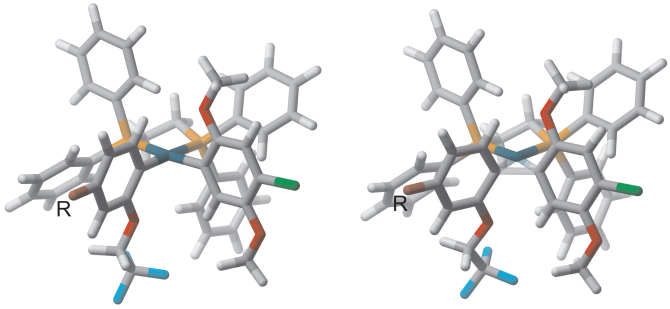


Figure S51. Structures of the reactant and TS for the reductive elimination of **3**.

The computed free energy barriers are listed in Table S16, along with Hammett constants and changes in the charge delocalized on the two aryl rings. As shown in Fig. S52, there is essentially no linear correlation between computed barrier heights and either the Hammett σ_p constants or the differences in charges of the reacting carbon atoms.

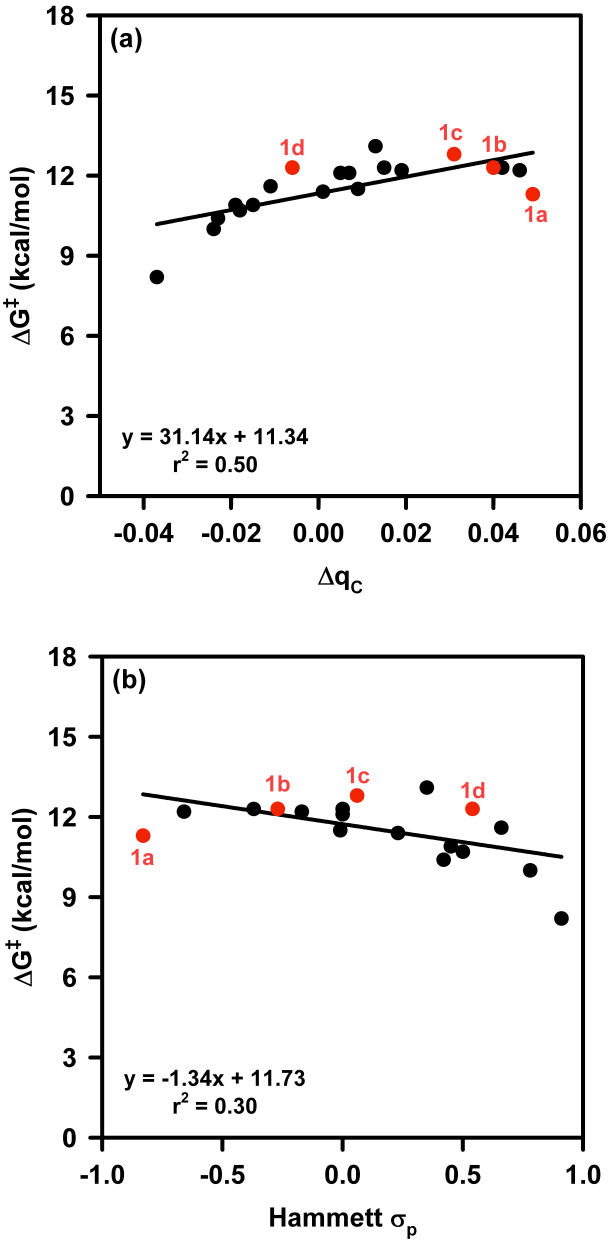


Figure S52. Plots of free energy barriers (kcal mol^{-1}) versus (a) the difference in charge between the two reacting carbon atoms (Δq_C) and (b) Hammett σ_p constants.

Changes in the ring charges were calculated to test whether the ability of the aryl rings to delocalize the increasing electron density on the catalyst during the reductive elimination is responsible for the lowering of the reaction barriers. Charges were computed for each atom in the reactants and TSs for all 20 substituted systems based on natural population analyses (NPA). The total charge on the two reacting phenyl rings, excluding the reacting carbons but including all aryl substituents, was calculated for the reactant and TS. The difference in these ring charges (TS – reactant) is reported as ΔCharge in Table S15.

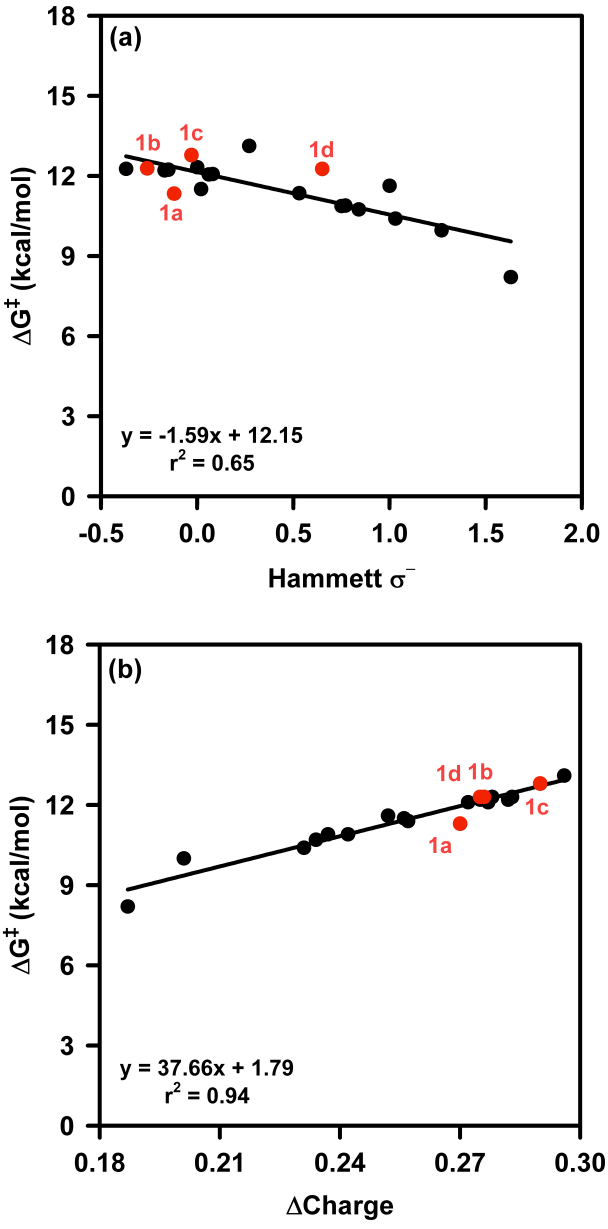


Figure S53. Plots of free energy barriers (kcal mol^{-1}) versus (a) Hammett σ^- constants and (b) change in charge on two aryl rings between **3** and the transition state, excluding the carbon atoms bound to the Ni.

Table S16. Computed free energy barriers ($\Delta G^{‡}$, kcal mol^{-1}), Hammett σ_p and σ^- constants, the change in charge on the two aryl rings (ΔCharge), the charges on the reacting carbons [q_{C1} and qc2, where C1 and C2 refer to the carbons on the substituted and monomer rings, respectively], and the difference in charges at the reacting carbons (Δq_C).

R	$\Delta G^{‡}$	σ_p	σ^-	ΔCharge	q_{C1}	q_{C2}	Δq_C
NH_2	12.2	–0.66	–0.15	0.275	-0.228	-0.182	0.046
$N(CH_3)_2$	11.3	–0.83	–0.12	0.270	-0.231	-0.182	0.049
CH_3	12.2	–0.17	–0.17	0.282	-0.201	-0.183	0.019
H	12.3	0.00	0.00	0.283	-0.197	-0.182	0.015
OCH_3	12.3	–0.27	–0.26	0.276	-0.221	-0.181	0.040
CCH	11.4	0.23	0.53	0.257	-0.183	-0.182	0.001
F	12.8	0.06	–0.03	0.290	-0.214	-0.183	0.031
CF_3	12.3	0.54	0.65	0.275	-0.178	-0.184	-0.006
CN	11.6	0.66	1.00	0.252	-0.172	-0.183	-0.011
NO_2	10.0	0.78	1.27	0.201	-0.161	-0.184	-0.024
CHO	10.4	0.42	1.03	0.231	-0.161	-0.184	-0.023
$COCH_3$	10.7	0.50	0.84	0.234	-0.166	-0.184	-0.018
SCH_3	12.1	0.00	0.06	0.272	-0.188	-0.184	0.005
$COOCH_3$	10.9	0.45	0.75	0.242	-0.168	-0.183	-0.015
NO	8.2	0.91	1.63	0.187	-0.146	-0.183	-0.037
OCF_3	13.1	0.35	0.27	0.296	-0.196	-0.183	0.013
OH	12.3	–0.37	–0.37	0.278	-0.224	-0.182	0.042
COOH	10.9	0.45	0.77	0.237	-0.165	-0.184	-0.019
CH_2OH	12.1	0.00	0.08	0.277	-0.189	-0.182	0.007
Ph	11.5	–0.01	0.02	0.256	-0.191	-0.182	0.009

VIII. Optimized Cartesian Coordinates

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NH2 Reactant

Ni	0.0296040	0.3970530	-0.1924740
P	1.7525870	1.4910740	0.6632850
P	-1.1685440	1.1377810	1.5226590
C	1.3190460	1.9699820	2.4283960
C	1.9731440	3.1577330	-0.1224860
C	3.4775900	0.8439130	0.7422900
C	-1.4854460	-0.4360700	-1.0329010
C	1.0586710	-0.3061300	-1.6682610
C	-0.1457890	2.4318250	2.4321140
C	-1.4302910	-0.1273390	2.8537920
C	-2.8430620	1.8893880	1.3354460
H	1.9940080	2.7534260	2.8116240
H	1.4363450	1.0738300	3.0614240
C	3.0926500	3.9657720	0.1582580
C	0.9652070	3.6456690	-0.9755600
C	4.1629870	0.6289140	-0.4725560
C	4.1172840	0.5224590	1.9550120
C	-2.2760550	0.3074190	-1.9344750
C	-1.8736320	-1.7632460	-0.7754240
C	1.1383400	0.3467590	-2.9119950
C	1.8036570	-1.4977540	-1.5581570
H	-0.5235670	2.5901430	3.4555780
H	-0.2347900	3.3830920	1.8807200
C	-2.3790620	0.0568010	3.8790910
C	-0.6131610	-1.2728660	2.8676860
C	-3.8998370	1.0536750	0.9151500
C	-3.1025970	3.2549080	1.5624090
C	3.1975750	5.2456080	-0.4003830
H	3.8925560	3.5883650	0.8041710
C	1.0733370	4.9296800	-1.5310180
H	0.1028660	3.0101000	-1.2082610
C	5.4635510	0.1107570	-0.4673080
H	3.6760580	0.8620100	-1.4240990
C	5.4194360	0.0019130	1.9547150
H	3.6085790	0.6726900	2.9115910
C	-3.4069090	-0.2549100	-2.5482650
O	-1.8744610	1.6223450	-2.1655430
C	-3.0120440	-2.3532830	-1.3659880
H	-1.2663240	-2.3650890	-0.0947120
C	1.9219690	-0.1267760	-3.9774930
H	0.5547420	1.2592390	-3.0674130
C	2.5881320	-2.0044270	-2.6074380
O	1.7220440	-2.1547940	-0.3186520
C	-2.5010360	-0.8889730	4.9047270
H	-3.0335460	0.9344120	3.8688250
C	-0.7338720	-2.2153440	3.8995820
H	0.1110060	-1.4274220	2.0605980
C	-5.1870150	1.5746980	0.7386860
H	-3.7144510	-0.0072830	0.7245810
C	-4.3936260	3.7727930	1.3827550
H	-2.3047770	3.9289940	1.8867890
C	2.1869920	5.7299990	-1.2448850
H	4.0734150	5.8652450	-0.1805760
H	0.2876590	5.3024760	-2.1964590
C	6.0957650	-0.2031700	0.7449870
H	5.9817080	-0.0505040	-1.4180020
H	5.9046930	-0.2421530	2.9055210
C	-3.7696260	-1.5754510	-2.2584580
H	-4.0282380	0.3061930	-3.2495910
C	-2.6577090	2.3923470	-3.0743640
O	-3.4390270	-3.6396320	-1.1331600
C	2.6552120	-1.3151710	-3.8360800
H	1.9529370	0.4267950	-4.9239960
H	3.1702480	-2.9251650	-2.4985910
C	2.4970460	-3.3265490	-0.1740000
C	-1.6775520	-2.0249100	4.9173510
H	-3.2448420	-0.7408320	5.6947910
H	-0.0947740	-3.1031770	3.8990400
C	-5.4386420	2.9343260	0.9731520
H	-5.9951580	0.9124890	0.4124430
H	-4.5807900	4.8353950	1.5703690
H	2.2723440	6.7297110	-1.6835730
H	7.1135050	-0.6072830	0.7464450
Cl	-5.2013200	-2.2605710	-3.0281390
H	-3.6981610	2.5081330	-2.7191920
H	-2.1827640	3.3822770	-3.1224310
H	-2.6644870	1.9455500	-4.0859880

C	-2.6817910	-4.4268100	-0.2153870	C	-2.4319280	0.3970300	3.9054020
C	2.2749060	-3.8930960	1.2210200	C	-0.7362750	-1.0722710	2.9760740
H	2.2036500	-4.1127260	-0.8960840	C	3.5711010	5.0224870	-0.5758440
H	3.5797240	-3.1270430	-0.2856360	H	4.0886100	3.4163240	0.7784850
H	-1.7767800	-2.7644350	5.7188560	C	1.4794990	4.7740360	-1.7810760
H	-6.4469520	3.3388120	0.8365780	H	0.3624690	2.9521700	-1.3684980
H	-1.6482390	-4.5850050	-0.5715270	C	5.2928920	-0.1559350	2.2914540
H	-3.2005080	-5.3935120	-0.1615570	H	3.4968010	0.7282160	3.0900770
H	-2.6546000	-3.9669770	0.7888080	C	5.4684110	-0.2465860	-0.1231750
F	0.9756700	-4.2433140	1.4443400	H	3.7909960	0.5432850	-1.2340230
F	3.0296600	-5.0243570	1.3708500	C	-5.1743790	1.7186680	0.5116250
F	2.6332400	-3.0323280	2.2107670	H	-3.7149540	0.1277830	0.5774250
N	3.5024100	-1.7865120	-4.8678230	C	-4.3925010	3.9200870	1.1586870
H	3.2276760	-1.4579040	-5.7940320	H	-2.3282550	4.0657770	1.7632760
H	3.6080170	-2.8016300	-4.8810180	C	-2.5836170	-0.4711330	4.9942480
				H	-3.0493880	1.2992700	3.8411750
92				C	-0.8828950	-1.9357230	4.0716480
NH2 Transition State				H	-0.0268500	-1.3098750	2.1763010
C	-1.5639590	-1.9288530	-1.0120310	C	2.6356630	5.5138990	-1.4994020
C	-3.3520340	-0.3394550	-2.4380310	H	4.4789860	5.5950450	-0.3572920
C	-1.1410880	-0.6130290	-1.3686860	H	0.7508140	5.1514940	-2.5064310
H	-4.0873030	0.2670910	-2.9699170	C	6.0157440	-0.5055500	1.1435150
Ni	0.0411080	0.4126720	-0.1825240	H	5.7094990	-0.3543250	3.2847340
P	1.7970100	1.4501610	0.6586710	H	6.0270170	-0.5123520	-1.0271920
P	-1.1960550	1.2453130	1.4503380	C	-5.4264190	3.0840080	0.7157510
C	1.2957410	2.0859360	2.3605970	H	-5.9731320	1.0566370	0.1617910
C	2.1878360	3.0487520	-0.2096670	H	-4.5799510	4.9867930	1.3228990
C	3.4801190	0.7270670	0.9113320	C	-1.8073420	-1.6368870	5.0811190
C	-0.1563500	2.5845660	2.2772490	H	-3.3131140	-0.2381220	5.7774130
C	-2.8544330	2.0234830	1.2127130	H	-0.2787340	-2.8464890	4.1301180
C	-1.5023380	0.1049210	2.8870010	H	2.8120830	6.4709400	-2.0017080
H	1.3594280	1.2421250	3.0694100	H	6.9997060	-0.9771590	1.2340280
H	1.9765460	2.8798370	2.7115180	H	-6.4245090	3.4938950	0.5292360
C	3.3487840	3.7976630	0.0665420	H	-1.9289900	-2.3139500	5.9332030
C	1.2572710	3.5444980	-1.1429960	C	0.5848440	-0.4976080	-1.8484440
C	4.0366170	0.4578200	2.1779430	C	0.8027230	0.2282260	-3.0547390
C	4.2102350	0.3554820	-0.2399640	C	2.4200930	-1.9857030	-2.6282370
H	-0.2053830	3.4889070	1.6460610	C	1.7540750	-0.1232590	-4.0122430
H	-0.5523220	2.8409300	3.2742020	C	2.5696310	-1.2529920	-3.8264110
C	-3.8991960	1.1930970	0.7503320	H	1.8560180	0.4821900	-4.9207530
C	-3.1156780	3.3948180	1.4072390	H	-0.8612830	-2.5543780	-0.4629140

H	3.0757760	-2.8459990	-2.4627250
H	0.1754520	1.0988970	-3.2462480
C	1.4732010	-1.6098270	-1.6722350
O	1.3683510	-2.2865870	-0.4544220
C	2.3538390	-3.2650060	-0.1781420
C	2.0994820	-3.8391070	1.2094520
H	2.3163590	-4.1103360	-0.8907760
H	3.3689630	-2.8268350	-0.1861900
F	0.8853400	-4.4505340	1.3067820
F	3.0523880	-4.7820630	1.4789900
F	2.1605380	-2.9046890	2.1926090
C	-2.8183300	-2.4548520	-1.3536130
O	-3.2549950	-3.7129440	-1.0155910
C	-2.3706650	-4.5354460	-0.2557310
H	-1.4404870	-4.7508390	-0.8111250
H	-2.9175290	-5.4721760	-0.0836260
H	-2.1187660	-4.0714930	0.7140010
C	-2.1093640	0.1806020	-2.0711110
O	-1.7578050	1.4991730	-2.3231490
C	-2.7074430	2.3209490	-3.0038760
H	-3.6423540	2.4170940	-2.4244430
H	-2.2364640	3.3089980	-3.0964230
H	-2.9342230	1.9291340	-4.0123530
C	-3.7072270	-1.6503990	-2.0917500
Cl	-5.2846940	-2.2685430	-2.5643790
N	3.4656510	-1.6867670	-4.8192100
H	3.7681960	-0.9569220	-5.4633890
H	4.2603280	-2.2282930	-4.4801010

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N(CH3)2 Reactant

Ni	-0.1771030	0.3910450	-0.1880310
P	1.1190180	2.1230880	0.2726470
P	-1.8099510	1.4587110	0.8745100
C	0.2577650	3.1745570	1.5730900
C	1.1825830	3.3024690	-1.1594120
C	2.8806360	2.0247740	0.8089130
C	-1.3290790	-1.0317720	-0.7730250
C	1.2361620	-0.5868500	-1.0648360
C	-1.2338790	3.2199000	1.2102190
C	-2.1169310	0.8275450	2.5895800
C	-3.5163920	1.6312590	0.1926530
H	0.6935690	4.1862890	1.6262190
H	0.3966860	2.6871710	2.5534550
C	2.0834510	4.3852160	-1.1939300
C	0.2575680	3.1387200	-2.2081850
C	3.8236380	1.4940630	-0.0974060
C	3.3101400	2.4198370	2.0904540
C	-2.0494780	-0.8733960	-1.9760310
C	-1.5151460	-2.2303510	-0.0610760
C	1.4737080	-0.5007820	-2.4483460
C	2.1099440	-1.4394640	-0.3634200
H	-1.8351890	3.6917820	2.0046140
H	-1.3696870	3.8023840	0.2831280
C	-3.2457350	1.2211570	3.3356640
C	-1.1660420	-0.0276880	3.1757710
C	-4.3029610	0.4651930	0.0768170
C	-4.0476680	2.8589650	-0.2473310
C	2.0528460	5.2952460	-2.2582460
H	2.8197310	4.5100590	-0.3928900
C	0.2281380	4.0556340	-3.2697420
H	-0.4297280	2.2841890	-2.1926630
C	5.1690260	1.3782800	0.2724030
H	3.5031860	1.1650920	-1.0905820
C	4.6581070	2.2970010	2.4573630
H	2.5994810	2.8274460	2.8151210
C	-2.9177910	-1.8717490	-2.4450480
O	-1.8540170	0.3290160	-2.6551640
C	-2.3910760	-3.2472140	-0.4983570
H	-0.9478880	-2.3853600	0.8601460
C	2.5145630	-1.1803570	-3.1006360
H	0.8107810	0.1176400	-3.0618810
C	3.1504020	-2.1516380	-0.9817040
O	1.8741500	-1.5505690	1.0198800
C	-3.4131080	0.7708000	4.6508870
H	-4.0038330	1.8683320	2.8824020
C	-1.3350080	-0.4745640	4.4946920
H	-0.2971720	-0.3476230	2.5904520
C	-5.5942180	0.5330660	-0.4596570
H	-3.9030800	-0.4986610	0.4052380
C	-5.3413500	2.9220110	-0.7853390
H	-3.4622620	3.7796600	-0.1724580

C	1.1233310	5.1329840	-3.2967250
H	2.7596790	6.1315140	-2.2793710
H	-0.4913840	3.9223240	-4.0844060
C	5.5906770	1.7798410	1.5488260
H	5.8899380	0.9684690	-0.4423600
H	4.9773820	2.6100570	3.4569160
C	-3.0859090	-3.0470600	-1.7039000
H	-3.4793830	-1.7656860	-3.3756130
C	-2.5684560	0.5120620	-3.8753240
O	-2.6171870	-4.4289250	0.1681520
C	3.3872010	-2.0207610	-2.3742930
H	2.6243310	-1.0551480	-4.1801910
H	3.7864080	-2.8154670	-0.3957720
C	2.8317550	-2.2673380	1.7697300
C	-2.4572170	-0.0762320	5.2325090
H	-4.2959210	1.0772290	5.2220030
H	-0.5903840	-1.1410860	4.9394590
C	-6.1177410	1.7604920	-0.8911400
H	-6.1903340	-0.3810320	-0.5438480
H	-5.7426680	3.8852900	-1.1176520
H	1.1029960	5.8437410	-4.1295590
H	6.6438230	1.6887720	1.8346560
Cl	-4.1896130	-4.2866400	-2.3013870
H	-3.6617800	0.4861420	-3.7149660
H	-2.2843830	1.5061150	-4.2480710
H	-2.2903380	-0.2488680	-4.6280500
C	-1.9158590	-4.6372210	1.3926860
C	2.4669470	-2.1791150	3.2447320
H	2.8570270	-3.3424050	1.5055960
H	3.8487350	-1.8481880	1.6500160
H	-2.5922450	-0.4300850	6.2599720
H	-7.1286130	1.8109640	-1.3089920
H	-0.8221350	-4.6503510	1.2376080
H	-2.2446090	-5.6207540	1.7547420
H	-2.1681520	-3.8661040	2.1427440
F	1.2507700	-2.7340030	3.5188440
F	3.3968300	-2.8646030	3.9782800
F	2.4401830	-0.9036180	3.7133560
N	4.4610800	-2.6904370	-2.9924680
C	5.0856080	-3.7994280	-2.2829030
H	4.3774560	-4.6224230	-2.0446700
H	5.8957150	-4.2108240	-2.9017440
H	5.5432250	-3.4572810	-1.3394030
C	4.4537890	-2.7878150	-4.4476100
H	4.4837660	-1.7865030	-4.9070130
H	5.3561860	-3.3232550	-4.7759920
H	3.5645550	-3.3217070	-4.8454310

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N(CH3)2 Transition State

C	-1.2093050	-2.2832070	-0.5412030
C	-2.8106780	-1.4780870	-2.6720300
C	-0.8843780	-1.0508620	-1.1838450
H	-3.4779960	-1.1776780	-3.4821860
Ni	-0.1508300	0.4465170	-0.1473120
P	1.2096970	1.9663480	0.6937700
P	-1.8308860	1.3954390	0.9367660
C	0.2697540	2.8331010	2.0771670
C	1.5078330	3.3848840	-0.4730360
C	2.8950320	1.6683900	1.3925480
C	-1.1816160	3.0333160	1.6111350
C	-3.4572980	1.8263290	0.1696660
C	-2.3576610	0.5501350	2.5067030
H	0.2959100	2.1757320	2.9639540
H	0.7397120	3.7937060	2.3485420
C	2.4471360	4.4026380	-0.2138050
C	0.7254970	3.4541610	-1.6417970
C	3.2335120	1.8795700	2.7442480
C	3.8729140	1.1326370	0.5252390
H	-1.2047340	3.7672110	0.7872640
H	-1.8204560	3.4134350	2.4259900
C	-4.2792790	0.7588540	-0.2544140
C	-3.8870360	3.1467810	-0.0712550
C	-3.5502530	0.8775680	3.1825030
C	-1.5032360	-0.4222310	3.0591810
C	2.5947590	5.4732320	-1.1053620
H	3.0743260	4.3527700	0.6829130
C	0.8708270	4.5303460	-2.5297000
H	0.0084800	2.6508150	-1.8504380
C	4.5183620	1.5714300	3.2154550
H	2.4983140	2.2896160	3.4429850
C	5.1568890	0.8359780	0.9964820

