Supporting Information

Stereo- and Regio-Selective Synthesis of Silicon-Containing Diborylalkenes via Platinum-Catalyzed Mono-Lateral Diboration of Dialkynlsilanes

Peng-Wei Long,[a]† Jia-Le Xie,[a]† Jing-Jing Yang,[a] Si-Qi Lu,[a] Zheng Xu,*[a] Fei Ye,[a] and Li-Wen Xu*[ab]

[a] Key Laboratory of Organosilicon Chemistry and Material Technology of Ministry of Education, and Key Laboratory of Organosilicon Material Technology of Zhejiang Province, Hangzhou Normal University, P. R. China
E-mail: zhengxu@hznu.edu.cn; liwenxu@hznu.edu.cn (XLW)
[b] State Key Laboratory for Oxo Synthesis and Selective Oxidation, Suzhou Research Institute and Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, P. R. China
† P.W. Long and J. L. Xie contributed equally to this work.

Table of Contents

Experimental Information

Ⅰ. General Information

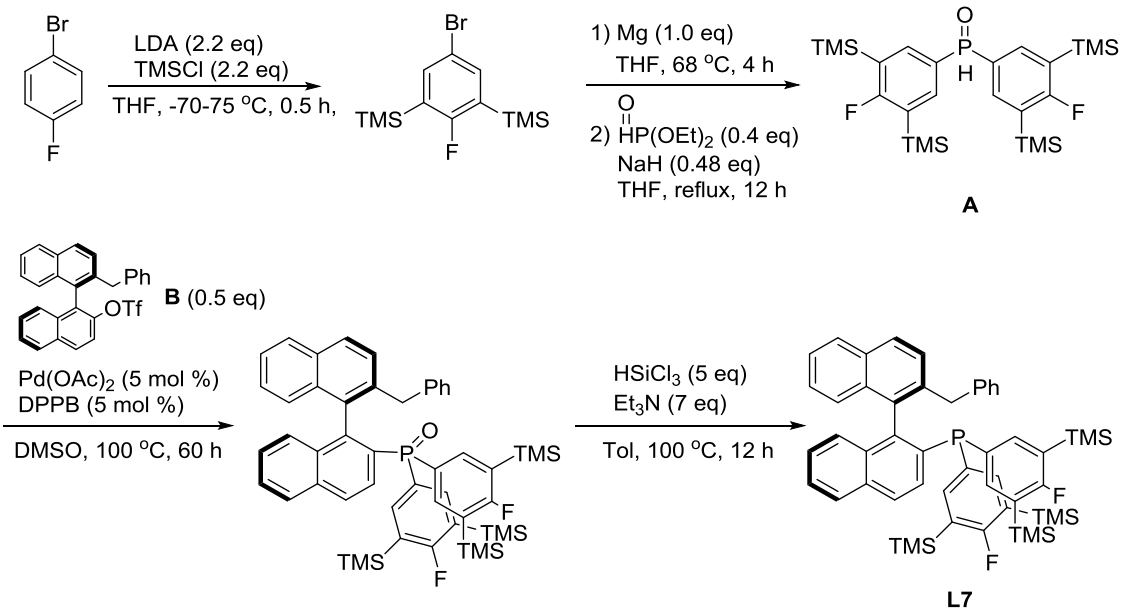
Unless specifically stated, all reagents were commercially obtained and where appropriate, purified prior to use. For example, all the aldehydes recrystallized or distilled prior to use. Dichloromethane, toluene, were freshly distilled from CaH_2, THF was freshly distilled from sodium metal prior to use. Ether (Et_2O), tetrahydrofuran (THF) and 1, 4-dioxane were dried and distilled from metal sodium and benzophenone. Alcohol solvents were dried and distilled from metal magnesium. Other commercially available reagents and solvents were used directly without purification. Reactions were monitored by thin layer chromatography (TLC) using silica gel plates. Flash column chromatography was performed over silica (200-300 mesh). ^{1}H, ^{13}C, ^{19}F and ^{29}Si NMR spectra were recorded on a Bruker 400 MHz or 500 MHz spectrometer in $CDCl_3$. Multiplicities were given as: s (singlet); d (doublet); dd (doublets of doublet); t (triplet); q (quartet); or m (multiplets). High resolution mass spectra (HRMS) of the products were obtained on a Bruker Daltonics micro TOF-spectrometer.

Ⅱ. Preparation of $Pt(dba)_3$

$Pt(dba)_3$ was prepared using the literature[1] procedure1 with slight modification. To a two-neck 250-mL round-bottomed flask equipped with a magnetic stir bar and reflux condenser was added trans-dibenzylideneacetone (2.4 g, 10.0 mmol, 7.0 eq), tetrabutylammonium chloride (1.2 g, 4.3 mmol, 3.0 eq), and sodium acetate (2.1 g, 25.7 mmol, 18.0 eq). Salts were dissolved in methanol and the solution was warmed to 70 ℃ and allowed to stir for 5 min. To a 50-mL pear-shaped flask was added potassium tetrachloroplatinate (593 mg, 1.4 mmol, 1.0 eq). The potassium salt was dissolved in water (4.0 mL) with mild heating. The two-neck roundbottomed flask was charged with the potassium tetrachloroplatinate solution and the reaction was

allowed to stir at 70 ℃ for 3 h. After 3 h, the reaction was cooled to ambient temperature, transferred to a 500 mL round-bottomed flask and concentrated by rotary evaporation to half the volume. The reaction mixture was filtered on a Büchner funnel; solids were washed with copious amounts of water and methanol until no yellow dibenzylideneacetone crystals were visible. The platinum catalyst was placed under the high vacuum for 24 h to remove residual methanol and water, and $Pt(dba)_3$ was obtained as a dark brown solid (572 mg, 45% yield).

Ⅲ. Synthesis of novel P-ligand L7



The preparation of 1-Bromo-4-fluoro-3,5-bis(trimethylsilyl)benzene was according to literature procedure.[2] LDA (2 M, 55 mL, 110 mmol, 2.2 eq) was added dropwise to a solution of 1-bromo-4-fluorobenzene (7.8 g, 50 mmol, 1.0 eq) in THF (70 mL) containing TMSCl (12.0 g, 110 mmol, 2.2 eq) at -70 ℃. The resultant solution was stirred for 30 min at -75 ℃ and hydrolyzed with dilute aqueous H_2SO_4. The yellow organic phase was separated, and the water phase was extracted with ether. Evaporation of the combined organic solutions left a pale-yellow oil. The oil was distilled in vacuo to give a crude product as a colorless oil. Methanol (10 mL) was added, and the solution was left to stand overnight in a -20 ℃ freezer. Crystals that