H	3.6259110	0.9467500	-0.5254920	F	2.9972570	-3.5863890	3.4457460
C	-5.5052820	1.0088060	-0.8820130	F	1.8699730	-1.6999730	3.4367380
H	-3.9601120	-0.2749310	-0.0877150	C	-2.2776700	-3.1015570	-0.9354620
C	-5.1128290	3.3941160	-0.7069670	O	-2.6182310	-4.2872230	-0.3297500
H	-3.2754130	3.9972860	0.2434860	C	-1.8393090	-4.7025210	0.7906890
C	-3.8763960	0.2457270	4.3893640	H	-0.7857040	-4.8782920	0.5090500
H	-4.2335770	1.6195520	2.7565110	H	-2.2888400	-5.6469910	1.1256810
C	-1.8266780	-1.0476150	4.2721330	H	-1.8808460	-3.9631360	1.6094970
H	-0.5850790	-0.6912720	2.5267280	C	-1.7546960	-0.6633210	-2.2576310
C	1.8051120	5.5402410	-2.2634940	O	-1.5154490	0.5804610	-2.8235490
H	3.3304170	6.2576220	-0.8969500	C	-2.4018340	1.0239340	-3.8513320
H	0.2583450	4.5760320	-3.4365230	H	-3.4366230	1.1099310	-3.4754690
C	5.4852640	1.0533690	2.3440070	H	-2.0407780	2.0175200	-4.1499830
H	4.7637170	1.7434710	4.2689510	H	-2.3786970	0.3505200	-4.7276310
H	5.9060220	0.4329000	0.3064910	C	-3.0711000	-2.6935830	-2.0243040
C	-5.9276530	2.3276260	-1.1100580	Cl	-4.4154310	-3.6893410	-2.5688400
H	-6.1318730	0.1671840	-1.1948460	N	4.4424880	-2.1860870	-3.3027510
H	-5.4343810	4.4272490	-0.8778030	C	4.9090860	-1.5362150	-4.5209850
C	-3.0141040	-0.7159490	4.9378110	C	5.4137270	-2.9602550	-2.5451210
H	-4.8095620	0.5025980	4.9021820	H	5.2143450	-0.4812450	-4.3589010
H	-1.1523780	-1.8009260	4.6915460	H	5.7727420	-2.0891590	-4.9161400
H	1.9231610	6.3777340	-2.9592420	H	4.1271380	-1.5502910	-5.2979680
H	6.4892160	0.8182880	2.7124220	H	4.9355960	-3.8348610	-2.0724720
H	-6.8874360	2.5221150	-1.5999350	H	6.1832610	-3.3431210	-3.2299000
H	-3.2724440	-1.2100900	5.8803420	H	5.9219880	-2.3730630	-1.7498880
C	0.8784170	-0.7381320	-1.3406920				
C	1.2846840	-0.3139360	-2.6382310	93			
C	2.9893530	-2.0601280	-1.3265120	**CH3 Reactant**			
C	2.4505280	-0.7391690	-3.2737290	Ni	0.0347180	0.3969280	-0.1958080
C	3.3193180	-1.6667110	-2.6516730	P	1.7547160	1.4944440	0.6604680
H	2.6687020	-0.3493420	-4.2704320	P	-1.1703880	1.1466720	1.5129130
H	-0.5798860	-2.6021850	0.2888270	C	1.3145690	1.9781640	2.4223240
H	3.6756320	-2.7081290	-0.7819950	C	1.9795360	3.1580950	-0.1297010
H	0.6323030	0.3728330	-3.1780270	C	3.4793800	0.8467250	0.7506910
C	1.8283090	-1.5995310	-0.7025200	C	-1.4832290	-0.4395470	-1.0303370
O	1.5447460	-1.9308100	0.6266340	C	1.0560770	-0.3174990	-1.6665660
C	2.5280460	-2.6629480	1.3329970	C	-0.1490360	2.4432730	2.4197750
C	2.0541340	-2.8656140	2.7661770	C	-1.4358360	-0.1133270	2.8475610
H	2.6935180	-3.6671700	0.8987230	C	-2.8433260	1.8984140	1.3158710
H	3.4901530	-2.1193910	1.3691270	H	1.9903100	2.7610990	2.8051850
F	0.8843450	-3.5623600	2.8364380	H	1.4277970	1.0834800	3.0581240

C	3.0994220	3.9656500	0.1510570	C	6.1004920	-0.1933070	0.7730860
C	0.9737100	3.6446780	-0.9861030	H	6.0018840	-0.0436700	-1.3899760
C	4.1729130	0.6301530	-0.4591690	H	5.8946200	-0.2297430	2.9321090
C	4.1120150	0.5291680	1.9680990	C	-3.7732110	-1.5761110	-2.2458940
C	-2.2723610	0.3029610	-1.9338770	H	-4.0267370	0.3015080	-3.2458440
C	-1.8748110	-1.7641800	-0.7657890	C	-2.6448540	2.3820570	-3.0873360
C	1.1405040	0.3361900	-2.9091320	O	-3.4481440	-3.6359120	-1.1114490
C	1.7952980	-1.5141330	-1.5485930	C	2.6522870	-1.3418810	-3.8313330
H	-0.5295240	2.6062270	3.4414610	H	1.9646690	0.4018830	-4.9149150
H	-0.2344260	3.3926300	1.8645600	H	3.1411580	-2.9541100	-2.4898870
C	-2.3865580	0.0752390	3.8702740	C	2.4790280	-3.3363370	-0.1539650
C	-0.6191070	-1.2590320	2.8672160	C	-1.6878480	-2.0029100	4.9175220
C	-3.9010910	1.0603070	0.9029980	H	-3.2560380	-0.7152830	5.6872540
C	-3.1002850	3.2667510	1.5283580	H	-0.1038550	-3.0858710	3.9060430
C	3.2069530	5.2436080	-0.4113570	C	-5.4362440	2.9444510	0.9400090
H	3.8973340	3.5896720	0.8002460	H	-5.9961410	0.9180380	0.3995910
C	1.0846040	4.9267430	-1.5454210	H	-4.5754290	4.8500480	1.5181540
H	0.1107770	3.0097240	-1.2183390	H	2.2861100	6.7247370	-1.7010870
C	5.4751250	0.1165160	-0.4437670	H	7.1193430	-0.5943820	0.7819150
H	3.6912680	0.8595540	-1.4144570	Cl	-5.2087020	-2.2594520	-3.0091310
C	5.4153010	0.0116090	1.9776590	H	-3.6853770	2.5056330	-2.7351260
H	3.5968640	0.6803890	2.9210230	H	-2.1650030	3.3692350	-3.1421490
C	-3.4063010	-0.2583880	-2.5428200	H	-2.6513520	1.9271340	-4.0951880
O	-1.8670120	1.6154460	-2.1706390	C	-2.6891410	-4.4239220	-0.1956860
C	-3.0166590	-2.3527290	-1.3513110	C	2.2621900	-3.8902380	1.2468600
H	-1.2684730	-2.3650160	-0.0833760	H	2.1776160	-4.1257830	-0.8689460
C	1.9272160	-0.1511430	-3.9684050	H	3.5621460	-3.1442110	-0.2739320
H	0.5666090	1.2551080	-3.0631070	H	-1.7890210	-2.7394200	5.7215390
C	2.5751010	-2.0230240	-2.5992840	H	-6.4436160	3.3494190	0.7981670
O	1.7104820	-2.1604270	-0.3030360	H	-1.6580300	-4.5864080	-0.5567920
C	-2.5108130	-0.8666710	4.8991700	H	-3.2109670	-5.3886520	-0.1375060
H	-3.0407260	0.9530300	3.8554400	H	-2.6556590	-3.9622510	0.8074610
C	-0.7423040	-2.1976430	3.9023180	F	0.9625910	-4.2324250	1.4808220
H	0.1064720	-1.4170430	2.0620200	F	3.0125350	-5.0232180	1.4026160
C	-5.1870870	1.5819890	0.7199110	F	2.6298260	-3.0221290	2.2272830
H	-3.7175360	-0.0029460	0.7237340	C	3.4713310	-1.9100930	-4.9703900
C	-4.3900810	3.7851950	1.3419490	H	3.6679970	-1.1491450	-5.7426590
H	-2.3015030	3.9427100	1.8463840	H	4.4463220	-2.2960990	-4.6260940
C	2.1986740	5.7265290	-1.2594550	H	2.9509530	-2.7496930	-5.4664380
H	4.0828970	5.8630410	-0.1914510				
H	0.3007650	5.2983870	-2.2136120				

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CH3 Transition State

C	-1.5322190	-1.9389630	-1.0596890
C	-3.3132240	-0.3319730	-2.4748790
C	-1.1047920	-0.6215740	-1.4046850
H	-4.0467760	0.2812170	-3.0012300
Ni	0.0398070	0.4170230	-0.1806690
P	1.7819160	1.4569100	0.6734900
P	-1.2219180	1.2358130	1.4436440
C	1.2647150	2.0698560	2.3788250
C	2.1727270	3.0654060	-0.1751570
C	3.4638370	0.7334070	0.9300780
C	-0.1877630	2.5665430	2.2911060
C	-2.8752730	2.0221840	1.1931300
C	-1.5485710	0.0847610	2.8666260
H	1.3258930	1.2172290	3.0771970
H	1.9403830	2.8613210	2.7450410
C	3.3286010	3.8152010	0.1191210
C	1.2492280	3.5669380	-1.1122670
C	4.0175420	0.4669800	2.1984770
C	4.1968060	0.3629930	-0.2195220
H	-0.2334370	3.4775100	1.6692470
H	-0.5904750	2.8121940	3.2880440
C	-3.9181070	1.1988400	0.7142030
C	-3.1337810	3.3932530	1.3925870
C	-2.4947390	0.3654760	3.8729090
C	-0.7798500	-1.0905830	2.9575380
C	3.5524830	5.0470380	-0.5090550
H	4.0634760	3.4288070	0.8334580
C	1.4731450	4.8033120	-1.7362840
H	0.3590740	2.9736360	-1.3528740
C	5.2751260	-0.1434540	2.3153060
H	3.4749840	0.7370770	3.1090950
C	5.4561320	-0.2363680	-0.0992180
H	3.7804860	0.5480000	-1.2152560
C	-5.1884220	1.7304430	0.4634920
H	-3.7360350	0.1335600	0.5383740
C	-4.4055610	3.9250150	1.1316760
H	-2.3483800	4.0591740	1.7621540
C	-2.6601840	-0.5125200	4.9518610
H	-3.1138720	1.2664300	3.8069820
C	-0.9400320	-1.9634730	4.0436050
H	-0.0570910	-1.3187270	2.1669570
C	2.6239720	5.5442790	-1.4364220
H	4.4566230	5.6201360	-0.2770040
H	0.7504920	5.1851060	-2.4653780
C	6.0009240	-0.4924100	1.1689460
H	5.6902460	-0.3397550	3.3096250
H	6.0158720	-0.5032080	-1.0019740
C	-5.4374110	3.0957960	0.6717820
H	-5.9859960	1.0734100	0.1016580
H	-4.5907150	4.9914970	1.2997450
C	-1.8811690	-1.6762760	5.0409890
H	-3.4022690	-0.2884840	5.7257510
H	-0.3330440	-2.8721210	4.1041170
H	2.8021140	6.5064230	-1.9281900
H	6.9856180	-0.9620090	1.2619620
H	-6.4315610	3.5107250	0.4757630
H	-2.0133410	-2.3607140	5.8855680
C	0.6044790	-0.4976700	-1.8400230
C	0.8547550	0.2377010	-3.0361480
C	2.4826080	-1.9566460	-2.5643570
C	1.8461760	-0.1073990	-3.9580390
C	2.6697130	-1.2245800	-3.7569130
H	1.9758640	0.5081080	-4.8562030
H	-0.8318920	-2.5699130	-0.5141710
H	3.1519000	-2.8007360	-2.3710190
H	0.2256420	1.1028420	-3.2449070
C	1.5010370	-1.6035810	-1.6362090
O	1.3665520	-2.2823400	-0.4202650
C	2.3468370	-3.2614600	-0.1258320
C	2.0512670	-3.8551910	1.2448930
H	2.3346180	-4.0966290	-0.8511050
H	3.3605840	-2.8213090	-0.0975990
F	0.8343350	-4.4679150	1.2968370
F	2.9952340	-4.8016480	1.5304290
F	2.0813160	-2.9349840	2.2434430
C	-2.7864360	-2.4594510	-1.4084300
O	-3.2268780	-3.7189660	-1.0849730
C	-2.3462010	-4.5521850	-0.3313290
H	-1.4151600	-4.7632180	-0.8867090
H	-2.8958030	-5.4893570	-0.1715490

H	-2.0964830	-4.0994950	0.6440220
C	-2.0693990	0.1819500	-2.1023780
O	-1.7171180	1.5001080	-2.3415770
C	-2.6597700	2.3290170	-3.0252030
H	-3.5971710	2.4272040	-2.4504890
H	-2.1832640	3.3148610	-3.1107160
H	-2.8812950	1.9419640	-4.0364040
C	-3.6713250	-1.6449380	-2.1408430
Cl	-5.2478260	-2.2549300	-2.6219770
C	3.7098620	-1.6486040	-4.7666630
H	4.6509610	-1.9639370	-4.2831290
H	3.9496440	-0.8306640	-5.4649560
H	3.3631810	-2.5038760	-5.3760590

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H Reactant

Ni	0.0837520	0.3733520	-0.2641910
P	1.9198400	1.3251770	0.5321300
P	-0.9270380	0.9783140	1.6206500
C	1.6484830	1.6812940	2.3584800
C	2.1530830	3.0395670	-0.1376430
C	3.6147180	0.6049510	0.4240490
C	-1.5380550	-0.3024220	-1.0458620
C	0.9427610	-0.1949940	-1.8907000
C	0.2058500	2.1806880	2.5216550
C	-1.0739640	-0.3888070	2.8644630
C	-2.5973950	1.7607470	1.6753620
H	2.3797770	2.4153070	2.7359790
H	1.7857580	0.7394440	2.9165910
C	3.3354610	3.7695020	0.0944850
C	1.0952560	3.6418860	-0.8448860
C	4.2045990	0.4744930	-0.8517110
C	4.3255490	0.1559660	1.5537610
C	-2.3799330	0.5828000	-1.7514440
C	-1.9558270	-1.6405040	-0.9316240
C	0.9454690	0.5995120	-3.0537140
C	1.6364480	-1.4220400	-1.9700740
H	-0.0778550	2.2737980	3.5828550
H	0.0976710	3.1710490	2.0478090
C	-1.8360010	-0.2393750	4.0407870
C	-0.3580450	-1.5812190	2.6529800
C	-3.7089320	0.9793170	1.2945150
C	-2.8023750	3.1016530	2.0538780
C	3.4543710	5.0855070	-0.3689870
H	4.1711740	3.3025570	0.6263110
C	1.2177810	4.9621430	-1.3038910
H	0.1824680	3.0671000	-1.0412150
C	5.4826620	-0.0813210	-0.9852110
H	3.6636620	0.8057900	-1.7432440
C	5.6039930	-0.4033020	1.4140050
H	3.8924410	0.2376730	2.5545630
C	-3.5912140	0.1466510	-2.3117570
O	-1.9427800	1.9028490	-1.8475430
C	-3.1731730	-2.1070150	-1.4730200
H	-1.3094660	-2.3499820	-0.4093070
C	1.6149430	0.2146620	-4.2290770
H	0.4000600	1.5481900	-3.0485020
C	2.3023720	-1.8346860	-3.1365260
O	1.6247100	-2.2014200	-0.8008630
C	-1.8727500	-1.2661190	4.9920150
H	-2.4140700	0.6756190	4.2079570
C	-0.3956620	-2.6073510	3.6089090
H	0.2249380	-1.7032330	1.7340120
C	-4.9967790	1.5281420	1.3067730
H	-3.5662240	-0.0607210	0.9867470
C	-4.0941720	3.6477940	2.0619310
H	-1.9604330	3.7330460	2.3517570
C	2.3947470	5.6843000	-1.0673850
H	4.3787880	5.6444310	-0.1890360
H	0.3936410	5.4249030	-1.8567640
C	6.1868730	-0.5205380	0.1456910
H	5.9281510	-0.1720170	-1.9811160
H	6.1442720	-0.7454900	2.3027930
C	-3.9819990	-1.1892850	-2.1655540
H	-4.2526000	0.8183060	-2.8630530
C	-2.7819310	2.8185610	-2.5486420
O	-3.6315740	-3.3993750	-1.3741720
C	2.2926380	-1.0064960	-4.2710390
H	1.5940790	0.8663910	-5.1095880
H	2.8329420	-2.7897420	-3.1895960
C	2.3726990	-3.3993920	-0.8420600
C	-1.1518440	-2.4510050	4.7776430

H	-2.4718870	-1.1439140	5.9005320	H	2.3357780	2.4380930	2.7303100
H	0.1628200	-3.5314050	3.4333420	C	3.5216980	3.6537690	0.0930470
C	-5.1935560	2.8622930	1.6915770	C	1.3557320	3.5646900	-1.0039400
H	-5.8484340	0.9086000	1.0088360	C	4.2521100	0.0687440	1.7581000
H	-4.2388650	4.6902620	2.3647250	C	4.2465380	0.2339180	-0.6634860
H	2.4909790	6.7124210	-1.4318030	H	0.1411640	3.2850110	1.8880270
H	7.1869060	-0.9533070	0.0381070	H	-0.1515870	2.4681180	3.4479290
Cl	-5.5129450	-1.7164090	-2.8638270	C	-3.7490410	1.3731110	0.9871720
H	-3.7736130	2.9117210	-2.0695060	C	-2.7217610	3.4543180	1.6931650
H	-2.2716750	3.7910400	-2.5075750	C	-2.1955270	0.1970560	3.9340310
H	-2.9127270	2.5233100	-3.6062270	C	-0.7648570	-1.3683530	2.7507840
C	-2.8015020	-4.3412590	-0.6962520	C	3.7371290	4.9312640	-0.4396500
H	2.8105140	-1.3304660	-5.1797900	H	4.2937270	3.1873890	0.7143540
C	2.2578290	-4.0964640	0.5059460	C	1.5714980	4.8460620	-1.5322750
H	1.9937140	-4.1030430	-1.6079190	H	0.4348380	3.0147830	-1.2320540
H	3.4465090	-3.2120300	-1.0321480	C	5.4915950	-0.5860430	1.7085580
H	-1.1855500	-3.2544770	5.5208420	H	3.7878760	0.2477080	2.7321680
H	-6.2020430	3.2886670	1.7018610	C	5.4877180	-0.4123050	-0.7087560
H	-1.8258430	-4.4589330	-1.2006710	H	3.7654490	0.5440150	-1.5969670
H	-3.3484150	-5.2930180	-0.7331860	C	-4.9822700	2.0236670	0.8633520
H	-2.6347030	-4.0538050	0.3574720	H	-3.6786560	0.3057370	0.7537910
F	0.9720620	-4.4330220	0.8139120	C	-3.9573590	4.1056530	1.5608660
F	2.9825670	-5.2559790	0.4749760	H	-1.8550110	4.0322630	2.0265540
F	2.7334160	-3.3477520	1.5363800	C	-2.4012680	-0.7540890	4.9410050
				H	-2.6910610	1.1714980	3.9993230
90				C	-0.9665070	-2.3177540	3.7637030
H Transition State				H	-0.1379500	-1.6083900	1.8857600
C	-1.5794230	-1.8798830	-1.1703520	C	2.7615160	5.5304190	-1.2513220
C	-3.4375970	-0.1468380	-2.3116210	H	4.6716950	5.4603370	-0.2242610
C	-1.1537570	-0.5489370	-1.4577060	H	0.8121230	5.3074680	-2.1724810
H	-4.1992070	0.5148220	-2.7280860	C	6.1155310	-0.8250700	0.4769180
Ni	0.1030020	0.3929640	-0.2641510	H	5.9718040	-0.9057710	2.6394680
P	1.9473160	1.2875490	0.5360830	H	5.9666960	-0.5937490	-1.6767930
P	-1.0061230	1.1441400	1.4983670	C	-5.0918640	3.3930680	1.1510510
C	1.5903720	1.7297620	2.3307000	H	-5.8613220	1.4561410	0.5407800
C	2.3263420	2.9604670	-0.1820690	H	-4.0322470	5.1740180	1.7908370
C	3.6163530	0.4930150	0.5740450	C	-1.7846960	-2.0122060	4.8589790
C	0.1686100	2.3101620	2.4045010	H	-3.0486090	-0.5144840	5.7914430
C	-2.6021690	2.0780660	1.4150290	H	-0.4878520	-3.2994800	3.6912690
C	-1.3709190	-0.1009090	2.8304620	H	2.9338370	6.5280930	-1.6687440
H	1.6486640	0.7995320	2.9220710	H	7.0857540	-1.3311270	0.4398750

H	-6.0572100	3.9009700	1.0561730	C	0.8868410	2.4224590	2.2907420
H	-1.9489180	-2.7551960	5.6465180	C	1.6684670	3.2317060	-0.3703400
C	0.5238660	-0.4241610	-2.0126630	C	3.2658710	1.2332640	0.9860930
C	0.6927880	0.3909090	-3.1733850	C	-1.4399220	-0.6612890	-0.9933020
C	2.3075570	-1.8669200	-2.9699710	C	1.1454220	-0.4810840	-1.3872820
C	1.6022810	0.0945550	-4.1916990	C	-0.5967960	2.7693060	2.0980750
C	2.4057130	-1.0472680	-4.1089410	C	-1.7533990	0.2199410	2.8249710
H	1.6781080	0.7624660	-5.0565250	C	-3.1475510	1.8620630	0.8995190
H	-0.8504940	-2.5606410	-0.7327370	H	1.4745960	3.3054160	2.5929520
H	2.9692630	-2.7336900	-2.8920840	H	0.9985580	1.6496290	3.0707280
H	3.1120360	-1.3037400	-4.9043210	C	2.7141490	4.1581990	-0.1890020
H	0.0655650	1.2768110	-3.2700610	C	0.6706410	3.4932460	-1.3285590
C	1.4072650	-1.5574510	-1.9470690	C	4.0745380	0.8948160	-0.1200570
O	1.3448670	-2.3099720	-0.7693140	C	3.8158090	1.1684000	2.2808520
C	2.3496030	-3.2919910	-0.5885260	C	-2.1747660	-0.0899430	-2.0535910
C	2.1485350	-3.9527690	0.7686990	C	-1.7794010	-1.9688420	-0.6021510
H	2.2949860	-4.0919410	-1.3504620	C	1.3131460	-0.0297900	-2.7059270
H	3.3590800	-2.8415550	-0.6057580	C	1.9426890	-1.5860890	-1.0120650
F	0.9408800	-4.5803600	0.8688800	H	-1.0766480	3.0568900	3.0481070
F	3.1149250	-4.9025670	0.9467980	H	-0.6916030	3.6141690	1.3950150
F	2.2352880	-3.0808650	1.8054680	C	-2.7300690	0.5610550	3.7823850
C	-2.8702570	-2.3533320	-1.4446080	C	-0.9516120	-0.9173360	3.0322290
O	-3.3090420	-3.6261630	-1.1773210	C	-4.1056550	0.8971620	0.5215130
C	-2.3814940	-4.5319010	-0.5795530	C	-3.5140660	3.2218060	0.9028550
H	-1.5079240	-4.7054640	-1.2326520	C	2.7552690	5.3329080	-0.9506470
H	-2.9334540	-5.4723990	-0.4505130	H	3.5061660	3.9548670	0.5394910
H	-2.0373390	-4.1682530	0.4042850	C	0.7136560	4.6736780	-2.0854420
C	-2.1524310	0.3163180	-2.0206340	H	-0.1314670	2.7611120	-1.4830690
O	-1.7875510	1.6381320	-2.2102250	C	5.4080610	0.5133130	0.0707050
C	-2.7644000	2.5309120	-2.7508360	H	3.6583820	0.9260750	-1.1316770
H	-3.6365590	2.6218360	-2.0801700	C	5.1512610	0.7829220	2.4665250
H	-2.2651320	3.5059700	-2.8294110	H	3.2100800	1.4167860	3.1570960
H	-3.0960620	2.2093090	-3.7546920	C	-3.2087280	-0.7962030	-2.6885950
C	-3.7966340	-1.4727700	-2.0352280	O	-1.8193620	1.2078940	-2.4209230
Cl	-5.4233250	-2.0188480	-2.4127870	C	-2.8186530	-2.7021570	-1.2145260
				H	-1.2096340	-2.4380600	0.2038780
94				C	2.2282800	-0.6045010	-3.6126200
OCH3 Reactant				H	0.7021550	0.8060210	-3.0604600
Ni	-0.0579790	0.3690120	-0.1425220	C	2.8534320	-2.1933260	-1.8860730
P	1.5111920	1.7035300	0.6697270	O	1.7696410	-2.0455500	0.3026300
P	-1.4510500	1.2756850	1.3321290	C	-2.8930730	-0.2204190	4.9324500

H	-3.3751480	1.4312450	3.6217210	H	-2.5469810	-4.0589800	1.1377460
C	-1.1160910	-1.6970520	4.1869830	F	1.1369770	-3.8428510	2.4049400
H	-0.2019250	-1.1921670	2.2826900	F	3.2768110	-4.2845620	2.6509560
C	-5.4016880	1.2884420	0.1655540	F	2.5182840	-2.2543110	3.0148630
H	-3.8373580	-0.1631950	0.5030410	O	3.9275700	-2.3603370	-3.9736240
C	-4.8136090	3.6092640	0.5441560	C	4.0675110	-1.9302710	-5.3259860
H	-2.7942520	3.9936900	1.1894870	H	4.4163810	-0.8826780	-5.3862120
C	1.7538970	5.5933970	-1.8986200	H	4.8231830	-2.5904410	-5.7728390
H	3.5742260	6.0456940	-0.8070140	H	3.1180300	-2.0303380	-5.8827490
H	-0.0644750	4.8717250	-2.8300320				
C	5.9507270	0.4577660	1.3630670	94			
H	6.0235930	0.2544960	-0.7967770	**OCH3 Transition State**			
H	5.5656160	0.7390100	3.4791280	C	-1.4218150	-2.0800250	-0.9096550
C	-3.5261480	-2.0917940	-2.2645740	C	-3.0800770	-0.7081690	-2.6772090
H	-3.7859530	-0.3693240	-3.5116460	C	-1.0056270	-0.7820890	-1.3339040
C	-2.5533240	1.8100590	-3.4843850	H	-3.7686280	-0.1843160	-3.3426650
O	-3.1945710	-3.9763470	-0.8603970	Ni	-0.0354280	0.4167600	-0.1127110
C	2.9994550	-1.6949110	-3.1947440	P	1.5698960	1.5952230	0.8358770
H	2.3112370	-0.1978920	-4.6237230	P	-1.4988930	1.3488170	1.2551050
H	3.4679020	-3.0529370	-1.6075930	C	0.8405880	2.3226340	2.4127630
C	2.6753380	-3.0370220	0.7444840	C	2.0130150	3.1438910	-0.0962220
C	-2.0850040	-1.3494630	5.1370340	C	3.2315790	0.9590240	1.3385200
H	-3.6573360	0.0492190	5.6690300	C	-0.5990020	2.7700350	2.1094870
H	-0.4882740	-2.5801150	4.3372260	C	-3.1153580	2.0742990	0.7282140
C	-5.7603430	2.6441660	0.1767130	C	-2.0019690	0.3214740	2.7212480
H	-6.1322620	0.5271100	-0.1254310	H	0.8321690	1.5268550	3.1779080
H	-5.0846050	4.6702750	0.5572000	H	1.4502290	3.1587040	2.7958270
H	1.7896980	6.5112410	-2.4948090	C	3.0828960	3.9742100	0.2921860
H	6.9939460	0.1592380	1.5096540	C	1.2234320	3.5140840	-1.2013220
Cl	-4.8340780	-2.9601850	-3.0677830	C	3.6347780	0.7994490	2.6793850
H	-3.6272360	1.8994760	-3.2387340	C	4.1063500	0.5344240	0.3136980
H	-2.1299430	2.8158750	-3.6142000	H	-0.5825550	3.6265930	1.4137360
H	-2.4396390	1.2462750	-4.4289360	H	-1.1260710	3.0842700	3.0260940
C	-2.4603370	-4.6116780	0.1849110	C	-4.0928170	1.1865390	0.2269860
C	2.3913950	-3.3411630	2.2085530	C	-3.4009700	3.4541810	0.7452290
H	2.5646760	-3.9866970	0.1869360	C	-3.0623180	0.6896110	3.5729100
H	3.7254340	-2.6984370	0.6660380	C	-1.2593530	-0.8379630	3.0126080
H	-2.2164280	-1.9611170	6.0357370	C	3.3527710	5.1568640	-0.4079080
H	-6.7752450	2.9470130	-0.1011500	H	3.7164560	3.6873190	1.1384440
H	-1.3930050	-4.7210820	-0.0778720	C	1.4927860	4.7014310	-1.8987310
H	-2.9124490	-5.6062980	0.2975120	H	0.4027000	2.8583200	-1.5140700

C	4.8832440	0.2395540	2.9882690	H	2.4482510	-4.0614950	-0.1142100
H	2.9792950	1.1123410	3.4972740	H	3.3763950	-2.6942910	0.6047240
C	5.3549610	-0.0165350	0.6248270	F	0.7609780	-4.2652250	1.9182250
H	3.8078450	0.6380900	-0.7349750	F	2.8961000	-4.5140970	2.3812590
C	-5.3285060	1.6663510	-0.2227360	F	1.8844330	-2.6115230	2.8148350
H	-3.8880880	0.1115700	0.1925960	C	-2.6038640	-2.6940230	-1.3488780
C	-4.6373080	3.9329280	0.2864220	O	-3.0303280	-3.9384340	-0.9539170
H	-2.6658560	4.1694550	1.1256830	C	-2.2093590	-4.6569710	-0.0340580
C	-3.3694190	-0.0874600	4.6969060	H	-1.2116360	-4.8651150	-0.4597130
H	-3.6586150	1.5806950	3.3500110	H	-2.7335040	-5.6048760	0.1469840
C	-1.5623710	-1.6103410	4.1437310	H	-2.0944410	-4.1112030	0.9187270
H	-0.4445050	-1.1323890	2.3423340	C	-1.9094570	-0.1013520	-2.2190450
C	2.5563310	5.5236730	-1.5037440	O	-1.5765870	1.2030040	-2.5523150
H	4.1889280	5.7936910	-0.0996160	C	-2.4626680	1.9152560	-3.4180040
H	0.8741710	4.9814720	-2.7581170	H	-3.4619550	2.0287570	-2.9623650
C	5.7486040	-0.1667050	1.9640680	H	-2.0132780	2.9080860	-3.5555150
H	5.1802330	0.1258440	4.0362980	H	-2.5559430	1.4177630	-4.4006520
H	6.0234570	-0.3307750	-0.1836840	C	-3.4259600	-1.9997460	-2.2563970
C	-5.6062900	3.0416810	-0.1937110	Cl	-4.9095080	-2.7310990	-2.8526690
H	-6.0767980	0.9604020	-0.5975500	O	4.1201260	-1.8804520	-3.8771030
H	-4.8449170	5.0081060	0.3145530	C	4.4338730	-1.2519910	-5.1204790
C	-2.6184510	-1.2372690	4.9856270	H	3.6063460	-1.3563920	-5.8449870
H	-4.1995540	0.2040100	5.3493420	H	4.6688200	-0.1807040	-4.9842250
H	-0.9759270	-2.5087240	4.3609310	H	5.3213560	-1.7736800	-5.5025190
H	2.7691680	6.4481000	-2.0509840				
H	6.7247680	-0.5991670	2.2066530	92			
H	-6.5737510	3.4160580	-0.5441560	**CCH Reactant**			
H	-2.8609040	-1.8440490	5.8644260	Ni	-0.0110690	0.4000050	-0.1733350
C	0.7496730	-0.6225980	-1.5965910	P	1.5878130	1.6814360	0.6707710
C	1.1014410	0.0136180	-2.8184650	P	-1.3700530	1.2513620	1.3698080
C	2.7428130	-2.0591900	-1.9757670	C	0.9886300	2.3534590	2.3206050
C	2.1991180	-0.3514890	-3.6083180	C	1.7693910	3.2388420	-0.3186640
C	3.0196940	-1.4083020	-3.1956830	C	3.3320650	1.1569840	0.9585220
H	2.3901780	0.1947830	-4.5351780	C	-1.4247010	-0.5791200	-1.0394220
H	-0.7723390	-2.6208000	-0.2227920	C	1.1479090	-0.4020030	-1.4759600
H	3.4330910	-2.8472520	-1.6662150	C	-0.4942330	2.7179670	2.1607800
H	0.4657340	0.8250590	-3.1724790	C	-1.6129820	0.1387710	2.8314210
C	1.6552280	-1.6672970	-1.1976670	C	-3.0799530	1.8468910	1.0137550
O	1.4115040	-2.2429940	0.0494350	H	1.5893290	3.2211110	2.6407690
C	2.3783160	-3.1626960	0.5265470	H	1.1033470	1.5562550	3.0752060
C	1.9659640	-3.6269510	1.9170300	C	2.8493520	4.1238440	-0.1305700

C	0.7574960	3.5675960	-1.2412400	H	6.0538880	0.1695940	-0.8739810
C	4.1256540	0.8347020	-0.1633740	H	5.6332080	0.5246650	3.4186930
C	3.8874200	1.0356120	2.2468600	C	-3.5681330	-1.9144710	-2.3161500
C	-2.1654200	0.0473240	-2.0636790	H	-3.8098680	-0.1450720	-3.4984680
C	-1.7858580	-1.8918930	-0.6870910	C	-2.5165610	1.9990480	-3.4295320
C	1.3242570	0.1561410	-2.7586230	O	-3.2584940	-3.8521920	-0.9815650
C	1.9041290	-1.5636890	-1.1948910	C	2.9565450	-1.5318050	-3.3971370
H	-0.9560840	2.9819370	3.1264240	H	2.3224470	0.0919490	-4.6870850
H	-0.5954280	3.5824180	1.4827020	H	3.3693310	-3.0264060	-1.9029180
C	-2.5684120	0.4249750	3.8274170	C	2.5186300	-3.2378440	0.3999050
C	-0.7827240	-0.9879020	2.9735790	C	-1.8445350	-1.5184560	5.0927690
C	-4.0435910	0.8982390	0.6099620	H	-3.4297650	-0.1746960	5.7194300
C	-3.4531190	3.2014920	1.1092400	H	-0.2481570	-2.6859500	4.2040400
C	2.9101360	5.3243760	-0.8494090	C	-5.7182520	2.6499260	0.4231410
H	3.6523470	3.8679070	0.5685910	H	-6.0880000	0.5518000	0.0074170
C	0.8205660	4.7738410	-1.9545120	H	-5.0428320	4.6553370	0.9006210
H	-0.0708510	2.8674500	-1.4046510	H	1.9457410	6.5900880	-2.3234070
C	5.4500740	0.4135770	0.0058490	H	7.0346660	-0.0265380	1.4217840
H	3.7074830	0.9119100	-1.1717220	Cl	-4.9123660	-2.7225450	-3.1204820
C	5.2139240	0.6110190	2.4108860	H	-3.5865740	2.1062650	-3.1742450
H	3.2941580	1.2719660	3.1348520	H	-2.0707770	2.9979920	-3.5342140
C	-3.2270570	-0.6132500	-2.7023180	H	-2.4211050	1.4585630	-4.3892320
O	-1.7898100	1.3503070	-2.3877700	C	-2.5351270	-4.5333370	0.0424190
C	-2.8558890	-2.5778310	-1.3017120	C	2.2192970	-3.6603270	1.8310320
H	-1.2131050	-2.4028960	0.0908310	H	2.2988270	-4.1027600	-0.2545230
C	2.2097580	-0.3769240	-3.7046950	H	3.5994540	-3.0105660	0.3380940
H	0.7426020	1.0412050	-3.0328330	H	-1.9371980	-2.1644220	5.9720670
C	2.7880240	-2.1277950	-2.1227100	H	-6.7433520	2.9610960	0.1968080
O	1.7214760	-2.1137850	0.0822460	H	-1.4749700	-4.6730500	-0.2340100
C	-2.6817340	-0.4009510	4.9522660	H	-3.0189670	-5.5144990	0.1393470
H	-3.2348140	1.2868800	3.7167500	H	-2.5934250	-3.9975780	1.0068540
C	-0.8966550	-1.8110570	4.1038600	F	0.9153310	-4.0190680	2.0107500
H	-0.0521320	-1.2206430	2.1913670	F	2.9855100	-4.7466020	2.1481490
C	-5.3527330	1.2999710	0.3196820	F	2.4962040	-2.6874340	2.7400270
H	-3.7695870	-0.1572240	0.5207430	C	3.8659280	-2.1001450	-4.3378800
C	-4.7658780	3.5991960	0.8161780	C	4.6455030	-2.5852470	-5.1400180
H	-2.7285320	3.9600270	1.4184870	H	5.3223620	-3.0143280	-5.8529220
C	1.8944380	5.6524480	-1.7602310				
H	3.7558620	6.0041530	-0.7016330				
H	0.0318560	5.0241790	-2.6716220				
C	5.9983520	0.3021970	1.2921670				

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C	-1.3899520	-2.1209120	-0.8846840
C	-3.1259140	-0.7994980	-2.6167620
C	-1.0106010	-0.8241870	-1.3410410
H	-3.8429700	-0.2976270	-3.2686450
Ni	-0.0207030	0.4265110	-0.1835090
P	1.5995590	1.6410450	0.6793790
P	-1.4462920	1.3555330	1.2384290
C	0.9259760	2.3667740	2.2801500
C	1.9932560	3.1868530	-0.2759050
C	3.2821440	1.0127640	1.1111720
C	-0.5277390	2.7998280	2.0282520
C	-3.0912020	2.0527200	0.7620830
C	-1.8789570	0.3471440	2.7383150
H	0.9538720	1.5752520	3.0490150
H	1.5423370	3.2100630	2.6350770
C	3.0512640	4.0413900	0.0919230
C	1.1836330	3.5294510	-1.3748210
C	3.7420700	0.8591520	2.4338930
C	4.1175180	0.6020070	0.0491110
H	-0.5464910	3.6422130	1.3153940
H	-1.0202760	3.1268870	2.9592050
C	-4.0762070	1.1455240	0.3139790
C	-3.3935640	3.4287010	0.7725880
C	-2.8860660	0.7401980	3.6422080
C	-1.1399710	-0.8215000	2.9997810
C	3.2885500	5.2222740	-0.6222500
H	3.7023540	3.7746410	0.9314410
C	1.4215250	4.7144200	-2.0875970
H	0.3734030	2.8538200	-1.6711650
C	5.0111340	0.3187980	2.6886300
H	3.1166720	1.1613290	3.2789120
C	5.3862470	0.0692430	0.3064580
H	3.7752040	0.7050720	-0.9857580
C	-5.3351790	1.6032180	-0.0918210
H	-3.8591150	0.0727020	0.2864660
C	-4.6538910	3.8853350	0.3581120
H	-2.6525900	4.1581520	1.1123430
C	-3.1430150	-0.0208340	4.7892470
H	-3.4817570	1.6370510	3.4418670
C	-1.3938090	-1.5787340	4.1531790
H	-0.3670210	-1.1356820	2.2902920
C	2.4723570	5.5616600	-1.7123900
H	4.1159910	5.8780710	-0.3311330
H	0.7892890	4.9722630	-2.9438760
C	5.8379790	-0.0737950	1.6277380
H	5.3545570	0.2099160	3.7228330
H	6.0235270	-0.2344040	-0.5304600
C	-5.6293330	2.9752730	-0.0702050
H	-6.0891370	0.8830590	-0.4259580
H	-4.8742630	4.9580390	0.3797140
C	-2.3953010	-1.1799550	5.0480700
H	-3.9315300	0.2899390	5.4829720
H	-0.8106550	-2.4843840	4.3471900
H	2.6611560	6.4837190	-2.2721060
H	6.8305190	-0.4901460	1.8284460
H	-6.6149850	3.3323810	-0.3861010
H	-2.5983070	-1.7742000	5.9451720
C	0.7354090	-0.6343900	-1.6445470
C	1.0399220	-0.0351440	-2.9082440
C	2.7108540	-2.0887120	-2.0538690
C	2.1001330	-0.4326970	-3.7152590
C	2.9559980	-1.4833410	-3.3155500
H	2.2772400	0.0707290	-4.6705870
H	-0.7091130	-2.6403500	-0.2120350
H	3.4019890	-2.8690660	-1.7275490
H	0.3937340	0.7690040	-3.2602260
C	1.6548980	-1.6723140	-1.2497840
O	1.4519020	-2.2081530	0.0256390
C	2.4357200	-3.1113440	0.4997600
C	2.0732450	-3.5262000	1.9191780
H	2.4842070	-4.0323330	-0.1109230
H	3.4361700	-2.6420900	0.5260230
F	0.8675570	-4.1619110	1.9848280
F	3.0174660	-4.3979610	2.3818730
F	2.0224910	-2.4797610	2.7832530
C	-2.5732680	-2.7611750	-1.2778990
O	-2.9659360	-4.0064460	-0.8573700
C	-2.0959230	-4.7087230	0.0310560
H	-1.1130330	-4.9001280	-0.4347530
H	-2.5960700	-5.6647980	0.2343770

H	-1.9530020	-4.1583770	0.9772420
C	-1.9492470	-0.1677810	-2.2057170
O	-1.6480070	1.1326590	-2.5675070
C	-2.5664970	1.8184750	-3.4232130
H	-3.5533610	1.9302360	-2.9412050
H	-2.1316170	2.8126520	-3.5919010
H	-2.6797570	1.3004960	-4.3925460
C	-3.4351420	-2.0893320	-2.1669780
Cl	-4.9231210	-2.8521750	-2.7026370
C	4.0423770	-1.9139570	-4.1234850
C	4.9790380	-2.2813240	-4.8151290
H	5.7924560	-2.6080250	-5.4331780

90

F Reactant

Ni	0.0387340	0.3966220	-0.1952090
P	1.7691580	1.4720280	0.6732000
P	-1.1533110	1.1168940	1.5350030
C	1.3402310	1.9215420	2.4463560
C	1.9961590	3.1489920	-0.0869550
C	3.4903570	0.8127480	0.7395750
C	-1.4910300	-0.4159680	-1.0309420
C	1.0482640	-0.2901110	-1.6889140
C	-0.1214990	2.3918380	2.4599510
C	-1.4163940	-0.1674050	2.8463300
C	-2.8238400	1.8807570	1.3629120
H	2.0210560	2.6940070	2.8411580
H	1.4529250	1.0141810	3.0640170
C	3.1211790	3.9460090	0.2033530
C	0.9887400	3.6557330	-0.9297920
C	4.1862370	0.6419820	-0.4762210
C	4.1170770	0.4394070	1.9440600
C	-2.2818290	0.3440670	-1.9179590
C	-1.8875380	-1.7422620	-0.7827270
C	1.1087430	0.3842350	-2.9229910
C	1.7924160	-1.4858850	-1.5941950
H	-0.4962260	2.5370060	3.4864100
H	-0.2063850	3.3515290	1.9228430
C	-2.3648880	0.0044650	3.8739490
C	-0.6004500	-1.3139730	2.8451250
C	-3.8887420	1.0585010	0.9367790
C	-3.0725120	3.2442970	1.6127570
C	3.2325530	5.2330890	-0.3369130
H	3.9200850	3.5544660	0.8419870
C	1.1035300	4.9469840	-1.4667460
H	0.1208350	3.0301740	-1.1689280
C	5.4840000	0.1170520	-0.4803120
H	3.7107570	0.9197750	-1.4216420
C	5.4164780	-0.0878440	1.9346840
H	3.6006280	0.5539530	2.9013470
C	-3.4245200	-0.2015560	-2.5248780
O	-1.8687340	1.6566830	-2.1413140
C	-3.0375060	-2.3155870	-1.3676340
H	-1.2806150	-2.3557620	-0.1121290
C	1.8788390	-0.0703460	-4.0108570
H	0.5224450	1.2981200	-3.0533260
C	2.5658020	-1.9819510	-2.6593450
O	1.7227640	-2.1555940	-0.3655320
C	-2.4879430	-0.9546320	4.8869630
H	-3.0180650	0.8830130	3.8756680
C	-0.7223090	-2.2697680	3.8645290
H	0.1238750	-1.4589370	2.0364110
C	-5.1735180	1.5909460	0.7770420
H	-3.7124620	-0.0008010	0.7292140
C	-4.3611700	3.7734370	1.4498930
H	-2.2684610	3.9081990	1.9425620
C	2.2230480	5.7358300	-1.1719460
H	4.1125140	5.8441940	-0.1100890
H	0.3184670	5.3345160	-2.1243450
C	6.1031840	-0.2485230	0.7242280
H	6.0119330	-0.0074420	-1.4311620
H	5.8916100	-0.3719820	2.8793540
C	-3.7974300	-1.5209390	-2.2436730
H	-4.0470400	0.3720740	-3.2148430
C	-2.6556120	2.4446260	-3.0326230
O	-3.4744760	-3.5992070	-1.1438500
C	2.5910210	-1.2505500	-3.8482700
H	1.9137980	0.4708540	-4.9604880
H	3.1474060	-2.9049570	-2.6070630
C	2.4901130	-3.3380650	-0.2502530
C	-1.6659440	-2.0916360	4.8845740
H	-3.2315430	-0.8159950	5.6788680

H	-0.0842290	-3.1582660	3.8526040	C	3.2980080	3.8270540	0.2465530
C	-5.4143990	2.9483210	1.0343890	C	1.2451620	3.5765990	-1.0279150
H	-5.9882680	0.9391890	0.4463470	C	4.0430770	0.3359810	2.1344680
H	-4.5399250	4.8341060	1.6554830	C	4.2242830	0.4282320	-0.2838510
H	2.3137130	6.7411470	-1.5963550	H	-0.1777910	3.4091590	1.7974450
H	7.1187700	-0.6576560	0.7187560	H	-0.5547140	2.6646800	3.3751370
Cl	-5.2435440	-2.1840040	-3.0032150	C	-3.9133090	1.3007950	0.7086440
H	-3.6901000	2.5665950	-2.6629830	C	-3.0123630	3.4624250	1.3432250
H	-2.1713640	3.4301940	-3.0756980	C	-2.5649240	0.3496300	3.8340320
H	-2.6789650	2.0089260	-4.0486220	C	-0.9906430	-1.2186260	2.8547580
C	-2.7056210	-4.4106240	-0.2569920	C	3.5074940	5.0819440	-0.3393540
C	2.2741760	-3.9278370	1.1363320	H	4.0293200	3.4323660	0.9600070
H	2.1829980	-4.1062260	-0.9852150	C	1.4547360	4.8355670	-1.6103170
H	3.5727750	-3.1436140	-0.3681600	H	0.3705120	2.9742570	-1.3011780
H	-1.7661490	-2.8416330	5.6760950	C	5.3069180	-0.2689860	2.2027750
H	-6.4209050	3.3614010	0.9112000	H	3.4961390	0.5250630	3.0628290
H	-1.6807230	-4.5687720	-0.6371390	C	5.4886250	-0.1682920	-0.2121710
H	-3.2305540	-5.3743350	-0.2130140	H	3.8076240	0.6932840	-1.2613160
H	-2.6557900	-3.9719600	0.7557600	C	-5.1509700	1.8960230	0.4382010
F	0.9739490	-4.2712400	1.3619540	H	-3.7907250	0.2232640	0.5581980
F	3.0216340	-5.0654540	1.2605820	C	-4.2515970	4.0575670	1.0633230
F	2.6455630	-3.0854630	2.1373220	H	-2.1944520	4.0935690	1.7026600
F	3.3530760	-1.7347190	-4.8840470	C	-2.8145920	-0.5537140	4.8746620
				H	-3.0978960	1.3060610	3.8076030
90				C	-1.2372950	-2.1199270	3.9009710
F Transition State				H	-0.2871680	-1.4767430	2.0565430
C	-1.5045660	-1.9636720	-1.0856490	C	2.5852080	5.5891380	-1.2676560
C	-3.3074130	-0.3447210	-2.4585860	H	4.3958230	5.6652060	-0.0741590
C	-1.0857120	-0.6401080	-1.4179680	H	0.7372410	5.2253330	-2.3402300
H	-4.0491410	0.2732520	-2.9675670	C	6.0355950	-0.5188390	1.0322850
Ni	0.0496810	0.4040170	-0.1847360	H	5.7242530	-0.5401620	3.1783430
P	1.7960470	1.4176400	0.6918050	H	6.0492370	-0.3589780	-1.1333660
P	-1.2171260	1.2072900	1.4462320	C	-5.3256850	3.2772720	0.6154260
C	1.2908160	1.9409410	2.4289270	H	-5.9821970	1.2758110	0.0871580
C	2.1626760	3.0640530	-0.0908970	H	-4.3778610	5.1360640	1.2073210
C	3.4879300	0.6988870	0.8909210	C	-2.1495670	-1.7890960	4.9112750
C	-0.1536150	2.4646350	2.3675860	H	-3.5338800	-0.2942340	5.6588490
C	-2.8283170	2.0751220	1.1764670	H	-0.7186670	-3.0836020	3.9218540
C	-1.6464890	0.0254480	2.8148260	H	2.7526370	6.5691060	-1.7268290
H	1.3419070	1.0489270	3.0771850	H	7.0246580	-0.9850450	1.0880580
H	1.9770820	2.7015210	2.8387170	H	-6.2945590	3.7418680	0.4050030

H	-2.3481500	-2.4944320	5.7250390	C	1.0286620	3.3561190	-1.1952340
C	0.6144600	-0.5017530	-1.8514320	C	2.6074940	2.2556680	0.9773210
C	0.8566790	0.2378290	-3.0483370	C	-1.2915730	-1.1028490	-0.7808350
C	2.5185510	-1.9453460	-2.5541520	C	1.2604120	-0.5265650	-0.8975860
C	1.8542700	-0.0830160	-3.9749400	C	-1.5809870	3.2396370	0.9614240
C	2.6598860	-1.1854170	-3.7190030	C	-2.4583060	0.8747440	2.3748990
H	1.9993390	0.5109730	-4.8813650	C	-3.6816100	1.4913070	-0.1755450
H	-0.7973880	-2.6005950	-0.5564870	H	0.2513890	4.3192800	1.5111260
H	3.2140760	-2.7700030	-2.3867340	H	-0.0553940	2.8360690	2.4611430
H	0.2121870	1.0905070	-3.2595130	C	1.8758840	4.4816100	-1.2105310
C	1.5243770	-1.5961510	-1.6352430	C	0.2048830	3.0934460	-2.3068970
O	1.3935460	-2.2727410	-0.4238450	C	3.6614930	1.7732720	0.1719310
C	2.3976590	-3.2240080	-0.1101860	C	2.8918280	2.6901770	2.2863590
C	2.1049730	-3.8024360	1.2681530	C	-1.8632220	-1.0949980	-2.0705570
H	2.4086560	-4.0687740	-0.8239320	C	-1.5366150	-2.2238610	0.0320550
H	3.3988800	-2.7568090	-0.0824140	C	1.6134780	-0.4685360	-2.2603410
F	0.9006200	-4.4411350	1.3175930	C	2.1147460	-1.2855260	-0.0637150
F	3.0666010	-4.7221020	1.5759360	H	-2.2734820	3.7077850	1.6801630
F	2.1039680	-2.8647620	2.2492600	H	-1.6646860	3.7771310	0.0016460
C	-2.7608020	-2.4839970	-1.4264990	C	-3.6714450	1.2373520	2.9938710
O	-3.1914570	-3.7501670	-1.1181120	C	-1.5133530	0.1223360	3.0965560
C	-2.2925970	-4.5980310	-0.4034430	C	-4.3930690	0.2813720	-0.3240710
H	-1.3711450	-4.7891860	-0.9818080	C	-4.2378250	2.6785730	-0.6898830
H	-2.8342770	-5.5421210	-0.2583940	C	1.8918240	5.3361030	-2.3199390
H	-2.0273300	-4.1702680	0.5790620	H	2.5352730	4.6829700	-0.3597890
C	-2.0586070	0.1668660	-2.1005570	C	0.2210880	3.9556890	-3.4133770
O	-1.7077760	1.4853900	-2.3397340	H	-0.4398180	2.2057350	-2.3032910
C	-2.6561540	2.3173240	-3.0130190	C	4.9710290	1.7400940	0.6658680
H	-3.5847060	2.4214280	-2.4255050	H	3.4587690	1.4237590	-0.8449950
H	-2.1760160	3.3004880	-3.1074980	C	4.2049390	2.6528940	2.7772970
H	-2.8928030	1.9281600	-4.0198620	H	2.0951460	3.0618950	2.9370120
C	-3.6587440	-1.6620690	-2.1344470	C	-2.6522370	-2.1646360	-2.5227940
Cl	-5.2395970	-2.2698140	-2.6007500	O	-1.6067950	0.0302780	-2.8523870
F	3.6410910	-1.5415110	-4.6074210	C	-2.3343510	-3.3094700	-0.3900680
				H	-1.0917390	-2.2569340	1.0295880
93				C	2.7543900	-1.1020780	-2.7771480
CF3 Reactant				H	0.9710570	0.0886140	-2.9480630
Ni	-0.2593360	0.4153430	-0.2020550	C	3.2553490	-1.9366040	-0.5512740
P	0.9007330	2.2426630	0.2808550	O	1.7563470	-1.3360300	1.2884690
P	-2.0371710	1.4383660	0.6606340	C	-3.9280880	0.8592360	4.3173670
C	-0.1284070	3.2854850	1.4560200	H	-4.4236920	1.8052370	2.4366380

C	-1.7719240	-0.2507390	4.4239180	F	0.8913170	-2.5195550	3.7105460
H	-0.5775390	-0.1760710	2.6122530	F	2.9730150	-2.5770520	4.4150930
C	-5.6391810	0.2686650	-0.9619630	F	1.9939310	-0.6502120	4.0155570
H	-3.9714660	-0.6530320	0.0583430	C	4.7751480	-2.5754030	-2.4403140
C	-5.4855070	2.6598690	-1.3301560	F	4.4986070	-3.8919460	-2.7294150
H	-3.7101800	3.6315610	-0.5923480	F	5.2731140	-2.0298700	-3.5906350
C	1.0630400	5.0754700	-3.4218140	F	5.8102470	-2.6040640	-1.5361380
H	2.5570990	6.2058660	-2.3269040				
H	-0.4206680	3.7472050	-4.2756760	93			
C	5.2468440	2.1807370	1.9686130	**CF3 Transition State**			
H	5.7781290	1.3656230	0.0283320	C	-1.0720930	-2.3747820	-0.4668390
H	4.4108720	2.9963800	3.7963210	C	-2.5710060	-1.7654900	-2.7342820
C	-2.8863230	-3.2589710	-1.6823980	C	-0.7721090	-1.1609920	-1.1539320
H	-3.1004760	-2.1760950	-3.5183850	H	-3.1998170	-1.5437990	-3.5983420
C	-2.1814880	0.0636450	-4.1578890	Ni	-0.2709000	0.4642620	-0.1397830
O	-2.6175210	-4.4181970	0.3697450	P	0.9362140	2.1087190	0.6719270
C	3.5795350	-1.8349220	-1.9172100	P	-2.0872240	1.3623780	0.7740330
H	2.9967310	-1.0232260	-3.8405410	C	-0.1401480	2.9839450	1.9456510
H	3.9135550	-2.5171210	0.0987630	C	1.2332520	3.4736910	-0.5535560
C	2.6473980	-2.0196120	2.1500260	C	2.5839220	1.9242790	1.4826010
C	-2.9777330	0.1170810	5.0348220	C	-1.5698120	3.0698110	1.3860890
H	-4.8757120	1.1407290	4.7884510	C	-3.6740030	1.6589330	-0.1287760
H	-1.0310830	-0.8367260	4.9754460	C	-2.6752900	0.5724940	2.3488270
C	-6.1894020	1.4562790	-1.4655230	H	-0.1310190	2.3774200	2.8681360
H	-6.1791230	-0.6774120	-1.0681740	H	0.2548170	3.9845160	2.1897470
H	-5.9078410	3.5923990	-1.7189880	C	2.1566230	4.5129960	-0.3263920
H	1.0799370	5.7432770	-4.2893770	C	0.4658510	3.4816970	-1.7344400
H	6.2719090	2.1548580	2.3523620	C	2.8218890	2.2113150	2.8414150
Cl	-3.8904380	-4.5856270	-2.2627920	C	3.6413760	1.4087360	0.7008610
H	-3.2855070	0.0311960	-4.1173030	H	-1.5872710	3.7554650	0.5213010
H	-1.8664240	1.0171970	-4.6039870	H	-2.2762580	3.4538450	2.1407800
H	-1.8129130	-0.7677640	-4.7865490	C	-4.3767890	0.5255490	-0.5934620
C	-2.0387820	-4.4912620	1.6723000	C	-4.1886530	2.9383510	-0.4178820
C	2.1137520	-1.9306220	3.5728220	C	-3.9427660	0.8366780	2.9055240
H	2.7321590	-3.0931810	1.8959800	C	-1.7955680	-0.2918680	3.0275140
H	3.6576190	-1.5695060	2.1414220	C	2.3027050	5.5453620	-1.2621390
H	-3.1815220	-0.1798510	6.0688540	H	2.7730200	4.5094820	0.5787770
H	-7.1649760	1.4428670	-1.9624100	C	0.6086080	4.5206790	-2.6656400
H	-0.9352410	-4.4912280	1.6259530	H	-0.2357860	2.6593000	-1.9192520
H	-2.3860140	-5.4442720	2.0933020	C	4.0888650	1.9964520	3.4037020
H	-2.3777810	-3.6599500	2.3162210	H	2.0225230	2.6089490	3.4734620

C	4.9068740	1.2029920	1.2634590
H	3.4756930	1.1701530	-0.3549640
C	-5.5688650	0.6700670	-1.3123180
H	-3.9912990	-0.4780820	-0.3870900
C	-5.3789300	3.0806060	-1.1470300
H	-3.6731100	3.8377850	-0.0692790
C	-4.3176960	0.2492060	4.1206170
H	-4.6454840	1.4932670	2.3822240
C	-2.1687630	-0.8702790	4.2493780
H	-0.8172840	-0.5132610	2.5882040
C	1.5272960	5.5525500	-2.4314160
H	3.0271600	6.3462110	-1.0797100
H	0.0080720	4.5195370	-3.5814840
C	5.1347970	1.4956950	2.6170540
H	4.2578250	2.2283500	4.4605970
H	5.7172490	0.8114960	0.6400910
C	-6.0741450	1.9490320	-1.5929790
H	-6.1045280	-0.2216300	-1.6539560
H	-5.7673410	4.0828880	-1.3572700
C	-3.4307950	-0.6025940	4.7961500
H	-5.3077410	0.4559390	4.5408860
H	-1.4737690	-1.5373410	4.7687310
H	1.6453830	6.3595150	-3.1621260
H	6.1245480	1.3331590	3.0559770
H	-7.0065550	2.0619770	-2.1556610
H	-3.7266430	-1.0610640	5.7455160
C	0.9220180	-0.7126490	-1.1604140
C	1.4201310	-0.3051300	-2.4410640
C	3.1308780	-1.8194960	-0.8506560
C	2.6817630	-0.6448670	-2.9223650
C	3.5484000	-1.4211240	-2.1389030
H	2.9959760	-0.2974410	-3.9102990
H	-0.4805170	-2.6158740	0.4152750
H	3.8342590	-2.3756460	-0.2281410
H	0.7669370	0.2935020	-3.0747320
C	1.8744330	-1.4609150	-0.3725500
O	1.4798930	-1.7590520	0.9334990
C	2.4530560	-2.3630510	1.7704460
C	1.8500750	-2.5612160	3.1546060
H	2.7611250	-3.3583860	1.3993750
H	3.3480650	-1.7233680	1.8762930
F	0.7605880	-3.3818950	3.1353340
F	2.7823100	-3.1409890	3.9657340
F	1.4658620	-1.3962290	3.7384380
C	-2.0659010	-3.2710310	-0.8826170
O	-2.3831930	-4.4408870	-0.2430290
C	-1.6564390	-4.7634580	0.9438410
H	-0.5803830	-4.8958230	0.7344640
H	-2.0789310	-5.7139240	1.2952000
H	-1.7885660	-3.9904330	1.7203340
C	-1.5903770	-0.8704680	-2.2975910
O	-1.3942400	0.3541270	-2.9065830
C	-2.1584960	0.6497110	-4.0795900
H	-3.2374550	0.6980350	-3.8519830
H	-1.8148920	1.6363310	-4.4175870
H	-1.9763920	-0.0930540	-4.8765340
C	-2.8050120	-2.9594350	-2.0413330
Cl	-4.0498180	-4.0545690	-2.6151420
C	4.8780900	-1.8664280	-2.6534430
F	5.3558160	-1.0630230	-3.6506750
F	5.8415290	-1.8935460	-1.6690760
F	4.8541670	-3.1446470	-3.1734070

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CN Reactant

Ni	-0.0002350	0.4068650	-0.1721830
P	1.6130940	1.6577570	0.6926960
P	-1.3463250	1.2376600	1.3941580
C	1.0240980	2.2969800	2.3584280
C	1.8128680	3.2339180	-0.2611610
C	3.3494110	1.0998410	0.9628820
C	-1.4331150	-0.5462350	-1.0388330
C	1.1350320	-0.3798470	-1.4990870
C	-0.4548160	2.6807920	2.2092460
C	-1.5867710	0.0960590	2.8332490
C	-3.0526630	1.8508530	1.0564950
H	1.6356480	3.1500530	2.6964620
H	1.1305160	1.4819250	3.0947560
C	2.8993720	4.1045740	-0.0445550
C	0.8099110	3.5936640	-1.1821220
C	4.1479110	0.8284660	-0.1688910
C	3.8926720	0.8993150	2.2464360

C	-2.1767780	0.1055180	-2.0447200	H	-3.8385110	-0.0455810	-3.4642230
C	-1.8040310	-1.8607050	-0.7038050	C	-2.5297530	2.0882100	-3.3649520
C	1.2942620	0.2001090	-2.7750870	O	-3.3035380	-3.7976710	-1.0122960
C	1.8862410	-1.5538710	-1.2469700	C	2.8974010	-1.4846560	-3.4581040
H	-0.9121060	2.9304160	3.1807530	H	2.2620660	0.1612850	-4.7213390
H	-0.5487170	3.5591690	1.5482320	H	3.3324800	-3.0135850	-2.0022580
C	-2.5406310	0.3626110	3.8360800	C	2.4951100	-3.2700780	0.3035320
C	-0.7549670	-1.0320910	2.9525710	C	-1.8132140	-1.6044680	5.0624030
C	-4.0286600	0.9144870	0.6540340	H	-3.3983280	-0.2743810	5.7174460
C	-3.4116440	3.2081770	1.1669250	H	-0.2167060	-2.7528770	4.1495270
C	2.9760760	5.3208210	-0.7346950	C	-5.6881650	2.6832910	0.4979130
H	3.6948150	3.8260280	0.6546000	H	-6.0819780	0.5923740	0.0683820
C	0.8892530	4.8155610	-1.8667110	H	-4.9896570	4.6781850	0.9859380
H	-0.0253530	2.9069230	-1.3655900	H	2.0338060	6.6288470	-2.1857060
C	5.4650180	0.3800380	-0.0139910	H	7.0319440	-0.1595770	1.3866560
H	3.7403750	0.9696320	-1.1746210	Cl	-4.9662340	-2.6155490	-3.1143150
C	5.2119480	0.4477640	2.3963900	H	-3.5935190	2.1991170	-3.0868600
H	3.2956120	1.0941540	3.1418700	H	-2.0763880	3.0850020	-3.4559820
C	-3.2524010	-0.5331270	-2.6823170	H	-2.4573550	1.5681850	-4.3377640
O	-1.7898680	1.4095400	-2.3508930	C	-2.5821580	-4.5020570	-0.0024190
C	-2.8888620	-2.5242150	-1.3171950	C	2.1962880	-3.7231050	1.7258280
H	-1.2303290	-2.3908310	0.0604490	H	2.2533450	-4.1127140	-0.3714070
C	2.1592810	-0.3214130	-3.7450130	H	3.5792770	-3.0608290	0.2400540
H	0.7134200	1.0926770	-3.0237160	H	-1.9040030	-2.2673570	5.9291520
C	2.7518430	-2.1090020	-2.1962820	H	-6.7124310	3.0059620	0.2845220
O	1.7162960	-2.1222650	0.0198740	H	-1.5267790	-4.6551170	-0.2897510
C	-2.6515170	-0.4852130	4.9448050	H	-3.0802620	-5.4766620	0.0869220
H	-3.2073150	1.2263970	3.7435830	H	-2.6243930	-3.9767100	0.9684980
C	-0.8661290	-1.8768510	4.0669810	F	0.8873940	-4.0631580	1.9026890
H	-0.0253650	-1.2490930	2.1649380	F	2.9455000	-4.8286950	2.0101440
C	-5.3366020	1.3308790	0.3795300	F	2.4943300	-2.7767450	2.6557520
H	-3.7655310	-0.1428470	0.5545120	C	3.7961270	-2.0392040	-4.4206910
C	-4.7232880	3.6203870	0.8897240	N	4.5395220	-2.4920330	-5.2043480
H	-2.6770670	3.9571900	1.4757510				
C	1.9699360	5.6790510	-1.6447660	91			
H	3.8265750	5.9893230	-0.5651130	**CN Transition State**			
H	0.1079470	5.0901740	-2.5829500	C	-1.3846180	-2.1144330	-0.9260330
C	6.0012300	0.1899700	1.2682470	C	-3.1263540	-0.7554930	-2.6240260
H	6.0736740	0.1776530	-0.9010140	C	-1.0065920	-0.8100450	-1.3591890
H	5.6217450	0.3002490	3.4009000	H	-3.8452440	-0.2405000	-3.2633830
C	-3.6042750	-1.8363860	-2.3133820	Ni	-0.0194150	0.4251140	-0.1768170

P	1.6047330	1.6302830	0.6877260	H	6.0291560	-0.2140010	-0.5724830
P	-1.4400030	1.3384460	1.2664760	C	-5.6287010	2.9717680	-0.0053310
C	0.9401890	2.3390450	2.2989810	H	-6.0966230	0.8821950	-0.3654450
C	1.9959820	3.1824680	-0.2560290	H	-4.8661060	4.9508880	0.4471770
C	3.2851260	0.9857640	1.1005140	C	-2.3641350	-1.2211810	5.0647230
C	-0.5141490	2.7762540	2.0584230	H	-3.8920640	0.2502510	5.5226650
C	-3.0865540	2.0404070	0.8028850	H	-0.7893430	-2.5254610	4.3420000
C	-1.8628450	0.3198340	2.7612620	H	2.6634310	6.4956600	-2.2240450
H	0.9707650	1.5402440	3.0600490	H	6.8300110	-0.5420300	1.7785890
H	1.5600060	3.1777870	2.6583110	H	-6.6160550	3.3323510	-0.3116120
C	3.0646580	4.0251450	0.1084200	H	-2.5611470	-1.8206840	5.9595830
C	1.1748470	3.5430850	-1.3405830	C	0.7352360	-0.6077510	-1.6491240
C	3.7418410	0.7919240	2.4189590	C	1.0399480	0.0088010	-2.9075910
C	4.1219200	0.6060350	0.0281680	C	2.7058880	-2.0661480	-2.0789400
H	-0.5358840	3.6232880	1.3512010	C	2.0943080	-0.3815740	-3.7231880
H	-1.0006510	3.0978970	2.9943030	C	2.9420800	-1.4402670	-3.3314540
C	-4.0768810	1.1372160	0.3590110	H	2.2728920	0.1333240	-4.6717490
C	-3.3854760	3.4168950	0.8218070	H	-0.7018500	-2.6471090	-0.2657280
C	-2.8612170	0.7099190	3.6761780	H	3.3982830	-2.8495850	-1.7637160
C	-1.1251930	-0.8527860	3.0083800	H	0.3971670	0.8212130	-3.2457660
C	3.3015030	5.2120340	-0.5957680	C	1.6535530	-1.6568480	-1.2690970
H	3.7242660	3.7445100	0.9366210	O	1.4514350	-2.2049780	-0.0007700
C	1.4124850	4.7342040	-2.0430420	C	2.4323360	-3.1192210	0.4617070
H	0.3558800	2.8769410	-1.6343810	C	2.0635390	-3.5558730	1.8731170
C	5.0098940	0.2427780	2.6594840	H	2.4791980	-4.0299030	-0.1640670
H	3.1155930	1.0696560	3.2716510	H	3.4334300	-2.6523710	0.4981900
C	5.3896330	0.0640360	0.2715420	F	0.8548620	-4.1872140	1.9227870
H	3.7830360	0.7429420	-1.0039130	F	3.0023010	-4.4374310	2.3246780
C	-5.3380440	1.5991290	-0.0349780	F	2.0127740	-2.5222820	2.7526960
H	-3.8624680	0.0639630	0.3271150	C	-2.5709560	-2.7447920	-1.3253160
C	-4.6481070	3.8779270	0.4191430	O	-2.9655380	-3.9955330	-0.9277230
H	-2.6405430	4.1433500	1.1591600	C	-2.0955730	-4.7175790	-0.0542540
C	-3.1105520	-0.0581500	4.8201190	H	-1.1153890	-4.9050520	-0.5270440
H	-3.4559440	1.6098400	3.4872380	H	-2.5993990	-5.6747260	0.1334220
C	-1.3715290	-1.6170090	4.1587700	H	-1.9480320	-4.1841660	0.9007380
H	-0.3584870	-1.1644730	2.2911520	C	-1.9458920	-0.1339260	-2.2069000
C	2.4743530	5.5692670	-1.6717940	O	-1.6433690	1.1706480	-2.5465990
H	4.1375200	5.8583030	-0.3082220	C	-2.5665360	1.8767240	-3.3823710
H	0.7717080	5.0063890	-2.8884020	H	-3.5487600	1.9814070	-2.8899390
C	5.8381740	-0.1191890	1.5888270	H	-2.1292890	2.8724330	-3.5340240
H	5.3515180	0.1032190	3.6905100	H	-2.6879540	1.3784660	-4.3607090

C	-3.4353390	-2.0525960	-2.1972820	H	2.6953530	1.8352880	3.2793910
Cl	-4.9263960	-2.8013580	-2.7383110	C	-2.9882390	-1.2696470	-2.7334950
C	4.0322570	-1.8597000	-4.1431540	O	-1.7673250	0.8543370	-2.6078270
N	4.9374400	-2.2046900	-4.8052120	C	-2.5722130	-2.9653010	-1.0271610
				H	-1.0906060	-2.4261580	0.4492330
92				C	2.4587940	-0.6784850	-3.3293110
NO2 Reactant				H	0.8184560	0.6710380	-3.0180870
Ni	-0.1204270	0.4222120	-0.1517650	C	3.0502810	-2.0820070	-1.4164440
P	1.2724550	1.9651480	0.6157210	O	1.7823940	-1.8205120	0.6551250
P	-1.7014260	1.3659340	1.0960140	C	-3.3345280	0.1163420	4.7062590
C	0.4556570	2.7876570	2.0942070	H	-3.8460270	1.5530530	3.1717500
C	1.4426180	3.3888810	-0.5587560	C	-1.3479840	-1.2202380	4.3030510
C	3.0084020	1.6218090	1.1325780	H	-0.3020020	-0.8246960	2.4406360
C	-1.3602770	-0.8133970	-0.9577870	C	-5.5401730	0.9207640	-0.3276480
C	1.2083210	-0.4504270	-1.2102010	H	-3.8990450	-0.3524470	0.2689840
C	-1.0240830	2.9980890	1.7434410	C	-5.1567310	3.3098320	-0.1759530
C	-2.0381550	0.4524110	2.6723080	H	-3.2232540	3.9273210	0.5465400
C	-3.3942610	1.7545080	0.4756690	C	1.5732170	5.5929110	-2.3026490
H	0.9549590	3.7371900	2.3493180	H	3.2185660	6.2755250	-1.0631390
H	0.5459210	2.1076530	2.9585250	H	-0.0738760	4.6599730	-3.3560170
C	2.4019520	4.4007560	-0.3553440	C	5.6688660	0.9966280	1.8298250
C	0.5522140	3.4869050	-1.6452040	H	6.0014110	0.7679980	-0.3027260
C	3.9564090	1.3110880	0.1343170	H	5.0286130	1.2909180	3.8811350
C	3.4085690	1.6065630	2.4825600	C	-3.2449080	-2.5302560	-2.1830920
C	-2.0542330	-0.4192570	-2.1207440	H	-3.5306110	-0.9816230	-3.6363450
C	-1.6306250	-2.0924530	-0.4400630	C	-2.4538760	1.2723510	-3.7875600
C	1.4490410	-0.0929100	-2.5556600	O	-2.8840580	-4.2158030	-0.5536320
C	2.0367850	-1.4698570	-0.6737020	C	3.2510470	-1.6691800	-2.7436260
H	-1.6041090	3.3503110	2.6123290	H	2.6358110	-0.3847760	-4.3659910
H	-1.1149730	3.7497930	0.9410340	H	3.7031460	-2.8632840	-1.0250670
C	-3.1360110	0.7831570	3.4913450	C	2.6615340	-2.7732890	1.2280810
C	-1.1478570	-0.5567600	3.0832110	C	-2.4404490	-0.8855110	5.1136810
C	-4.2467260	0.6781100	0.1497320	H	-4.1935840	0.3747770	5.3342110
C	-3.8602730	3.0722170	0.3034260	H	-0.6522090	-2.0052540	4.6129670
C	2.4663380	5.4964180	-1.2247410	C	-5.9995340	2.2358100	-0.4902290
H	3.1104550	4.3252120	0.4762600	H	-6.1892810	0.0751810	-0.5755800
C	0.6180530	4.5894940	-2.5104220	H	-5.5077430	4.3399210	-0.2977090
H	-0.1847930	2.6930500	-1.8149760	H	1.6274710	6.4487130	-2.9833970
C	5.2770050	1.0045260	0.4829890	H	6.7020640	0.7560840	2.1002180
H	3.6627410	1.3115950	-0.9196840	Cl	-4.4284630	-3.5791650	-2.9584340
C	4.7319540	1.2963550	2.8272740	H	-3.5478490	1.2985020	-3.6340200

H	-2.0975500	2.2894660	-4.0018800	C	-4.2724710	0.8588670	-0.0613070
H	-2.2189590	0.6182720	-4.6472400	C	-3.7684690	3.2256240	0.1251640
C	-2.1677700	-4.6866690	0.5879040	C	-3.3670090	0.8748490	3.3716430
C	2.2330970	-3.0280200	2.6663440	C	-1.4944210	-0.6292290	3.0040200
H	2.6270720	-3.7434120	0.6979140	C	2.7338470	5.4765750	-0.8705990
H	3.7061930	-2.4109730	1.2424150	H	3.2066000	4.2191880	0.8253650
H	-2.5999960	-1.4092060	6.0619260	C	0.9672420	4.6836330	-2.3340620
H	-7.0126810	2.4226070	-0.8608670	H	0.0584480	2.7882060	-1.7757420
H	-1.0829590	-4.7435200	0.3889090	C	4.6381220	1.1106150	3.0540750
H	-2.5567750	-5.6951930	0.7813200	H	2.6414190	1.8339180	3.4271430
H	-2.3450830	-4.0486930	1.4722930	C	5.2020160	0.6423110	0.7424610
F	0.9768720	-3.5533310	2.7507250	H	3.6419500	0.9881220	-0.7113540
F	3.0884600	-3.9261590	3.2360550	C	-5.5056840	1.1676270	-0.6470320
F	2.2494230	-1.9044070	3.4329360	H	-3.9949110	-0.1894760	0.0898950
N	4.3278510	-2.3019870	-3.5196150	C	-5.0026980	3.5319490	-0.4675180
O	5.0141820	-3.1786040	-2.9597920	H	-3.1090770	4.0455710	0.4238250
O	4.5011710	-1.9273060	-4.6924290	C	-3.6837330	0.1893960	4.5507430
				H	-3.9869700	1.7184850	3.0500090
92				C	-1.8102390	-1.3114470	4.1883330
NO2 Transition State				H	-0.6474850	-0.9512940	2.3896730
C	-1.2081660	-2.2673580	-0.6723360	C	1.9330000	5.6455840	-2.0105130
C	-2.8731960	-1.3144710	-2.6947920	H	3.4960110	6.2219890	-0.6203330
C	-0.9173810	-0.9902470	-1.2285830	H	0.3488080	4.8078050	-3.2291400
H	-3.5607120	-0.9628660	-3.4659840	C	5.5677260	0.6834810	2.0966970
Ni	-0.1345740	0.4577580	-0.1502460	H	4.9146440	1.1437250	4.1130930
P	1.2847400	1.9035900	0.7070700	H	5.9202370	0.3067770	-0.0124020
P	-1.7614050	1.3826520	1.0539730	C	-5.8756460	2.5058420	-0.8516370
C	0.4187770	2.6866870	2.1818660	H	-6.1804440	0.3581160	-0.9435330
C	1.5946920	3.3817120	-0.3705970	H	-5.2838250	4.5793790	-0.6200300
C	2.9752430	1.4700040	1.3048680	C	-2.9045900	-0.9034450	4.9615980
C	-1.0389040	2.9635610	1.7780330	H	-4.5439410	0.5065090	5.1497520
C	-3.3911950	1.8857790	0.3411030	H	-1.2025450	-2.1657730	4.5018640
C	-2.2661000	0.4712910	2.5896980	H	2.0694130	6.5238450	-2.6499110
H	0.4505830	1.9634480	3.0151350	H	6.5741370	0.3809860	2.4034260
H	0.9292190	3.6086450	2.5074310	H	-6.8414600	2.7466250	-1.3075200
C	2.5669510	4.3513690	-0.0537400	H	-3.1558890	-1.4389940	5.8829780
C	0.8004040	3.5534940	-1.5201190	C	0.8678240	-0.6455840	-1.3809350
C	3.3494670	1.5019380	2.6624120	C	1.2333510	-0.1874910	-2.6907860
C	3.9148820	1.0273890	0.3483110	C	2.9460830	-2.0101170	-1.4462680
H	-1.0636300	3.7397880	0.9940040	C	2.3725470	-0.6112690	-3.3624860
H	-1.6365190	3.3219570	2.6326970	C	3.2258520	-1.5384050	-2.7449720

H	2.6192860	-0.2338660	-4.3569760	C	0.4688310	2.6406000	-2.2822360
H	-0.5530160	-2.6404120	0.1141570	C	1.6896150	0.0686690	-2.8010750
H	3.6733120	-2.6860800	-0.9949140	C	3.0480520	1.9086020	-1.0242230
H	0.5722170	0.5238690	-3.1851660	H	-1.6182250	3.0507860	-2.8321570
C	1.8081190	-1.5686740	-0.7871120	H	-1.0686990	1.3836360	-3.1707050
O	1.5296410	-1.9475740	0.5270660	C	-2.9564660	4.0618570	-0.1759010
C	2.5155050	-2.7341800	1.1789980	C	-0.9177980	3.6120250	1.0745360
C	2.0507650	-3.0105520	2.6022840	C	-4.1501920	0.7598150	0.0401850
H	2.6622060	-3.7105740	0.6813820	C	-3.8425490	0.7736650	-2.3701370
H	3.4843810	-2.2050600	1.2293900	C	2.1368090	0.1605740	2.0665880
F	0.8660390	-3.6895650	2.6386760	C	1.8269340	-1.8183150	0.7276290
F	2.9812560	-3.7819110	3.2340870	C	-1.3597330	0.2287560	2.7121130
F	1.8858490	-1.8801040	3.3369820	C	-1.8667430	-1.5729180	1.1992420
C	-2.2786120	-3.0649700	-1.0995450	H	0.9443710	2.8736180	-3.2491170
O	-2.5925950	-4.2960190	-0.5884330	H	0.5271010	3.5388460	-1.6440510
C	-1.7365700	-4.8306970	0.4235510	C	2.6987960	0.3075720	-3.7554040
H	-0.7052060	-4.9580340	0.0503530	C	0.8597230	-1.0591020	-2.9400470
H	-2.1588990	-5.8127350	0.6731240	C	4.0354850	1.0062310	-0.5747540
H	-1.7273040	-4.1933220	1.3244750	C	3.3727890	3.2738010	-1.1430900
C	-1.8049290	-0.5266690	-2.2525560	C	-3.0846090	5.2937260	0.4775380
O	-1.5760620	0.7438190	-2.7406380	H	-3.7124880	3.7530260	-0.9055100
C	-2.4587000	1.2437390	-3.7510430	C	-1.0490980	4.8491540	1.7232520
H	-3.4921150	1.3218200	-3.3716620	H	-0.0812610	2.9446060	1.3147580
H	-2.0867750	2.2461560	-4.0004460	C	-5.4559740	0.2855500	-0.1323230
H	-2.4367620	0.6114730	-4.6562700	H	-3.7678370	0.9326480	1.0508910
C	-3.1061150	-2.5736350	-2.1302650	C	-5.1502440	0.2952180	-2.5374250
Cl	-4.4571780	-3.5327090	-2.7035990	H	-3.2289270	0.9563280	-3.2568490
N	4.4310660	-1.9908990	-3.4110550	C	3.2102390	-0.4565150	2.7289840
O	4.6779070	-1.5462850	-4.5533510	O	1.7233160	1.4595290	2.3549750
O	5.1702840	-2.8041220	-2.8068970	C	2.9109860	-2.4593810	1.3653120
				H	1.2781990	-2.3622740	-0.0450820
92				C	-2.2327520	-0.2993480	3.6666750
CHO Reactant				H	-0.8100680	1.1437730	2.9506170
Ni	-0.0022110	0.4118810	0.1405420	C	-2.7329930	-2.1302400	2.1457910
P	-1.6132370	1.6155760	-0.7861310	O	-1.6565530	-2.1536290	-0.0595170
P	1.3708290	1.2419730	-1.4035100	C	2.8649350	-0.5656880	-4.8374070
C	-0.9975320	2.2207630	-2.4554330	H	3.3648760	1.1694750	-3.6443310
C	-1.8699030	3.2137510	0.1162080	C	1.0260960	-1.9287520	-4.0279230
C	-3.3316490	1.0163520	-1.0806930	H	0.0889370	-1.2574400	-2.1872160
C	1.4254880	-0.5095370	1.0492740	C	5.3211560	1.4634150	-0.2624480
C	-1.1518440	-0.3761630	1.4498010	H	3.7987490	-0.0566490	-0.4684330

C	4.6621730	3.7269530	-0.8280400
H	2.6286920	3.9973950	-1.4878300
C	-2.1300940	5.6895830	1.4267490
H	-3.9352670	5.9445280	0.2497840
H	-0.3085100	5.1532770	2.4701240
C	-5.9603780	0.0534780	-1.4205710
H	-6.0811100	0.0969450	0.7462660
H	-5.5348190	0.1148130	-3.5465470
C	3.5929940	-1.7547870	2.3730660
H	3.7712960	0.0449030	3.5203170
C	2.4103340	2.1463550	3.4003280
O	3.3545370	-3.7265250	1.0735980
C	-2.9274720	-1.4905830	3.3905150
H	-2.3840780	0.1902800	4.6340240
H	-3.2836430	-3.0590390	1.9591840
C	-2.4062370	-3.3199710	-0.3390080
C	2.0273250	-1.6828890	-4.9763810
H	3.6543830	-0.3758980	-5.5722110
H	0.3775110	-2.8038190	-4.1258960
C	5.6388760	2.8233870	-0.3894910
H	6.0756000	0.7507260	0.0849940
H	4.9019090	4.7904460	-0.9312440
H	-2.2345320	6.6509840	1.9401980
H	-6.9825600	-0.3158520	-1.5526160
Cl	4.9521060	-2.5062990	3.2052550
H	3.4813960	2.2818030	3.1639570
H	1.9332600	3.1330010	3.4798050
H	2.3115920	1.6179740	4.3662110
C	2.6683590	-4.4450300	0.0492210
C	-2.0781180	-3.7877310	-1.7498680
H	-2.1581910	-4.1490070	0.3508500
H	-3.4956920	-3.1329020	-0.2939410
H	2.1610450	-2.3652400	-5.8222250
H	6.6458400	3.1780010	-0.1464520
H	1.6105420	-4.6194210	0.3146760
H	3.1877750	-5.4094100	-0.0297110
H	2.7195170	-3.9187920	-0.9207850
F	-0.7614540	-4.1086960	-1.9029070
F	-2.8044100	-4.9105950	-2.0296910
F	-2.3778750	-2.8606560	-2.6986140
C	-3.8566120	-2.0928290	4.3621640
O	-4.1422140	-1.6366710	5.4648680
H	-4.3255170	-3.0574400	4.0181250

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CHO Transition State

C	-1.4121570	-2.0863760	-0.9269490
C	-3.0740270	-0.7034700	-2.6861320
C	-1.0078610	-0.7835760	-1.3381680
H	-3.7621830	-0.1799620	-3.3519040
Ni	-0.0206130	0.4213940	-0.1331710
P	1.5943310	1.6163580	0.7584900
P	-1.4582410	1.3456960	1.2846390
C	0.9114840	2.3254170	2.3617690
C	2.0043860	3.1654530	-0.1809290
C	3.2641110	0.9586260	1.1906140
C	-0.5364450	2.7725050	2.1007720
C	-3.0861690	2.0626670	0.7820230
C	-1.9247260	0.3246060	2.7642300
H	0.9263860	1.5246630	3.1213100
H	1.5309340	3.1596630	2.7320790
C	3.0700900	4.0047510	0.1994340
C	1.2017280	3.5264090	-1.2789570
C	3.7048000	0.7674060	2.5148190
C	4.1090500	0.5690950	0.1283320
H	-0.5418520	3.6243460	1.3991280
H	-1.0359570	3.0910830	3.0308410
C	-4.0694300	1.1698100	0.3033810
C	-3.3775370	3.4405220	0.8082760
C	-2.9523780	0.7103250	3.6478170
C	-1.1906360	-0.8455800	3.0325900
C	3.3222490	5.1894730	-0.5030250
H	3.7156830	3.7227470	1.0381730
C	1.4549460	4.7153520	-1.9795310
H	0.3859940	2.8620700	-1.5854370
C	4.9663450	0.2109680	2.7717160
H	3.0709010	1.0529150	3.3592530
C	5.3703740	0.0202270	0.3887240
H	3.7822010	0.7027620	-0.9080190
C	-5.3169990	1.6432960	-0.1189400
H	-3.8601140	0.0957290	0.2660260
C	-4.6264500	3.9131430	0.3774240

H	-2.6375910	4.1590480	1.1725620	C	-2.1815210	-4.6853420	-0.0944190
C	-3.2349580	-0.0605870	4.7821410	H	-1.1841710	-4.8797560	-0.5266750
H	-3.5432650	1.6090390	3.4417760	H	-2.7007820	-5.6386900	0.0691110
C	-1.4701970	-1.6122540	4.1736630	H	-2.0691750	-4.1560030	0.8676220
H	-0.4008850	-1.1535510	2.3390860	C	-1.9064800	-0.0936560	-2.2166990
C	2.5136030	5.5473370	-1.5928120	O	-1.5821890	1.2116740	-2.5306840
H	4.1560840	5.8331880	-0.2036710	C	-2.4416860	1.9173380	-3.4320890
H	0.8298050	4.9875840	-2.8364320	H	-3.4532560	2.0369590	-3.0070100
C	5.8035990	-0.1604600	1.7113740	H	-1.9858370	2.9073750	-3.5647510
H	5.2958300	0.0733680	3.8069400	H	-2.5032470	1.4093790	-4.4108800
H	6.0176990	-0.2644650	-0.4471040	C	-3.4096370	-1.9998220	-2.2787090
C	-5.6003550	3.0172590	-0.0826080	Cl	-4.8837710	-2.7337470	-2.8828870
H	-6.0705030	0.9344340	-0.4772160	C	4.0891340	-1.9621670	-4.0536590
H	-4.8389540	4.9870420	0.4107250	O	4.4480090	-1.4927910	-5.1349310
C	-2.4926020	-1.2214680	5.0482070	H	4.6489150	-2.8336840	-3.6108340
H	-4.0392150	0.2440240	5.4602370				
H	-0.8910050	-2.5190800	4.3735570	95			
H	2.7152420	6.4715610	-2.1442290	**COCH3 Reactant**			
H	6.7907510	-0.5885320	1.9137080	Ni	-0.1285310	0.4298700	-0.1640760
H	-6.5769950	3.3869610	-0.4115670	P	1.2321110	1.9924280	0.6164500
H	-2.7158370	-1.8232780	5.9353400	P	-1.7424360	1.3673240	1.0446010
C	0.7641940	-0.6070050	-1.5833180	C	0.3849250	2.8051580	2.0844520
C	1.1015470	0.0108560	-2.8366060	C	1.3942820	3.4210760	-0.5542930
C	2.6918820	-2.1148650	-1.9985200	C	2.9688420	1.6895830	1.1575350
C	2.1557740	-0.4049540	-3.6344480	C	-1.3342500	-0.8397770	-0.9653080
C	2.9667250	-1.4911270	-3.2410220	C	1.2360710	-0.4393160	-1.1885400
H	2.3771240	0.1020950	-4.5790120	C	-1.0911860	3.0023600	1.7115180
H	-0.7575470	-2.6278810	-0.2452070	C	-2.1126980	0.4489560	2.6111420
H	3.3577320	-2.9254190	-1.6827830	C	-3.4211940	1.7495830	0.3819280
H	0.4835850	0.8430780	-3.1737790	H	0.8700670	3.7594520	2.3492060
C	1.6438300	-1.6845230	-1.1952140	H	0.4692080	2.1237250	2.9484020
O	1.4039060	-2.2323970	0.0709250	C	2.3302040	4.4513870	-0.3355220
C	2.3579510	-3.1674750	0.5431260	C	0.5196200	3.5022710	-1.6546130
C	1.9658270	-3.5980110	1.9498940	C	3.9265730	1.3521990	0.1772220
H	2.3930060	-4.0792520	-0.0823440	C	3.3643990	1.7481060	2.5076690
H	3.3692430	-2.7235820	0.5907880	C	-1.9990020	-0.4997040	-2.1621330
F	0.7458150	-4.2081640	1.9869600	C	-1.6175180	-2.0951000	-0.3984640
F	2.8838290	-4.4968250	2.4120680	C	1.5124740	-0.0736530	-2.5249860
F	1.9241530	-2.5644020	2.8304390	C	2.0528700	-1.4557510	-0.6402820
C	-2.5870230	-2.7042480	-1.3759330	H	-1.6885950	3.3456640	2.5722040
O	-3.0083660	-3.9533390	-1.0007510	H	-1.1756660	3.7566610	0.9108670

C	-3.2458490	0.7496750	3.3925050	C	2.6452980	-2.7421180	1.2881280
C	-1.2099100	-0.5360200	3.0528240	C	-2.5593590	-0.8982980	5.0400320
C	-4.2561990	0.6704490	0.0209720	H	-4.3534740	0.3124330	5.1991500
C	-3.8903960	3.0655510	0.2042670	H	-0.7251800	-1.9688520	4.6006610
C	2.3863110	5.5490120	-1.2030320	C	-5.9980050	2.2221170	-0.6631020
H	3.0271710	4.3889160	0.5069610	H	-6.1707200	0.0609180	-0.7699210
C	0.5767150	4.6066690	-2.5180920	H	-5.5256980	4.3277150	-0.4400760
H	-0.1975290	2.6931200	-1.8364320	H	1.5560500	6.4861460	-2.9739470
C	5.2528070	1.0946780	0.5441700	H	6.6786630	0.9610050	2.1750120
H	3.6363210	1.2936190	-0.8761920	Cl	-4.3446960	-3.7025030	-2.9208300
C	4.6932330	1.4851580	2.8706010	H	-3.4449480	1.1421460	-3.8100480
H	2.6432640	2.0003710	3.2901210	H	-1.9790430	2.1115490	-4.1753620
C	-2.9129390	-1.3810790	-2.7618360	H	-2.0799740	0.4082810	-4.7340650
O	-1.7053570	0.7529850	-2.6953830	C	-2.2186250	-4.6150740	0.7647360
C	-2.5424970	-2.9959820	-0.9691980	C	2.2102670	-2.9704110	2.7289680
H	-1.1024870	-2.3854740	0.5202860	H	2.6192560	-3.7255080	0.7806010
C	2.5445390	-0.6564880	-3.2665920	H	3.6898630	-2.3775930	1.3051920
H	0.8921920	0.6921740	-2.9995540	H	-2.7361360	-1.4254550	5.9833530
C	3.0799030	-2.0671910	-1.3697990	H	-6.9999920	2.4053900	-1.0646520
O	1.7702620	-1.8070870	0.6897820	H	-1.1249580	-4.6912900	0.6310820
C	-3.4667040	0.0778440	4.6009910	H	-2.6262480	-5.6054380	1.0079820
H	-3.9653800	1.4997520	3.0482500	H	-2.4375400	-3.9138340	1.5900040
C	-1.4316710	-1.2034780	4.2666620	F	0.9580380	-3.5038820	2.8191750
H	-0.3376220	-0.7822050	2.4371730	F	3.0697080	-3.8526980	3.3213210
C	-5.5353930	0.9088290	-0.4954490	F	2.2159780	-1.8329820	3.4739700
H	-3.9057300	-0.3588350	0.1426510	C	4.4346320	-2.2764570	-3.5171940
C	-5.1724530	3.2988380	-0.3143090	O	4.6831550	-1.8762990	-4.6568220
H	-3.2669220	3.9228710	0.4731540	C	5.2496530	-3.4221060	-2.9185570
C	1.5081590	5.6288260	-2.2945600	H	5.7725300	-3.1106900	-1.9976300
H	3.1205340	6.3426770	-1.0295050	H	4.6062540	-4.2794020	-2.6556080
H	-0.1031110	4.6635760	-3.3744550	H	5.9949020	-3.7491050	-3.6558530
C	5.6404570	1.1611970	1.8906630				
H	5.9857620	0.8416370	-0.2285130	95			
H	4.9864180	1.5373750	3.9242360	**COCH3 Transition State**			
C	-3.1827450	-2.6164080	-2.1619240	C	-1.1472810	-2.3021170	-0.6473380
H	-3.4317840	-1.1359470	-3.6908280	C	-2.8032580	-1.4205450	-2.7069150
C	-2.3457300	1.1075870	-3.9202180	C	-0.8631830	-1.0345880	-1.2318360
O	-2.8682540	-4.2232810	-0.4439650	H	-3.4890210	-1.0954500	-3.4913140
C	3.3442810	-1.6656620	-2.7003040	Ni	-0.1475960	0.4446450	-0.1441170
H	2.7459990	-0.3493220	-4.2972540	P	1.2196850	1.9425960	0.7010860
H	3.6927360	-2.8550090	-0.9253460	P	-1.8170630	1.3489510	1.0118760

C	0.3154310	2.7311560	2.1507620	H	-6.1690100	0.2061630	-1.0665540
C	1.4870100	3.4093210	-0.4061060	H	-5.3877600	4.4505070	-0.7426390
C	2.9207510	1.5897990	1.3245820	C	-2.9737190	-0.8752540	4.9556460
C	-1.1442120	2.9590630	1.7242370	H	-4.7447810	0.3783880	4.9907870
C	-3.4454950	1.8098950	0.2667250	H	-1.1374430	-1.9863670	4.6439030
C	-2.3314480	0.4576860	2.5581980	H	1.8636010	6.5125350	-2.7564430
H	0.3573330	2.0253630	2.9985910	H	6.5537670	0.6818060	2.4781700
H	0.7952230	3.6737190	2.4637860	H	-6.8843120	2.5758970	-1.4534790
C	2.4182700	4.4229440	-0.1043190	H	-3.2267840	-1.3953700	5.8853960
C	0.6985520	3.5227730	-1.5667320	C	0.8914760	-0.6577020	-1.3645670
C	3.2856240	1.6812940	2.6821470	C	1.2775850	-0.1813090	-2.6620440
C	3.8821230	1.1492720	0.3884390	C	3.0060120	-1.9660270	-1.4072550
H	-1.1792630	3.7218380	0.9274920	C	2.4421530	-0.5760770	-3.3044850
H	-1.7631940	3.3135920	2.5652210	C	3.3289810	-1.4975970	-2.7070630
C	-4.2924270	0.7596740	-0.1494350	H	2.6939900	-0.1819690	-4.2935840
C	-3.8535200	3.1387560	0.0380670	H	-0.4947660	-2.6475320	0.1536240
C	-3.5065220	0.7860190	3.2636190	H	3.7056010	-2.6381700	-0.9054420
C	-1.4865640	-0.5477330	3.0639570	H	0.6091920	0.5149450	-3.1682770
C	2.5502590	5.5341060	-0.9466400	C	1.8497900	-1.5481640	-0.7576930
H	3.0537600	4.3366830	0.7836140	O	1.5628270	-1.9294680	0.5594560
C	0.8298950	4.6389750	-2.4060520	C	2.5618270	-2.6673910	1.2393910
H	-0.0099920	2.7226450	-1.8106050	C	2.0942390	-2.9221900	2.6661390
C	4.5853690	1.3521080	3.0940280	H	2.7431880	-3.6541020	0.7727270
H	2.5607360	2.0133940	3.4309720	H	3.5150160	-2.1091860	1.2871600
C	5.1810820	0.8307620	0.8024630	F	0.9328710	-3.6371590	2.7138430
H	3.6167670	1.0605940	-0.6703990	F	3.0458930	-3.6487030	3.3233110
C	-5.5216650	1.0341670	-0.7599420	F	1.8912190	-1.7797270	3.3719170
H	-3.9905850	-0.2801630	0.0123260	C	-2.2039760	-3.1227320	-1.0643050
C	-5.0830880	3.4111030	-0.5803010	O	-2.5092990	-4.3442580	-0.5217630
H	-3.2222210	3.9766450	0.3473440	C	-1.6825420	-4.8194060	0.5415590
C	-3.8255920	0.1206780	4.4539830	H	-0.6375970	-4.9532680	0.2101720
H	-4.1812870	1.5551470	2.8737510	H	-2.1030260	-5.7931540	0.8251670
C	-1.8035450	-1.2072040	4.2604850	H	-1.7090390	-4.1383890	1.4097360
H	-0.5801850	-0.8152310	2.5112400	C	-1.7527550	-0.6063250	-2.2711100
C	1.7547120	5.6449900	-2.0973180	O	-1.5454000	0.6601680	-2.7802820
H	3.2807980	6.3142160	-0.7076210	C	-2.4270170	1.1230420	-3.8076820
H	0.2162220	4.7178290	-3.3095450	H	-3.4653120	1.1902440	-3.4390510
C	5.5374880	0.9313040	2.1561960	H	-2.0709530	2.1267850	-4.0747900
H	4.8537190	1.4313320	4.1527800	H	-2.3857900	0.4730930	-4.6997420
H	5.9186340	0.5055410	0.0614770	C	-3.0253480	-2.6700330	-2.1163790
C	-5.9219770	2.3616600	-0.9773250	Cl	-4.3574550	-3.6619090	-2.6829130

C	4.5519440	-1.9173430	-3.4311460
O	4.8397430	-1.4488450	-4.5400370
C	5.4678990	-2.9600510	-2.7871950
H	5.8635030	-2.6151470	-1.8154820
H	4.9359260	-3.9099920	-2.6048460
H	6.3125850	-3.1512450	-3.4625200

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SCH3 Reactant

Ni	0.1491180	-0.4089310	-0.2202230
P	-1.1667900	-2.1496850	0.1461180
P	1.7747560	-1.5511410	0.7736330
C	-0.3077610	-3.2786470	1.3807690
C	-1.2722970	-3.2452550	-1.3462010
C	-2.9178800	-2.0409280	0.7133780
C	1.3240060	1.0388870	-0.6937020
C	-1.2362110	0.6384080	-1.0445070
C	1.1811790	-3.3217900	1.0078760
C	2.0886960	-1.0247750	2.5218940
C	3.4759190	-1.6995880	0.0741870
H	-0.7568060	-4.2857300	1.3810210
H	-0.4347670	-2.8448210	2.3874160
C	-2.1826160	-4.3181400	-1.4180260
C	-0.3743620	-3.0265410	-2.4083990
C	-3.8681070	-1.4768420	-0.1646330
C	-3.3312820	-2.4559070	1.9938600
C	2.0567030	0.9552340	-1.8964390
C	1.5098070	2.1834900	0.1016170
C	-1.4671580	0.6113740	-2.4340110
C	-2.1032680	1.4556140	-0.2857210
H	1.7807490	-3.8434570	1.7717020
H	1.3072890	-3.8531550	0.0494260
C	3.2155770	-1.4716470	3.2408360
C	1.1443240	-0.2005870	3.1610690
C	4.2884960	-0.5460480	0.0529630
C	3.9787110	-2.8984020	-0.4671300
C	-2.1875480	-5.1649570	-2.5333360
H	-2.8991210	-4.4835800	-0.6064710
C	-0.3808340	-3.8801740	-3.5217900
H	0.3199430	-2.1788020	-2.3616420
C	-5.2045720	-1.3454580	0.2309250
H	-3.5614360	-1.1363340	-1.1582280
C	-4.6704900	-2.3186490	2.3866510
H	-2.6156460	-2.8901860	2.6977860
C	2.9404490	1.9749570	-2.2838760
O	1.8566210	-0.1945800	-2.6588150
C	2.4005420	3.2193240	-0.2537120
H	0.9333100	2.2793180	1.0249550
C	-2.5083540	1.3303230	-3.0452600
H	-0.8114590	0.0071080	-3.0684920
C	-3.1398060	2.1995400	-0.8717830
O	-1.8687630	1.4750270	1.0985560
C	3.3871820	-1.1041920	4.5810280
H	3.9689650	-2.0952940	2.7484750
C	1.3179870	0.1633170	4.5046410
H	0.2767660	0.1607930	2.5986160
C	5.5776500	-0.5985950	-0.4905210
H	3.9119280	0.3956310	0.4629200
C	5.2705160	-2.9462430	-1.0108560
H	3.3731150	-3.8089040	-0.4678520
C	-1.2851370	-4.9483300	-3.5858210
H	-2.9016880	-5.9935950	-2.5840550
H	0.3167900	-3.7039930	-4.3471590
C	-5.6098470	-1.7663700	1.5063630
H	-5.9307460	-0.9079870	-0.4615240
H	-4.9774560	-2.6471880	3.3850120
C	3.1096530	3.0946110	-1.4613260
H	3.5116120	1.9276920	-3.2133910
C	2.6031540	-0.3138400	-3.8684460
O	2.6289080	4.3495430	0.4945280
H	-2.6687700	1.2653820	-4.1264150
H	-3.8094640	2.8326150	-0.2837800
C	-2.8048510	2.1910740	1.8803820
C	2.4380540	-0.2875860	5.2148060
H	4.2681390	-1.4515540	5.1310450
H	0.5790430	0.8068300	4.9907760
C	6.0730450	-1.7978460	-1.0224830
H	6.1946700	0.3053800	-0.4998040
H	5.6497230	-3.8878860	-1.4217110
H	-1.2935970	-5.6092750	-4.4588080
H	-6.6557210	-1.6622990	1.8132060
Cl	4.2321720	4.3605030	-1.9575530

H	3.6913330	-0.3104330	-3.6759380	C	3.1402290	2.2261490	2.4508120
H	2.3194490	-1.2809850	-4.3063270	C	3.8290310	1.2674620	0.3295890
H	2.3539570	0.4927050	-4.5826830	H	-1.2909330	3.8234730	0.1706200
C	1.9032950	4.4893300	1.7151270	H	-1.9034020	3.7324310	1.8459710
C	-2.4293790	2.0458710	3.3481050	C	-4.3239520	0.6136180	-0.3152620
H	-2.8054660	3.2729940	1.6473720	C	-3.9933170	3.0075600	-0.5312590
H	-3.8321050	1.8007260	1.7543410	C	-3.5124680	1.4085510	3.0749750
H	2.5767160	0.0017530	6.2617390	C	-1.5482260	-0.0204010	3.0677360
H	7.0826500	-1.8368970	-1.4444470	C	2.6368130	5.2930810	-1.8578250
H	0.8136260	4.5254860	1.5376170	H	3.0850390	4.3870160	0.0546150
H	2.2346490	5.4443190	2.1445880	C	0.8881900	4.2314300	-3.1624660
H	2.1309450	3.6702530	2.4207720	H	-0.0260150	2.4748340	-2.2651800
F	-1.1979700	2.5639970	3.6273150	C	4.4191440	1.9823530	2.9728220
F	-3.3362680	2.7254040	4.1123950	H	2.3889600	2.6965140	3.0920560
F	-2.4255130	0.7542810	3.7723290	C	5.1068080	1.0325870	0.8512510
C	-3.3453470	2.1381270	-2.2642140	H	3.6073230	0.9778780	-0.7028470
S	-4.6997410	3.0653820	-3.0053190	C	-5.5672890	0.7276540	-0.9479120
C	-3.8221850	4.6021110	-3.5136070	H	-3.9745680	-0.3721590	0.0085270
H	-3.4038510	5.1266790	-2.6424360	C	-5.2364730	3.1178890	-1.1726090
H	-3.0219420	4.3784830	-4.2335430	H	-3.3990490	3.9120220	-0.3718570
H	-4.5714620	5.2474150	-3.9971640	C	-3.8164650	0.9819960	4.3736260
				H	-4.1732960	2.1207440	2.5694430
94				C	-1.8506530	-0.4418120	4.3712280
SCH3 Transition State				H	-0.6694800	-0.4155730	2.5475470
C	-1.1008280	-2.4003930	-0.2493050	C	1.8503070	5.2397410	-3.0185570
C	-2.7491390	-1.8893960	-2.4367890	H	3.3954790	6.0749000	-1.7448090
C	-0.8197960	-1.2435580	-1.0349000	H	0.2791030	4.1811230	-4.0712990
H	-3.4318110	-1.7007850	-3.2670660	C	5.4067420	1.3888400	2.1754550
Ni	-0.1722660	0.4358420	-0.2226730	H	4.6431050	2.2637500	4.0072780
P	1.1588170	2.0867010	0.3648670	H	5.8703160	0.5678590	0.2187640
P	-1.8787020	1.4946000	0.7168860	C	-6.0292340	1.9810950	-1.3780630
C	0.1936750	3.1298810	1.5995330	H	-6.1764380	-0.1684020	-1.1053670
C	1.4904240	3.3299370	-0.9772850	H	-5.5887500	4.1009110	-1.5033520
C	2.8300860	1.8759910	1.1215670	C	-2.9843770	0.0581200	5.0248470
C	-1.2582560	3.2336830	1.1033160	H	-4.7077940	1.3691730	4.8788500
C	-3.5241070	1.7550960	-0.0874500	H	-1.2008120	-1.1656980	4.8726930
C	-2.3717990	0.9128570	2.4118220	H	1.9936850	5.9801120	-3.8125490
H	0.2211450	2.6085710	2.5722670	H	6.4057810	1.2031510	2.5830640
H	0.6469590	4.1270450	1.7306950	H	-7.0026830	2.0701170	-1.8713370
C	2.4584750	4.3448010	-0.8425140	H	-3.2245480	-0.2748920	6.0400260
C	0.7117260	3.2771350	-2.1494940	C	0.8999060	-0.8812120	-1.2134560

C	1.3071860	-0.6228840	-2.5594750	P	-2.1352200	1.2871660	0.6925210
C	3.0887280	-2.0324160	-0.9548490	C	-0.3403820	3.2280700	1.5243070
C	2.5229250	-1.0523670	-3.0926570	C	0.7394490	3.4697330	-1.1482550
H	2.7788540	-0.8150740	-4.1302050	C	2.4514880	2.4225540	0.9453210
H	-0.4512690	-2.6061120	0.6004570	C	-1.2346900	-1.1709410	-0.7999090
H	3.8253960	-2.5477200	-0.3338680	C	1.2602720	-0.4163490	-0.9524720
H	0.6212680	-0.0708150	-3.2021480	C	-1.7968700	3.1022590	1.0544970
C	1.8786060	-1.5847980	-0.4248770	C	-2.4933730	0.6359260	2.3894360
O	1.5675720	-1.7491480	0.9288270	C	-3.7892310	1.2582250	-0.1255440
C	2.6001950	-2.2537430	1.7590920	H	-0.0299130	4.2824930	1.6121810
C	2.0971680	-2.2926430	3.1956460	H	-0.2162220	2.7476800	2.5099670
H	2.8890760	-3.2860670	1.4862160	C	1.4811900	4.6673930	-1.1320860
H	3.4954180	-1.6061610	1.7249410	C	-0.0673760	3.1692950	-2.2625570
F	1.0017570	-3.0938560	3.3421020	C	3.5174900	2.0543970	0.0967440
F	3.0810830	-2.7993250	3.9964180	C	2.7356550	2.8280290	2.2636180
F	1.7661730	-1.0679820	3.6791950	C	-1.8517860	-1.1801440	-2.0685440
C	-2.1476000	-3.2886990	-0.5329020	C	-1.3588500	-2.3264360	-0.0082470
O	-2.4459090	-4.4065060	0.2049450	C	1.5728850	-0.3308270	-2.3262100
C	-1.6423550	-4.6721150	1.3551550	C	2.1860540	-1.1177340	-0.1436460
H	-0.5867820	-4.8452180	1.0798640	H	-2.5052140	3.4936210	1.8029990
H	-2.0586860	-5.5867820	1.7975340	H	-1.9354110	3.6701180	0.1189860
H	-1.7000520	-3.8479930	2.0873970	C	-3.7171420	0.8936860	3.0388570
C	-1.7116980	-1.0042680	-2.1341210	C	-1.4879890	-0.0779700	3.0671970
O	-1.5181580	0.1690010	-2.8413490	C	-4.4308110	0.0113590	-0.2864130
C	-2.4279190	0.4660000	-3.9042870	C	-4.4180130	2.4178360	-0.6191350
H	-3.4598650	0.5670340	-3.5256950	C	1.4108270	5.5541920	-2.2136700
H	-2.0971380	1.4271780	-4.3198940	H	2.1265980	4.9018550	-0.2790460
H	-2.3925150	-0.3038050	-4.6962360	C	-0.1373670	4.0630710	-3.3417380
C	-2.9639720	-3.0288380	-1.6510330	H	-0.6309170	2.2283460	-2.2822080
Cl	-4.2799920	-4.1179000	-2.0588740	C	4.8380760	2.1047400	0.5587580
C	3.4238080	-1.7869350	-2.3051080	H	3.3157570	1.7285580	-0.9280990
S	5.0026820	-2.3358330	-2.9561190	C	4.0600890	2.8748500	2.7221120
C	4.5805740	-4.0388390	-3.5221270	H	1.9296230	3.1113210	2.9463600
H	3.8036550	-4.0123680	-4.2995770	C	-2.5704530	-2.2992290	-2.5190140
H	5.5020840	-4.4660140	-3.9466520	O	-1.7161770	-0.0199450	-2.8291490
H	4.2478170	-4.6651270	-2.6817340	C	-2.0846640	-3.4619450	-0.4279820
				H	-0.8724700	-2.3477500	0.9697930
96				C	2.7382730	-0.8845620	-2.8696200
COOCH3 Reactant				H	0.8731240	0.1788600	-2.9948890
Ni	-0.3031860	0.4096680	-0.2170570	C	3.3516980	-1.6918350	-0.6624770
P	0.7324790	2.3013220	0.2908720	O	1.8620010	-1.1970790	1.2193510

C	-3.9261900	0.4479320	4.3495950	H	-1.8698420	-5.6455360	2.0035970
H	-4.5132770	1.4326280	2.5148790	H	-1.9959220	-3.8712760	2.2682190
C	-1.6988380	-0.5179190	4.3823430	F	1.1714720	-2.4628860	3.6633710
H	-0.5425840	-0.2927780	2.5569760	F	3.2688490	-2.3271630	4.3087930
C	-5.6786520	-0.0656120	-0.9163400	F	2.1046840	-0.4993950	3.9427020
H	-3.9536940	-0.9021620	0.0803690	C	4.8587260	-2.1603990	-2.6461430
C	-5.6673470	2.3350810	-1.2510170	O	5.1737460	-2.0823870	-3.8260990
H	-3.9463800	3.3987660	-0.5127410	O	5.6328240	-2.8270980	-1.7233600
C	0.6003890	5.2538030	-3.3191050	C	6.8246850	-3.4354120	-2.2634570
H	1.9951280	6.4801860	-2.1967570	H	7.3153640	-3.9217480	-1.4106220
H	-0.7637690	3.8236000	-4.2072320	H	6.5671200	-4.1765180	-3.0348720
C	5.1134910	2.5158660	1.8712130	H	7.4845270	-2.6746010	-2.7070630
H	5.6543960	1.8185250	-0.1119840				
H	4.2657190	3.1948220	3.7488440	96			
C	-2.6867960	-3.4268770	-1.6980260	**COOCH3 Transition State**			
H	-3.0517940	-2.3248670	-3.4987600	C	-0.9918840	-2.4414850	-0.3032450
C	-2.3436570	-0.0036840	-4.1104260	C	-2.5161470	-2.0899390	-2.6103750
O	-2.2497040	-4.6062850	0.3146390	C	-0.7774330	-1.2580340	-1.0678020
C	3.6385160	-1.5728330	-2.0401760	H	-3.1502810	-1.9697500	-3.4903360
H	2.9597980	-0.7999850	-3.9375490	Ni	-0.3205850	0.4521570	-0.2016700
H	4.0604750	-2.2368910	-0.0367270	P	0.8079570	2.2142300	0.4678820
C	2.8289220	-1.8035590	2.0546940	P	-2.1727930	1.3421540	0.6367890
C	-2.9166880	-0.2561170	5.0235430	C	-0.3279940	3.1719720	1.6247190
H	-4.8820700	0.6474690	4.8452870	C	1.1198690	3.4775820	-0.8586240
H	-0.9114630	-1.0728850	4.9003590	C	2.4362520	2.1472190	1.3375100
C	-6.3011800	1.0945990	-1.3991750	C	-1.7478720	3.1337070	1.0351810
H	-6.1633110	-1.0401450	-1.0319460	C	-3.7874910	1.4299280	-0.2578300
H	-6.1460700	3.2468300	-1.6234710	C	-2.6891860	0.7235440	2.3108800
H	0.5508020	5.9465520	-4.1656250	H	-0.3159720	2.6668730	2.6060710
H	6.1472550	2.5551440	2.2298130	H	0.0223600	4.2077970	1.7681290
Cl	-3.6038340	-4.8167900	-2.2755690	C	1.9288910	4.6093650	-0.6358000
H	-3.4378230	-0.1349870	-4.0276680	C	0.4918050	3.3165830	-2.1079820
H	-2.1316160	0.9851360	-4.5402030	C	2.6092710	2.4889530	2.6931500
H	-1.9296500	-0.7829060	-4.7765290	C	3.5453920	1.6595930	0.6114280
C	-1.6167990	-4.6590080	1.5926380	H	-1.7752270	3.7058860	0.0915850
C	2.3301250	-1.7623070	3.4918140	H	-2.4851730	3.5750040	1.7265360
H	2.9968700	-2.8664170	1.7967180	C	-4.4594790	0.2140050	-0.5090840
H	3.7977470	-1.2711930	2.0178850	C	-4.3480460	2.6267270	-0.7457190
H	-3.0833190	-0.6052940	6.0479000	C	-3.9341670	1.0503430	2.8851640
H	-7.2780980	1.0313350	-1.8895520	C	-1.7762750	-0.0518890	3.0499260
H	-0.5194850	-4.5683400	1.5050980	C	2.0988430	5.5668540	-1.6434660

H	2.4402140	4.7353280	0.3245580	O	1.5417130	-1.5944230	1.0254930
C	0.6608260	4.2792030	-3.1146310	C	2.5548860	-2.0706730	1.8947930
H	-0.1203700	2.4255410	-2.2874040	C	1.9673080	-2.2267220	3.2904790
C	3.8641890	2.3585000	3.3060700	H	2.9360090	-3.0628730	1.5888800
H	1.7683130	2.8632200	3.2839060	H	3.4013890	-1.3619810	1.9532460
C	4.7979590	1.5371900	1.2248360	F	0.9463470	-3.1310070	3.3276620
H	3.4299020	1.3778280	-0.4402800	F	2.9408740	-2.6782810	4.1352050
C	-5.6701860	0.2007800	-1.2111670	F	1.4897460	-1.0620790	3.8028250
H	-4.0363870	-0.7283560	-0.1462500	C	-1.9133560	-3.4338680	-0.6651460
C	-5.5582500	2.6098570	-1.4554690	O	-2.1487280	-4.5818750	0.0464220
H	-3.8521190	3.5856730	-0.5690030	C	-1.3943310	-4.7842430	1.2426470
C	-4.2545420	0.6123500	4.1762810	H	-0.3120610	-4.8421070	1.0318270
H	-4.6621030	1.6395510	2.3175970	H	-1.7399780	-5.7449230	1.6464570
C	-2.0954220	-0.4818700	4.3465590	H	-1.5828860	-3.9843660	1.9795360
H	-0.8138810	-0.3205110	2.6017320	C	-1.6055270	-1.1006050	-2.2282570
C	1.4630490	5.4042440	-2.8839860	O	-1.4902820	0.0945930	-2.9123560
H	2.7345160	6.4402120	-1.4630260	C	-2.2783880	0.2689500	-4.0941320
H	0.1732540	4.1442830	-4.0858970	H	-3.3573100	0.2490720	-3.8621500
C	4.9618580	1.8865870	2.5742660	H	-2.0114580	1.2591660	-4.4864860
H	3.9825270	2.6326130	4.3597120	H	-2.0439420	-0.4993910	-4.8523280
H	5.6488440	1.1663240	0.6442130	C	-2.6643390	-3.2518300	-1.8438180
C	-6.2245840	1.3992510	-1.6863990	Cl	-3.8199930	-4.4718000	-2.3504450
H	-6.1817690	-0.7509520	-1.3874090	C	4.8883680	-1.7836370	-2.6439040
H	-5.9840810	3.5505560	-1.8207000	O	5.2887790	-1.5342370	-3.7759400
C	-3.3346840	-0.1518630	4.9104330	O	5.6725610	-2.4455360	-1.7186320
H	-5.2272490	0.8669510	4.6105150	C	6.9781380	-2.8227070	-2.2004090
H	-1.3751300	-1.0815450	4.9116050	H	7.5578130	-1.9352450	-2.4970080
H	1.6012750	6.1513920	-3.6724500	H	7.4627190	-3.3357280	-1.3595330
H	5.9418040	1.7902490	3.0529700	H	6.8948520	-3.4967540	-3.0663840
H	-7.1723030	1.3882450	-2.2345420				
H	-3.5876260	-0.4936500	5.9195150	91			
C	0.9280860	-0.7228110	-1.1316300	**NO Reactant**			
C	1.3818850	-0.4171970	-2.4568280	Ni	-0.0099310	0.4192260	0.1358090
C	3.1742920	-1.7297030	-0.7761810	P	-1.6335380	1.5876040	-0.8173230
C	2.6433230	-0.7543830	-2.9302100	P	1.3480740	1.2033890	-1.4475050
C	3.5616280	-1.4332540	-2.1059260	C	-1.0358000	2.1238820	-2.5162560
H	2.9411900	-0.4956380	-3.9504830	C	-1.8911980	3.2183560	0.0231750
H	-0.3901430	-2.5796150	0.5940100	C	-3.3487300	0.9614040	-1.0653170
H	3.9083010	-2.2111970	-0.1285930	C	1.4321250	-0.4740520	1.0540850
H	0.6902200	0.0930060	-3.1266940	C	-1.1305160	-0.3409740	1.4747230
C	1.9144160	-1.3785060	-0.3067160	C	0.4294630	2.5591660	-2.3739420

C	1.6698230	-0.0240720	-2.7967350	H	2.5717380	3.9718200	-1.5945010
C	3.0202000	1.8964190	-1.0979530	C	-2.1633120	5.7400430	1.2399600
H	-1.6651210	2.9333020	-2.9222060	H	-3.9594780	5.9499310	0.0404740
H	-1.1086720	1.2566790	-3.1942820	H	-0.3495830	5.2439730	2.3165760
C	-2.9762340	4.0539230	-0.3080640	C	-5.9621830	-0.0634390	-1.3259070
C	-0.9466430	3.6524290	0.9731600	H	-6.0683230	0.1054980	0.8356600
C	-4.1553820	0.7602940	0.0751640	H	-5.5529480	-0.1222760	-3.4551050
C	-3.8640460	0.6345090	-2.3342150	C	3.6255760	-1.6688730	2.3798730
C	2.1555440	0.2300740	2.0394080	H	3.8146890	0.1665060	3.4674580
C	1.8324590	-1.7910060	0.7667930	C	2.4499500	2.2605780	3.2994130
C	-1.3090760	0.2890380	2.7352850	O	3.3739360	-3.6805550	1.1467430
C	-1.8587530	-1.5387760	1.2531360	C	-2.8822950	-1.3941000	3.4475400
H	0.8955540	2.7555250	-3.3534080	H	-2.3092090	0.2901870	4.6751040
H	0.4868480	3.4830520	-1.7734760	H	-3.3004930	-2.9839540	2.0819480
C	2.6865750	0.1722300	-3.7525010	C	-2.4187190	-3.3221200	-0.2288340
C	0.8330230	-1.1507470	-2.8984990	C	2.0108390	-1.8596760	-4.9006660
C	4.0222480	1.0139740	-0.6415450	H	3.6501910	-0.5866560	-5.5348110
C	3.3272460	3.2631430	-1.2436340	H	0.3476670	-2.9366230	-4.0196170
C	-3.1101550	5.3088020	0.2984790	C	5.6049140	2.8529720	-0.5017830
H	-3.7270130	3.7168420	-1.0305380	H	6.0708730	0.7942330	0.0045930
C	-1.0840500	4.9121810	1.5754940	H	4.8398140	4.8010980	-1.0721710
H	-0.1108960	2.9958760	1.2438920	H	-2.2723840	6.7196340	1.7167070
C	-5.4538070	0.2545390	-0.0577340	H	-6.9779390	-0.4591320	-1.4271190
H	-3.7693710	1.0001910	1.0706500	Cl	5.0015500	-2.3885900	3.2110300
C	-5.1645300	0.1253960	-2.4619020	H	3.5140250	2.3908400	3.0312120
H	-3.2589890	0.7724210	-3.2348180	H	1.9706460	3.2476600	3.3563350
C	3.2428700	-0.3619690	2.7019520	H	2.3777170	1.7661090	4.2853540
O	1.7399250	1.5349740	2.2958010	C	2.6678760	-4.4379520	0.1641370
C	2.9297140	-2.4074430	1.4059790	C	-2.0931840	-3.8420990	-1.6214830
H	1.2740400	-2.3610220	0.0203650	H	-2.1676350	-4.1225540	0.4922380
C	-2.1712070	-0.2079500	3.7105630	H	-3.5076760	-3.1338040	-0.1859770
H	-0.7387180	1.1984290	2.9455130	H	2.1462620	-2.5752260	-5.7183150
C	-2.7195660	-2.0663530	2.2168180	H	6.6095970	3.2238090	-0.2741190
O	-1.6681740	-2.1438970	0.0052200	H	1.6172380	-4.6061460	0.4599320
C	2.8545510	-0.7431550	-4.7988870	H	3.1895070	-5.4026670	0.1084410
H	3.3567110	1.0341160	-3.6703190	H	2.6955710	-3.9465560	-0.8248670
C	1.0011250	-2.0624790	-3.9509810	F	-0.7765280	-4.1691420	-1.7640290
H	0.0558900	-1.3158050	-2.1440820	F	-2.8203930	-4.9729340	-1.8589550
C	5.3048770	1.4917270	-0.3483010	F	-2.3924280	-2.9497480	-2.6039820
H	3.7995240	-0.0497810	-0.5164170	N	-3.8041010	-2.0154150	4.3461380
C	4.6136560	3.7369390	-0.9476910	O	-3.9737740	-1.4364110	5.4299660

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C	-1.4566730	-2.0673870	-0.8874770
C	-3.0987510	-0.6886010	-2.6720860
C	-1.0576550	-0.7624130	-1.2902270
H	-3.7773100	-0.1697180	-3.3512740
Ni	-0.0128560	0.4290710	-0.1330540
P	1.6243440	1.6197730	0.7257100
P	-1.4142490	1.3667780	1.3135430
C	0.9812010	2.3249560	2.3453930
C	2.0193040	3.1661950	-0.2218840
C	3.2949590	0.9394190	1.1086220
C	-0.4682400	2.7844430	2.1149810
C	-3.0414350	2.0916240	0.8232040
C	-1.8691410	0.3437620	2.7933880
H	1.0068650	1.5203830	3.1006020
H	1.6140460	3.1533550	2.7056290
C	3.1007170	3.9956990	0.1347040
C	1.1939530	3.5344320	-1.3004440
C	3.7923120	0.7935890	2.4182200
C	4.0833300	0.4963360	0.0241350
H	-0.4813800	3.6384410	1.4161020
H	-0.9475960	3.1027960	3.0554220
C	-4.0335840	1.2036830	0.3543120
C	-3.3249800	3.4707390	0.8551660
C	-2.8815920	0.7377010	3.6909300
C	-1.1436470	-0.8347540	3.0477830
C	3.3453230	5.1795590	-0.5716970
H	3.7646080	3.7066990	0.9565600
C	1.4402390	4.7224560	-2.0049830
H	0.3665070	2.8766160	-1.5891180
C	5.0561260	0.2265900	2.6383340
H	3.2018080	1.1220360	3.2784630
C	5.3466160	-0.0641700	0.2479260
H	3.7117200	0.5937860	-1.0010000
C	-5.2828280	1.6841750	-0.0548380
H	-3.8301690	0.1286130	0.3140910
C	-4.5761200	3.9500220	0.4383080
H	-2.5776060	4.1849120	1.2127100
C	-3.1569580	-0.0337010	4.8265300
H	-3.4664920	1.6425420	3.4949520
C	-1.4167150	-1.6020870	4.1899700
H	-0.3663480	-1.1495050	2.3435610
C	2.5141300	5.5454190	-1.6416110
H	4.1916100	5.8156310	-0.2918350
H	0.7978620	5.0008990	-2.8469470
C	5.8367800	-0.2001720	1.5558030
H	5.4313760	0.1230610	3.6618480
H	5.9473290	-0.3962840	-0.6047620
C	-5.5586680	3.0594580	-0.0133670
H	-6.0436350	0.9798470	-0.4063880
H	-4.7832020	5.0247630	0.4756210
C	-2.4232000	-1.2030790	5.0790350
H	-3.9490890	0.2769180	5.5159840
H	-0.8446490	-2.5155360	4.3792330
H	2.7102950	6.4686900	-2.1964970
H	6.8249080	-0.6383160	1.7295570
H	-6.5368140	3.4344770	-0.3315410
H	-2.6409620	-1.8052770	5.9672080
C	0.7635350	-0.6077440	-1.5591370
C	1.0718420	-0.0208580	-2.8374790
C	2.6347010	-2.1722950	-1.9925380
C	2.0930670	-0.4692490	-3.6548640
C	2.8885710	-1.5636820	-3.2457860
H	2.3136000	0.0093150	-4.6138800
H	-0.8071970	-2.6065670	-0.1984610
H	3.3090910	-2.9854010	-1.7068890
H	0.4613900	0.8211350	-3.1665270
C	1.6146670	-1.7094850	-1.1765110
O	1.3815950	-2.2385030	0.0984350
C	2.3249220	-3.1930690	0.5574820
C	1.9480500	-3.6090480	1.9722380
H	2.3306160	-4.1061460	-0.0663640
H	3.3456730	-2.7702690	0.5842280
F	0.7153410	-4.1926400	2.0328440
F	2.8534590	-4.5236720	2.4251490
F	1.9415100	-2.5694550	2.8481280
C	-2.6217890	-2.6901230	-1.3553760
O	-3.0434450	-3.9408540	-0.9902370
C	-2.2200720	-4.6778680	-0.0837000
H	-1.2186390	-4.8628760	-0.5100720
H	-2.7361020	-5.6350730	0.0661630

H	-2.1187490	-4.1570280	0.8841430	C	1.7688600	5.4540180	-1.9087270
C	-1.9402100	-0.0748960	-2.1833200	H	2.2738550	4.7252260	0.0643480
O	-1.6117850	1.2304770	-2.4908580	C	0.2406410	4.0792250	-3.1988720
C	-2.4570870	1.9352200	-3.4070060	H	-0.4532780	2.2608480	-2.2292410
H	-3.4758650	2.0527870	-2.9990380	C	4.7351340	1.7920440	1.0775070
H	-2.0008530	2.9260280	-3.5316270	H	3.3296670	1.5204680	-0.5420380
H	-2.5008810	1.4274290	-4.3867210	C	3.8100110	2.5629640	3.1823300
C	-3.4338210	-1.9861850	-2.2695550	H	1.6825460	2.9055590	3.2270030
Cl	-4.8944630	-2.7263840	-2.8957100	C	-2.6562460	-2.0685170	-2.7597220
N	3.9768000	-2.1022900	-3.9707620	O	-1.6383200	0.1595070	-2.8982570
O	4.2075330	-1.5681970	-5.0791640	C	-2.4138940	-3.3443520	-0.6930160
				H	-1.2569650	-2.3693480	0.8480880
94				C	2.7276420	-1.0118420	-2.6717940
OCF3 Reactant				H	0.9464900	0.1778480	-2.8715910
Ni	-0.4170180	0.3939690	-0.1759420	C	3.1311200	-1.9333180	-0.4515260
P	0.6828180	2.2106670	0.4604130	O	1.5513980	-1.3996040	1.3400310
P	-2.2577160	1.3485970	0.6251470	C	-4.3277290	0.6012250	4.1524630
C	-0.4366190	3.1874040	1.6117000	H	-4.7348230	1.6233460	2.2910010
C	0.8845960	3.3953270	-0.9518120	C	-2.1703690	-0.4978280	4.3235790
C	2.3424340	2.2259880	1.2639890	H	-0.8845790	-0.3365310	2.5812300
C	-1.3949440	-1.1006210	-0.8912440	C	-5.7594250	0.1895990	-1.2105210
C	1.1558290	-0.4991060	-0.8319360	H	-4.1323020	-0.7443150	-0.1377400
C	-1.8543860	3.1424360	1.0244760	C	-5.6166780	2.5922100	-1.4999020
C	-2.7601920	0.7093870	2.2907300	H	-3.8902700	3.5595080	-0.6479660
C	-3.8572880	1.4086190	-0.2930290	C	1.0419830	5.2227620	-3.0864970
H	-0.0785310	4.2227890	1.7359690	H	2.4033400	6.3420790	-1.8200590
H	-0.4203450	2.6951090	2.5990870	H	-0.3207640	3.8936040	-4.1204920
C	1.6916760	4.5456500	-0.8457480	C	4.9144990	2.1662280	2.4175510
C	0.1622370	3.1640220	-2.1382480	H	5.5917390	1.4760220	0.4741940
C	3.4586450	1.8173660	0.5031270	H	3.9411490	2.8539560	4.2296930
C	2.5299420	2.5928150	2.6105380	C	-2.9081320	-3.2187180	-2.0032700
C	-1.9080760	-1.0190160	-2.2031590	H	-3.0585920	-2.0223710	-3.7738500
C	-1.6561530	-2.2763300	-0.1651350	C	-2.1537960	0.2685920	-4.2242090
C	1.5653310	-0.3947600	-2.1753050	O	-2.7090890	-4.5048830	-0.0192650
C	1.9712320	-1.2880060	0.0100020	C	3.4929160	-1.7670980	-1.7917930
H	-2.5983740	3.5700050	1.7164930	H	3.0230450	-0.9180710	-3.7202940
H	-1.8863330	3.7181380	0.0838300	H	3.7582500	-2.5616310	0.1835150
C	-4.0066730	1.0370880	2.8611800	C	2.4154630	-2.0993720	2.2158810
C	-1.8471710	-0.0665690	3.0282340	C	-3.4091900	-0.1647090	4.8863130
C	-4.5459460	0.1965910	-0.5124330	H	-5.3006790	0.8564540	4.5853780
C	-4.4018090	2.6047550	-0.7991180	H	-1.4532470	-1.1013860	4.8874980

C	-6.2989790	1.3859750	-1.7046690	C	-2.9001640	0.4777670	2.2809900
H	-6.2819920	-0.7585610	-1.3711480	H	-0.3915940	2.1260260	3.0334640
H	-6.0305930	3.5314900	-1.8815130	H	0.1163180	3.7538940	2.4999690
H	1.1069920	5.9317760	-3.9183560	C	2.2516690	4.3631140	0.2520340
H	5.9138370	2.1467800	2.8643760	C	0.6682430	3.5573450	-1.4047620
Cl	-3.8602100	-4.5205280	-2.7137970	C	2.4938640	1.7208510	3.2408000
H	-3.2572680	0.2088370	-4.2389150	C	3.5020890	1.1636390	1.1047000
H	-1.8433040	1.2572180	-4.5899640	H	-1.6132920	3.7128010	0.6858980
H	-1.7361710	-0.5099610	-4.8890180	H	-2.4243800	3.3582540	2.2377820
C	-2.1905640	-4.6497700	1.3023060	C	-4.5078280	0.6584240	-0.7010740
C	1.8235230	-2.0604260	3.6178680	C	-4.2252190	3.0497130	-0.4020780
H	2.5225600	-3.1642230	1.9343430	C	-4.1702450	0.7732750	2.8162040
H	3.4198280	-1.6383720	2.2595540	C	-2.0851540	-0.4654210	2.9356770
H	-3.6632530	-0.5065280	5.8950370	C	2.5438230	5.4632200	-0.5642470
H	-7.2489690	1.3772780	-2.2489940	H	2.7700170	4.2456470	1.2094450
H	-1.0863010	-4.6241950	1.3096790	C	0.9582140	4.6632050	-2.2175790
H	-2.5348270	-5.6346670	1.6451620	H	-0.0532890	2.7998650	-1.7334230
H	-2.5785630	-3.8685090	1.9804140	C	3.6916740	1.3866310	3.8896070
F	0.6053160	-2.6704370	3.6867740	H	1.6472230	2.0666870	3.8407840
F	2.6571440	-2.7214800	4.4747720	C	4.6993170	0.8392120	1.7539800
F	1.6666810	-0.7967440	4.0937290	H	3.4374560	1.0702030	0.0154830
O	4.6263020	-2.4830780	-2.2881620	C	-5.6706030	0.8890160	-1.4456680
C	5.8378740	-1.9048290	-2.1393900	H	-4.1702860	-0.3701120	-0.5377060
F	6.7549290	-2.7015890	-2.7266160	C	-5.3854740	3.2783630	-1.1571210
F	6.2059420	-1.7445180	-0.8263720	H	-3.6821020	3.9081250	0.0037720
F	5.9249050	-0.6657810	-2.7094150	C	-4.6108240	0.1406180	3.9856960
				H	-4.8241040	1.4919600	2.3113770
94				C	-2.5240310	-1.0899950	4.1124230
OCF3 Transition State				H	-1.1044330	-0.7124840	2.5160800
C	-1.2817380	-2.3218270	-0.7138300	C	1.8961400	5.6165530	-1.7994790
C	-2.7276420	-1.4659350	-2.9340550	H	3.2830660	6.2021010	-0.2369870
C	-0.9257540	-1.0659920	-1.2917160	H	0.4568180	4.7756260	-3.1847730
H	-3.3357880	-1.1451250	-3.7814690	C	4.7980090	0.9490590	3.1499330
Ni	-0.4013370	0.4470650	-0.1258890	H	3.7587230	1.4749270	4.9791610
P	0.8257690	1.9558090	0.9057310	H	5.5573230	0.4998220	1.1654920
P	-2.2278770	1.3343920	0.7736060	C	-6.1142750	2.2002820	-1.6766050
C	-0.3046760	2.7932980	2.1585180	H	-6.2308920	0.0386200	-1.8477810
C	1.3082640	3.4011460	-0.1598160	H	-5.7244610	4.3055480	-1.3294770
C	2.3845090	1.6179280	1.8396460	C	-3.7876150	-0.7896620	4.6378330
C	-1.6855870	2.9823490	1.5103790	H	-5.6022740	0.3737220	4.3885750
C	-3.7743380	1.7366700	-0.1589230	H	-1.8783920	-1.8182750	4.6132310

H	2.1283380	6.4757420	-2.4373980
H	5.7339150	0.6938200	3.6575230
H	-7.0239120	2.3798090	-2.2589550
H	-4.1344300	-1.2835670	5.5515200
C	0.7757890	-0.6867350	-1.2376300
C	1.3090050	-0.1971540	-2.4722270
C	2.9454940	-1.8848350	-0.9715140
C	2.5719710	-0.5368330	-2.9613400
C	3.3742560	-1.3913010	-2.2114950
H	2.9253440	-0.1490250	-3.9205640
H	-0.7153220	-2.6620690	0.1513680
H	3.6225060	-2.5246200	-0.4035480
H	0.6801220	0.4548850	-3.0769790
C	1.6878150	-1.5176030	-0.4890040
O	1.2552120	-1.9143580	0.7747070
C	2.1991740	-2.5872040	1.5929400
C	1.5503780	-2.8835810	2.9386970
H	2.5100470	-3.5558840	1.1590080
H	3.0937950	-1.9629740	1.7705280
F	0.4610770	-3.6962120	2.8213110
F	2.4544350	-3.5264920	3.7342740
F	1.1487610	-1.7643690	3.5939170
C	-2.3035900	-3.1401840	-1.2139140
O	-2.6722470	-4.3468200	-0.6765940
C	-1.9667280	-4.7992460	0.4800310
H	-0.8953270	-4.9562490	0.2630660
H	-2.4290270	-5.7586700	0.7469670
H	-2.0721080	-4.0916850	1.3205570
C	-1.7182080	-0.6508540	-2.4159590
O	-1.4616400	0.6095220	-2.9230870
C	-2.2767280	1.0780650	-4.0013500
H	-3.3351130	1.1473290	-3.6960320
H	-1.9011930	2.0812710	-4.2431030
H	-2.1838020	0.4312740	-4.8921990
C	-3.0169030	-2.7046680	-2.3477750
Cl	-4.2954970	-3.6987720	-3.0248600
O	4.6091970	-1.8523980	-2.7546280
C	5.7409030	-1.2285900	-2.3565690
F	6.7714080	-1.7528070	-3.0499640
F	5.7240050	0.1193570	-2.5681130
F	6.0102230	-1.4005030	-1.0194860

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OH Reactant

Ni	0.0318710	0.3966470	-0.1950050
P	1.7598780	1.4841280	0.6617940
P	-1.1594600	1.1275830	1.5297800
C	1.3302770	1.9567830	2.4292030
C	1.9836880	3.1527290	-0.1187590
C	3.4835180	0.8322480	0.7379060
C	-1.4916540	-0.4272330	-1.0293730
C	1.0465500	-0.2998510	-1.6834380
C	-0.1340060	2.4195830	2.4385180
C	-1.4114930	-0.1436110	2.8566800
C	-2.8361980	1.8775130	1.3558020
H	2.0072390	2.7379530	2.8134660
H	1.4481750	1.0581240	3.0585260
C	3.1061930	3.9564770	0.1624070
C	0.9753840	3.6465830	-0.9680590
C	4.1698460	0.6225750	-0.4772340
C	4.1214450	0.5022110	1.9492110
C	-2.2883830	0.3246010	-1.9181960
C	-1.8787810	-1.7559320	-0.7788660
C	1.1054790	0.3559620	-2.9255250
C	1.7972490	-1.4911010	-1.5807580
H	-0.5083660	2.5753890	3.4636050
H	-0.2247180	3.3722000	1.8897530
C	-2.3530560	0.0376450	3.8891110
C	-0.5955510	-1.2900910	2.8604330
C	-3.8949250	1.0427630	0.9386520
C	-3.0959150	3.2411680	1.5935360
C	3.2139500	5.2377000	-0.3925150
H	3.9060170	3.5748070	0.8059010
C	1.0864480	4.9319220	-1.5198830
H	0.1101310	3.0148530	-1.2004040
C	5.4686840	0.1002970	-0.4739830
H	3.6843290	0.8637600	-1.4275110
C	5.4222250	-0.0216980	1.9470930
H	3.6124440	0.6480130	2.9062590
C	-3.4264580	-0.2307060	-2.5249110
O	-1.8852490	1.6402030	-2.1443220
C	-3.0237160	-2.3393870	-1.3634640
H	-1.2661950	-2.3638450	-0.1083440

C	1.8802770	-0.1132870	-4.0031910	H	3.5850540	-3.1272480	-0.3370210
H	0.5171210	1.2665280	-3.0717090	H	-1.7420040	-2.7917720	5.7131970
C	2.5708500	-1.9967640	-2.6377390	H	-6.4461680	3.3242340	0.8955370
O	1.7298040	-2.1490270	-0.3438120	H	-1.6497940	-4.5794160	-0.6237040
C	-2.4692380	-0.9120120	4.9117630	H	-3.1939560	-5.3965100	-0.2006180
H	-3.0066970	0.9159250	3.8867120	H	-2.6329870	-3.9862650	0.7648730
C	-0.7106050	-2.2365790	3.8893390	F	0.9936930	-4.2469290	1.4105810
H	0.1232810	-1.4425290	2.0482310	F	3.0451270	-5.0323480	1.3161990
C	-5.1842860	1.5629300	0.7758530	F	2.6603860	-3.0439630	2.1698000
H	-3.7098050	-0.0167990	0.7402560	O	3.3967560	-1.8374890	-4.8572130
C	-4.3891550	3.7581280	1.4276600	H	3.2944080	-1.2910670	-5.6579860
H	-2.2966890	3.9144510	1.9160920				
C	2.2032200	5.7278340	-1.2335450	91			
H	4.0918860	5.8541400	-0.1721560	**OH Transition State**			
H	0.3003220	5.3094650	-2.1821020	C	-1.5391620	-1.9305170	-1.0517570
C	6.0989950	-0.2222770	0.7370080	C	-3.3446290	-0.3302780	-2.4434920
H	5.9878540	-0.0581200	-1.4246040	C	-1.1257160	-0.6069110	-1.3911830
H	5.9057990	-0.2727050	2.8968920	H	-4.0869610	0.2801510	-2.9608760
C	-3.7890710	-1.5526090	-2.2416660	Ni	0.0380470	0.4154730	-0.1781540
H	-4.0533370	0.3368780	-3.2160040	P	1.7930810	1.4352050	0.6856110
C	-2.6790950	2.4204520	-3.0353340	P	-1.2083630	1.2217550	1.4620120
O	-3.4504700	-3.6263870	-1.1376680	C	1.2872440	2.0277760	2.4012310
C	2.6107000	-1.2956160	-3.8525600	C	2.1823020	3.0526230	-0.1467660
H	1.8984830	0.4370800	-4.9527880	C	3.4748180	0.7039220	0.9223500
H	3.1512810	-2.9196950	-2.5672430	C	-0.1631380	2.5328950	2.3267110
C	2.5035600	-3.3254070	-0.2151020	C	-2.8561120	2.0229280	1.2240680
C	-1.6471770	-2.0490400	4.9141580	C	-1.5412410	0.0522040	2.8684280
H	-3.2075420	-0.7661740	5.7073640	H	1.3473750	1.1652940	3.0874100
H	-0.0726520	-3.1251910	3.8809030	H	1.9687990	2.8104620	2.7753130
C	-5.4361160	2.9205810	1.0211550	C	3.3401210	3.7989830	0.1487030
H	-5.9940070	0.9014820	0.4520550	C	1.2549240	3.5633400	-1.0751830
H	-4.5764830	4.8191490	1.6237880	C	4.0256250	0.3959340	2.1825920
H	2.2906770	6.7287570	-1.6690110	C	4.2072030	0.3630850	-0.2367430
H	7.1151640	-0.6301100	0.7368610	H	-0.2058110	3.4536450	1.7193110
Cl	-5.2296080	-2.2285770	-3.0017970	H	-0.5610010	2.7653000	3.3287460
H	-3.7148020	2.5333780	-2.6659850	C	-3.9080960	1.2120930	0.7433910
H	-2.2038850	3.4104740	-3.0788720	C	-3.1014150	3.3950860	1.4329630
H	-2.6990910	1.9842580	-4.0514020	C	-2.4884840	0.3224070	3.8765210
C	-2.6768800	-4.4286040	-0.2465570	C	-0.7762300	-1.1266270	2.9454980
C	2.2922180	-3.8993390	1.1784340	C	3.5622740	5.0359290	-0.4700460
H	2.2006220	-4.1043150	-0.9403880	H	4.0777630	3.4059020	0.8564790

C	1.4768510	4.8048830	-1.6895630	C	2.3813670	-3.2393790	-0.2122590
H	0.3627070	2.9729260	-1.3157490	C	2.1120230	-3.8478470	1.1575850
C	5.2792560	-0.2257130	2.2817210	H	2.3680220	-4.0669520	-0.9456610
H	3.4834180	0.6410860	3.1004720	H	3.3886390	-2.7847550	-0.1945870
C	5.4615440	-0.2497280	-0.1346240	F	0.9032830	-4.4752990	1.2207010
H	3.7936310	0.5821670	-1.2265710	F	3.0710620	-4.7844410	1.4222830
C	-5.1741970	1.7573160	0.5002580	F	2.1443390	-2.9343310	2.1620470
H	-3.7367720	0.1463660	0.5598550	C	-2.7925400	-2.4587390	-1.3935510
C	-4.3690040	3.9402420	1.1797820	O	-3.2200460	-3.7237070	-1.0730540
H	-2.3088010	4.0515370	1.8040500	C	-2.3269390	-4.5540960	-0.3313760
C	-2.6588840	-0.5692770	4.9434170	H	-1.3984330	-4.7543960	-0.8949070
H	-3.1044300	1.2262360	3.8213830	H	-2.8676460	-5.4967060	-0.1729840
C	-0.9414280	-2.0134170	4.0194530	H	-2.0735220	-4.1052580	0.6449070
H	-0.0525200	-1.3468840	2.1535620	C	-2.1023750	0.1913070	-2.0780110
C	2.6299840	5.5420190	-1.3888820	O	-1.7599970	1.5142020	-2.3155810
H	4.4678490	5.6063710	-0.2370210	C	-2.7182300	2.3409360	-2.9790020
H	0.7505500	5.1940640	-2.4111280	H	-3.6480480	2.4276980	-2.3902450
C	6.0032490	-0.5466980	1.1260290	H	-2.2505380	3.3311390	-3.0640490
H	5.6920840	-0.4545520	3.2700110	H	-2.9523360	1.9598510	-3.9898520
H	6.0179550	-0.4963180	-1.0450880	C	-3.6903570	-1.6480810	-2.1139680
C	-5.4100340	3.1235110	0.7180640	Cl	-5.2664670	-2.2678900	-2.5860780
H	-5.9789750	1.1098650	0.1370870	O	3.5937110	-1.5386750	-4.6820260
H	-4.5436890	5.0072610	1.3554730	H	3.5815700	-0.9387790	-5.4506440
C	-1.8838500	-1.7366420	5.0185990				
H	-3.4017650	-0.3530740	5.7187640	93			
H	-0.3376490	-2.9249650	4.0690570	**COOH Reactant**			
H	2.8066670	6.5084600	-1.8727340	Ni	-0.1283560	0.4263600	-0.1672870
H	6.9838920	-1.0270190	1.2057950	P	1.2440500	1.9849940	0.6017140
H	-6.4010250	3.5487220	0.5281350	P	-1.7298020	1.3705900	1.0524200
H	-2.0200720	-2.4319160	5.8536160	C	0.4083860	2.8061900	2.0713630
C	0.5877700	-0.4689850	-1.8581640	C	1.4075180	3.4092380	-0.5743210
C	0.8074330	0.2830160	-3.0475220	C	2.9815170	1.6738770	1.1352330
C	2.4661300	-1.9107590	-2.6277540	C	-1.3451560	-0.8359740	-0.9628550
C	1.7852310	-0.0317540	-3.9960580	C	1.2264780	-0.4516400	-1.1967060
C	2.6095010	-1.1441490	-3.7962700	C	-1.0694360	3.0067690	1.7072620
H	1.8974420	0.5934160	-4.8907930	C	-2.0846210	0.4575490	2.6255680
H	-0.8305980	-2.5598700	-0.5149950	C	-3.4160190	1.7528450	0.4088490
H	3.1558120	-2.7450760	-2.4836320	H	0.8983310	3.7597990	2.3297350
H	0.1638040	1.1419310	-3.2356780	H	0.4956510	2.1275770	2.9372180
C	1.4945590	-1.5709440	-1.6842610	C	2.3496380	4.4353180	-0.3624410
O	1.3831070	-2.2695140	-0.4825630	C	0.5286150	3.4917870	-1.6711760

C	3.9323280	1.3265460	0.1517320	H	5.0090860	1.5083100	3.8937820
C	3.3833130	1.7317020	2.4835880	C	-3.2080190	-2.5997230	-2.1561100
C	-2.0243860	-0.4832890	-2.1477740	H	-3.4767210	-1.1022990	-3.6650520
C	-1.6207810	-2.0976580	-0.4066310	C	-2.3961990	1.1448030	-3.8816690
C	1.4882760	-0.1021950	-2.5393790	O	-2.8692990	-4.2266830	-0.4621730
C	2.0503190	-1.4601850	-0.6407780	C	3.3174890	-1.6872330	-2.7025280
H	-1.6598370	3.3556310	2.5705670	H	2.7013090	-0.4006550	-4.3225940
H	-1.1571760	3.7577300	0.9037880	H	3.7091650	-2.8527400	-0.9350280
C	-3.2038260	0.7698920	3.4224030	C	2.6554970	-2.7352840	1.2880190
C	-1.1846280	-0.5349500	3.0558160	C	-2.5098160	-0.8827110	5.0619500
C	-4.2563220	0.6736220	0.0608190	H	-4.2898420	0.3454170	5.2451540
C	-3.8873680	3.0687830	0.2368660	H	-0.6919730	-1.9707240	4.5981980
C	2.4075640	5.5304020	-1.2330290	C	-6.0075130	2.2251300	-0.5991880
H	3.0498100	4.3714120	0.4772680	H	-6.1822100	0.0638930	-0.7019130
C	0.5876680	4.5936610	-2.5378040	H	-5.5316620	4.3308210	-0.3845830
H	-0.1936160	2.6859600	-1.8476240	H	1.5741560	6.4672070	-3.0026760
C	5.2572930	1.0559680	0.5136240	H	6.6878370	0.9094270	2.1389050
H	3.6371760	1.2685940	-0.9002870	Cl	-4.3791130	-3.6777130	-2.9124710
C	4.7111500	1.4571680	2.8414280	H	-3.4936620	1.1759770	-3.7544870
H	2.6678130	1.9914010	3.2687770	H	-2.0350640	2.1527540	-4.1289920
C	-2.9461680	-1.3576770	-2.7454810	H	-2.1418870	0.4567360	-4.7087410
O	-1.7366790	0.7751720	-2.6715720	C	-2.1884270	-4.6411780	0.7217410
C	-2.5519770	-2.9928010	-0.9763330	C	2.2230130	-2.9664180	2.7286700
H	-1.0935930	-2.3984680	0.5018430	H	2.6291820	-3.7162890	0.7769090
C	2.5140070	-0.6937160	-3.2854250	H	3.6994990	-2.3701280	1.3020650
H	0.8630150	0.6567730	-3.0179840	H	-2.6782820	-1.4073310	6.0082080
C	3.0758090	-2.0755000	-1.3660140	H	-7.0152540	2.4083050	-0.9861250
O	1.7772990	-1.7986070	0.6929970	H	-1.0983540	-4.7106300	0.5586080
C	-3.4139560	0.1016700	4.6347340	H	-2.5869350	-5.6377790	0.9543000
H	-3.9210760	1.5263420	3.0873410	H	-2.3887680	-3.9583710	1.5669120
C	-1.3959290	-1.1991810	4.2733310	F	0.9705740	-3.5003660	2.8198040
H	-0.3227220	-0.7892740	2.4289540	F	3.0829610	-3.8489910	3.3188510
C	-5.5427810	0.9118630	-0.4373190	F	2.2286820	-1.8300250	3.4761060
H	-3.9044920	-0.3556710	0.1786030	C	4.3944280	-2.2993220	-3.5093220
C	-5.1767510	3.3019670	-0.2633060	O	4.6748690	-2.0184010	-4.6674460
H	-3.2598240	3.9260710	0.4963180	O	5.1039830	-3.2637990	-2.8208610
C	1.5251180	5.6117800	-2.3209740	H	5.7724790	-3.5960750	-3.4554090
H	3.1464170	6.3208850	-1.0646520				
H	-0.0956000	4.6518900	-3.3913550	93			
C	5.6509470	1.1212990	1.8583470	**COOH Transition State**			
H	5.9836800	0.7906200	-0.2610160	C	-1.1701000	-2.2900770	-0.6653110

C	-2.8354930	-1.3772070	-2.7038480	H	3.3979860	6.2606380	-0.6529080
C	-0.8789050	-1.0212920	-1.2431210	H	0.3086770	4.7535890	-3.2789810
H	-3.5250510	-1.0394740	-3.4795180	C	5.5290900	0.8068150	2.1839440
Ni	-0.1456670	0.4474560	-0.1518320	H	4.8478710	1.3247600	4.1768690
P	1.2435630	1.9188200	0.7068440	H	5.9082930	0.3651820	0.0918860
P	-1.8020510	1.3611880	1.0164760	C	-5.9119260	2.4207460	-0.9378700
C	0.3460270	2.7134970	2.1575550	H	-6.1804780	0.2681630	-1.0341470
C	1.5449860	3.3896550	-0.3859700	H	-5.3558690	4.5033850	-0.6985170
C	2.9339470	1.5305520	1.3389130	C	-2.9491720	-0.8586030	4.9654310
C	-1.1099410	2.9621440	1.7303990	H	-4.7033710	0.4178910	5.0208350
C	-3.4314490	1.8398600	0.2848500	H	-1.1306210	-1.9927510	4.6330490
C	-2.3135810	0.4709120	2.5643980	H	1.9907140	6.5089590	-2.7032330
H	0.3769320	2.0035930	3.0023540	H	6.5363310	0.5295010	2.5114800
H	0.8378960	3.6481540	2.4755720	H	-6.8758750	2.6462300	-1.4055000
C	2.4957690	4.3810920	-0.0715470	H	-3.1994930	-1.3771220	5.8968210
C	0.7624170	3.5311460	-1.5475800	C	0.8757950	-0.6596940	-1.3834580
C	3.2939190	1.6130060	2.6983970	C	1.2564830	-0.1846810	-2.6823280
C	3.8896360	1.0677430	0.4079120	C	2.9908870	-1.9682400	-1.4245640
H	-1.1348220	3.7264120	0.9346290	C	2.4186590	-0.5814280	-3.3305510
H	-1.7244970	3.3235310	2.5717740	C	3.3026140	-1.4954060	-2.7233920
C	-4.2915390	0.7995700	-0.1292880	H	2.6640290	-0.1881720	-4.3213830
C	-3.8284040	3.1735570	0.0648360	H	-0.5148370	-2.6472990	0.1281320
C	-3.4772370	0.8129870	3.2821380	H	3.7058860	-2.6355670	-0.9410760
C	-1.4769450	-0.5466230	3.0594660	H	0.5873810	0.5117460	-3.1869200
C	2.6525860	5.4979220	-0.9020230	C	1.8328270	-1.5553860	-0.7784800
H	3.1266130	4.2728740	0.8172620	O	1.5452250	-1.9438020	0.5345770
C	0.9185330	4.6530090	-2.3750340	C	2.5423410	-2.6970080	1.2038020
H	0.0379100	2.7485260	-1.8011340	C	2.0709010	-2.9735730	2.6247250
C	4.5832380	1.2524140	3.1166770	H	2.7211700	-3.6748810	0.7189030
H	2.5734300	1.9618630	3.4438490	H	3.4969070	-2.1426660	1.2608740
C	5.1776270	0.7148550	0.8283680	F	0.9056570	-3.6837430	2.6582290
H	3.6279310	0.9858580	-0.6522180	F	3.0170760	-3.7148560	3.2723840
C	-5.5227470	1.0885470	-0.7291640	F	1.8707310	-1.8418600	3.3493710
H	-3.9984840	-0.2439320	0.0253300	C	-2.2381520	-3.0976800	-1.0795430
C	-5.0599230	3.4604090	-0.5429870	O	-2.5499610	-4.3204350	-0.5442150
H	-3.1865470	4.0038490	0.3729480	C	-1.7116340	-4.8171940	0.5004430
C	-3.7931000	0.1492810	4.4742410	H	-0.6730250	-4.9550640	0.1516010
H	-4.1456360	1.5918600	2.9006350	H	-2.1364220	-5.7911460	0.7767680
C	-1.7904970	-1.2043440	4.2578890	H	-1.7196350	-4.1482680	1.3782340
H	-0.5794480	-0.8247840	2.4975920	C	-1.7728510	-0.5770590	-2.2720350
C	1.8626640	5.6369080	-2.0535620	O	-1.5563120	0.6906200	-2.7751210

C	-2.4436480	1.1703880	-3.7897420	H	3.4317910	3.9583370	0.8196270
H	-3.4777680	1.2433310	-3.4107350	C	0.6539520	4.8657800	-1.7626830
H	-2.0813200	2.1734070	-4.0511550	H	-0.1811620	2.9056400	-1.3231030
H	-2.4168360	0.5280720	-4.6879370	C	5.3469070	0.5156850	0.1076430
C	-3.0645470	-2.6288900	-2.1203940	H	3.6017220	0.9805820	-1.0765480
Cl	-4.4115350	-3.6032430	-2.6822420	C	5.0972290	0.7074070	2.5129230
C	4.5212170	-1.9029560	-3.4336570	H	3.1595130	1.3228460	3.2303940
O	4.8704280	-1.5289440	-4.5492600	C	-3.2186130	-0.6560250	-2.7849930
O	5.3001610	-2.7923360	-2.7095750	O	-1.8591520	1.3493520	-2.3930710
H	6.0664290	-2.9887300	-3.2871550	C	-2.8089880	-2.6380190	-1.4193490
				H	-1.2047980	-2.4349280	0.0149540
94				C	2.2781130	-0.2131080	-3.6238770
CH2OH Reactant				H	0.7042180	1.1173710	-2.9906960
Ni	-0.0954150	0.4022500	-0.1589010	C	2.8725590	-1.9608540	-2.0687370
P	1.4541480	1.6946930	0.7593390	O	1.7259100	-2.0537300	0.0979500
P	-1.5092250	1.1675710	1.3754460	C	-2.9351210	-0.7072830	4.8045320
C	0.8062090	2.2729420	2.4272330	H	-3.4966790	1.0146080	3.6195080
C	1.6044330	3.2995310	-0.1575030	C	-1.0452140	-1.9963630	3.9912120
C	3.2093750	1.2123200	1.0538070	H	-0.1297630	-1.2784400	2.1566750
C	-1.4569880	-0.5961110	-1.0795570	C	-5.4585850	1.2001800	0.2044140
C	1.1226820	-0.3377140	-1.4495320	H	-3.8588130	-0.2402460	0.3962880
C	-0.6815970	2.6110600	2.2545810	C	-4.9252010	3.4854030	0.8126560
C	-1.7803670	-0.0184470	2.7739980	H	-2.9142470	3.8515940	1.4948170
C	-3.2179420	1.7517540	0.9936680	C	1.6858260	5.7745360	-1.4939630
H	1.3776750	3.1380850	2.8029380	H	3.4955860	6.1499230	-0.3567960
H	0.9263690	1.4415660	3.1432220	H	-0.1185590	5.1165430	-2.4971140
C	2.6431810	4.2146380	0.1042700	C	5.8914940	0.4145690	1.3964250
C	0.6130500	3.6289710	-1.1018690	H	5.9522230	0.2761890	-0.7720690
C	4.0151000	0.9119460	-0.0657300	H	5.5147020	0.6291200	3.5222590
C	3.7621290	1.1022800	2.3445940	C	-3.5207640	-1.9775300	-2.4358390
C	-2.1961170	0.0270030	-2.1070470	H	-3.8004610	-0.1905650	-3.5835420
C	-1.7793320	-1.9281870	-0.7645880	C	-2.5864690	1.9969470	-3.4343760
C	1.3169340	0.2550240	-2.7109770	O	-3.1707110	-3.9338950	-1.1371060
C	1.9261530	-1.4651620	-1.1617890	C	3.0655690	-1.3271690	-3.3121240
H	-1.1676250	2.8214020	3.2216780	H	2.4112480	0.2967370	-4.5856580
H	-0.7872480	3.5033850	1.6140670	H	3.4983740	-2.8268420	-1.8335510
C	-2.7991930	0.1774550	3.7276880	C	2.6586460	-3.0481230	0.4731200
C	-0.9093550	-1.1149470	2.9085220	C	-2.0569800	-1.7936460	4.9387000
C	-4.1528310	0.8063410	0.5201790	H	-3.7325800	-0.5512120	5.5387510
C	-3.6161240	3.0955250	1.1315830	H	-0.3638420	-2.8465620	4.0861310
C	2.6819910	5.4461360	-0.5618030	C	-5.8492980	2.5391020	0.3511000

H	-6.1713450	0.4544760	-0.1615490	H	0.7924200	1.5880430	3.0833920
H	-5.2217550	4.5329320	0.9312720	H	1.3436110	3.2411570	2.6902980
H	1.7201360	6.7365940	-2.0158680	C	2.8914740	4.1200520	0.1772890
H	6.9331350	0.1045410	1.5302770	C	1.0556060	3.5776180	-1.3174600
Cl	-4.8163640	-2.8148500	-3.2903490	C	3.6281460	0.9876970	2.5242040
H	-3.6648020	2.0604260	-3.1998810	C	4.0284420	0.6804650	0.1494260
H	-2.1745460	3.0132050	-3.5063750	H	-0.7244420	3.6282870	1.3329520
H	-2.4523670	1.4831700	-4.4042920	H	-1.2210150	3.0857510	2.9607310
C	-2.4511650	-4.6062300	-0.1044140	C	-4.1747210	1.0586160	0.2417000
C	2.3509050	-3.4987600	1.8933470	C	-3.5438320	3.3556140	0.7031400
H	2.5999700	-3.9452000	-0.1725960	C	-3.0542430	0.6616100	3.5789410
H	3.6958590	-2.6645690	0.4556960	C	-1.2559160	-0.8559310	2.9775670
H	-2.1669360	-2.4854940	5.7803430	C	3.1118230	5.3113200	-0.5251520
H	-6.8717730	2.8439010	0.1049290	H	3.5370150	3.8613980	1.0235980
H	-1.3785520	-4.6993640	-0.3511000	C	1.2761770	4.7728620	-2.0185860
H	-2.8990140	-5.6069850	-0.0394080	H	0.2648930	2.8862290	-1.6300310
H	-2.5584300	-4.0911600	0.8670950	C	4.9036630	0.4740400	2.8014320
F	1.1153520	-4.0677400	2.0065750	H	2.9906270	1.2993300	3.3568110
F	3.2652440	-4.4415120	2.2737730	C	5.3021220	0.1708190	0.4283380
F	2.4095980	-2.4862720	2.7988990	H	3.6950410	0.7506210	-0.8910420
C	4.1048440	-1.8495100	-4.2680900	C	-5.4335050	1.4912150	-0.1913150
H	3.9414200	-2.9286960	-4.4669520	H	-3.9375570	-0.0101340	0.2226560
H	4.0277070	-1.3130320	-5.2336760	C	-4.8034890	3.7872590	0.2608460
O	5.4234760	-1.6614000	-3.6907540	H	-2.8238450	4.1003140	1.0548610
H	6.0654160	-2.1133570	-4.2702810	C	-3.3231840	-0.1094650	4.7165530
				H	-3.6641020	1.5462030	3.3668530
94				C	-1.5215360	-1.6230250	4.1218040
CH2OH Transition State				H	-0.4567710	-1.1484400	2.2880810
C	-1.3521460	-2.1592040	-0.9010630	C	2.3025170	5.6409270	-1.6233850
C	-3.1176280	-0.8995260	-2.6480710	H	3.9203940	5.9832820	-0.2180200
C	-1.0129570	-0.8494270	-1.3535970	H	0.6489040	5.0230460	-2.8808890
H	-3.8471300	-0.4218540	-3.3044400	C	5.7443870	0.0670160	1.7566410
Ni	-0.0904360	0.4319910	-0.1738300	H	5.2403090	0.3951680	3.8407130
P	1.4855180	1.6820810	0.7290200	H	5.9420870	-0.1519410	-0.3990730
P	-1.5666570	1.3197370	1.2143480	C	-5.7536250	2.8576880	-0.1823130
C	0.7585960	2.3828990	2.3180760	H	-6.1671740	0.7555500	-0.5368790
C	1.8577830	3.2446340	-0.2100000	H	-5.0436750	4.8559140	0.2730290
C	3.1767910	1.1016740	1.1942600	C	-2.5555720	-1.2517970	4.9912230
C	-0.7006210	2.7791800	2.0377010	H	-4.1362460	0.1806100	5.3907190
C	-3.2154860	1.9853660	0.7060570	H	-0.9216790	-2.5149160	4.3286560
C	-2.0155160	0.2956370	2.6998310	H	2.4774850	6.5715160	-2.1735420

H	6.7400260	-0.3324950	1.9760490
H	-6.7392430	3.1950370	-0.5194430
H	-2.7677220	-1.8539860	5.8809430
C	0.7225780	-0.6028460	-1.6373200
C	1.0327220	0.0257760	-2.8798260
C	2.7854270	-1.9434210	-1.9970560
C	2.1534480	-0.3039370	-3.6455420
C	3.0390020	-1.3074840	-3.2309890
H	2.3380750	0.2346990	-4.5827130
H	-0.6597930	-2.6558590	-0.2230530
H	3.5176420	-2.6748450	-1.6460960
H	0.3583490	0.8004060	-3.2446970
C	1.6827750	-1.5923340	-1.2204470
O	1.4734240	-2.1467050	0.0456440
C	2.5039610	-2.9765730	0.5536370
C	2.1215630	-3.4217680	1.9583640
H	2.6399590	-3.8905180	-0.0545190
H	3.4653520	-2.4346320	0.6136240
F	0.9561660	-4.1320120	1.9812150
F	3.1026170	-4.2368050	2.4488920
F	1.9770960	-2.3871460	2.8257620
C	-2.5098040	-2.8397430	-1.3037700
O	-2.8613890	-4.0989330	-0.8851020
C	-1.9797060	-4.7639930	0.0197590
H	-0.9834280	-4.9228120	-0.4298310
H	-2.4481050	-5.7363360	0.2222880
H	-1.8697870	-4.2034790	0.9644110
C	-1.9667990	-0.2278600	-2.2285040
O	-1.7064650	1.0821690	-2.5909410
C	-2.6423450	1.7351410	-3.4520890
H	-3.6351490	1.8152670	-2.9757590
H	-2.2398310	2.7429820	-3.6208920
H	-2.7340260	1.2119420	-4.4211970
C	-3.3870740	-2.1994030	-2.1997660
Cl	-4.8450450	-3.0130760	-2.7476350
C	4.2216000	-1.7151640	-4.0672120
H	4.0489220	-2.7126420	-4.5242410
H	4.3598590	-0.9902890	-4.8931540
O	5.4072360	-1.7740880	-3.2360570
H	6.1040570	-2.2275210	-3.7457930

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Ph Reactant

Ni	0.5071000	-0.3719960	-0.2590910
P	-0.2452030	-2.4452460	-0.0344640
P	2.5351030	-1.1671020	0.1716220
C	1.1096830	-3.4683060	0.7728790
C	-0.4079340	-3.2836760	-1.6813300
C	-1.8003350	-2.9256360	0.8320580
C	1.1588550	1.4008570	-0.6213810
C	-1.2400960	0.3584940	-0.5983600
C	2.4435940	-3.0473120	0.1403660
C	3.1064030	-0.8505740	1.9058450
C	4.0190000	-0.7371940	-0.8363140
H	0.9240200	-4.5483260	0.6504200
H	1.1123770	-3.2386140	1.8521490
C	-1.0211900	-4.5453780	-1.8144680
C	0.1487990	-2.6625820	-2.8159590
C	-3.0289040	-2.5033050	0.2804680
C	-1.8064600	-3.6626560	2.0319250
C	1.5542280	1.7417900	-1.9320880
C	1.2817980	2.3905710	0.3705430
C	-1.7658710	0.4769300	-1.8994200
C	-2.0936380	0.7685300	0.4493600
H	3.3047080	-3.4945920	0.6636360
H	2.4732820	-3.3739400	-0.9128320
C	4.4427450	-1.0656100	2.2982260
C	2.1634730	-0.4362000	2.8645140
C	4.4977420	0.5889790	-0.7759270
C	4.6687630	-1.6596140	-1.6789700
C	-1.0677120	-5.1796330	-3.0622000
H	-1.4771870	-5.0278650	-0.9434300
C	0.1032190	-3.3041040	-4.0628780
H	0.6069460	-1.6711040	-2.7186490
C	-4.2350310	-2.8247600	0.9143550
H	-3.0416770	-1.9186030	-0.6442960
C	-3.0172620	-3.9795560	2.6644760
H	-0.8693010	-3.9977510	2.4852410
C	2.0586140	3.0173480	-2.2321710
O	1.4214470	0.7433100	-2.8956580
C	1.7948230	3.6780070	0.1026320
H	0.9591460	2.1573720	1.3882720

C	-3.0665440	0.9392890	-2.1520690	H	-3.3399070	0.3145410	2.8142380
H	-1.1318170	0.2128140	-2.7510900	H	4.1791400	-0.3190350	5.6267200
C	-3.3901950	1.2503800	0.2200480	H	7.1248440	0.3535860	-2.9568700
O	-1.5664260	0.6409070	1.7448820	H	0.4663080	4.1541340	2.4363880
C	4.8240860	-0.8756680	3.6321220	H	1.7556340	5.2967960	2.9499970
H	5.1900020	-1.3675290	1.5570010	H	2.1206610	3.5417790	2.8031530
C	2.5479280	-0.2511560	4.2008030	F	-0.6021080	1.5119070	4.2619610
H	1.1281320	-0.2524060	2.5574280	F	-2.5405650	1.0043780	5.1669370
C	5.6088380	0.9756470	-1.5343830	F	-1.2883690	-0.5691680	4.2798180
H	3.9996570	1.3211790	-0.1337890	C	-5.2821150	1.8327080	-1.3373560
C	5.7807760	-1.2671070	-2.4382800	C	-5.8238940	2.8942040	-0.5792160
H	4.3200290	-2.6938170	-1.7501490	C	-6.0952820	1.2575500	-2.3393350
C	-0.5028330	-4.5609700	-4.1878960	C	-7.1245300	3.3587050	-0.8093190
H	-1.5505130	-6.1579430	-3.1573910	H	-5.2021170	3.3838880	0.1776800
H	0.5355340	-2.8153100	-4.9421990	C	-7.3943320	1.7237680	-2.5734340
C	-4.2332620	-3.5640580	2.1066710	H	-5.7079370	0.4173250	-2.9250610
H	-5.1803090	-2.4914620	0.4743750	C	-7.9175580	2.7758690	-1.8079660
H	-3.0063210	-4.5555290	3.5956380	H	-7.5162290	4.1908260	-0.2143420
C	2.1799740	3.9728410	-1.2166960	H	-8.0061580	1.2555370	-3.3521870
H	2.3669890	3.2980080	-3.2414190	H	-8.9338550	3.1401690	-1.9901880
C	1.7933800	1.0728810	-4.2325220				
O	1.9477900	4.6723770	1.0394240	100			
C	-3.9037760	1.3354250	-1.0941410	**Ph Transition State**			
H	-3.4162910	1.0312970	-3.1861170	C	-0.9189160	-2.5195860	-0.0306800
H	-4.0467240	1.5303390	1.0485030	C	-2.1533710	-2.5822790	-2.5273150
C	-2.4367560	0.9536630	2.8132980	C	-0.7035040	-1.4135680	-0.9042910
C	3.8771700	-0.4701000	4.5850620	H	-2.6755000	-2.6253720	-3.4847910
H	5.8656950	-1.0392540	3.9280710	Ni	-0.5058350	0.4242670	-0.2196600
H	1.8068820	0.0730700	4.9371870	P	0.3838730	2.3503530	0.3626010
C	6.2546300	0.0493520	-2.3660300	P	-2.5158030	1.2326560	0.2577700
H	5.9669020	2.0082810	-1.4758450	C	-0.9611520	3.3186270	1.2562390
H	6.2794440	-1.9974110	-3.0842390	C	0.7547340	3.4753720	-1.0707480
H	-0.5423790	-5.0571150	-5.1632540	C	1.8875820	2.5495310	1.4176890
H	-5.1780960	-3.8142650	2.6001480	C	-2.2874610	3.0863670	0.5143090
Cl	2.8255820	5.5655890	-1.6104500	C	-3.9826940	1.1024530	-0.8622190
H	2.8630880	1.3415960	-4.3046910	C	-3.2415080	0.7229270	1.8907110
H	1.6103790	0.1692590	-4.8306170	H	-1.0305630	2.9252620	2.2852560
H	1.1801470	1.9015550	-4.6323200	H	-0.7152990	4.3924130	1.3156730
C	1.5452400	4.3834120	2.3774890	C	1.4650100	4.6827850	-0.9179550
C	-1.7026440	0.7168340	4.1256100	C	0.2773910	3.1171330	-2.3460280
H	-2.7521060	2.0145550	2.8000980	C	1.8642370	3.1047400	2.7123800

C	3.1102300	2.0522350	0.9143180	C	3.2039320	-1.4503380	-0.0632430
H	-2.2424090	3.5588440	-0.4821850	C	2.9055130	-0.8087040	-2.3643870
H	-3.1394310	3.5233150	1.0614780	C	3.7663270	-1.2812000	-1.3533380
C	-4.5107050	-0.1869270	-1.0920670	H	3.2845120	-0.6719090	-3.3825900
C	-4.5615950	2.1987110	-1.5317990	H	-0.4293870	-2.5000970	0.9421850
C	-4.5556590	1.0631150	2.2702840	H	3.8734140	-1.7351260	0.7524170
C	-2.4329890	0.0011040	2.7874580	H	0.9283560	-0.2236880	-2.9356990
C	1.6853060	5.5195330	-2.0193890	C	1.8628700	-1.1735240	0.1913690
H	1.8618750	4.9631590	0.0635770	O	1.3296530	-1.2489670	1.4827060
C	0.4956050	3.9590300	-3.4467990	C	2.2411360	-1.5006850	2.5374380
H	-0.2563210	2.1678980	-2.4701220	C	1.4758170	-1.4935900	3.8539240
C	3.0354200	3.1713270	3.4814170	H	2.7239810	-2.4916380	2.4447530
H	0.9324790	3.4932350	3.1334830	H	3.0223190	-0.7203720	2.5922900
C	4.2792210	2.1276900	1.6813730	F	0.5065070	-2.4536140	3.8974230
H	3.1489720	1.6029140	-0.0836360	F	2.3464220	-1.7498800	4.8753110
C	-5.6010040	-0.3688700	-1.9508010	F	0.8753130	-0.3047000	4.1158750
H	-4.0677130	-1.0545390	-0.5925840	C	-1.7018040	-3.6310120	-0.3729080
C	-5.6489130	2.0124910	-2.3988860	O	-1.9296840	-4.7090350	0.4451720
H	-4.1770050	3.2111450	-1.3781500	C	-1.3168510	-4.7002450	1.7345180
C	-5.0453370	0.6932390	3.5288750	H	-0.2152760	-4.6780380	1.6575380
H	-5.2042910	1.6054480	1.5739960	H	-1.6305210	-5.6373010	2.2133620
C	-2.9232320	-0.3640710	4.0499910	H	-1.6599100	-3.8434610	2.3402060
H	-1.4182490	-0.2771470	2.4848620	C	-1.3813440	-1.4745360	-2.1672580
C	1.1987830	5.1601820	-3.2856220	O	-1.2662840	-0.3612760	-2.9813850
H	2.2435090	6.4529930	-1.8904040	C	-1.9817890	-0.3635460	-4.2192770
H	0.1227480	3.6713430	-4.4355830	H	-3.0691880	-0.4476990	-4.0486110
C	4.2460950	2.6879810	2.9679480	H	-1.7624700	0.6030670	-4.6921570
H	2.9990430	3.6077750	4.4852230	H	-1.6423350	-1.1787990	-4.8835050
H	5.2194710	1.7455660	1.2704890	C	-2.3080880	-3.6584030	-1.6439700
C	-6.1751640	0.7308160	-2.6072240	Cl	-3.2874260	-5.0336570	-2.1281940
H	-6.0022440	-1.3754560	-2.1074790	C	5.1938990	-1.5723370	-1.6043610
H	-6.0908720	2.8775210	-2.9050840	C	5.9379920	-0.8274850	-2.5501340
C	-4.2290610	-0.0188010	4.4215070	C	5.8694980	-2.6019390	-0.9073020
H	-6.0695120	0.9574050	3.8133580	C	7.2900490	-1.0980780	-2.7854020
H	-2.2843700	-0.9240350	4.7400210	H	5.4539560	-0.0055850	-3.0877740
H	1.3746880	5.8139640	-4.1463100	C	7.2235710	-2.8690840	-1.1386770
H	5.1603590	2.7450920	3.5676540	H	5.3143130	-3.2269940	-0.1997440
H	-7.0285760	0.5881250	-3.2781380	C	7.9438840	-2.1191370	-2.0795220
H	-4.6153640	-0.3088450	5.4042700	H	7.8414090	-0.4989770	-3.5182620
C	0.9501190	-0.7366740	-0.8313670	H	7.7163210	-3.6793380	-0.5902570
C	1.5591900	-0.5555570	-2.1106510	H	9.0023880	-2.3297840	-2.2629960

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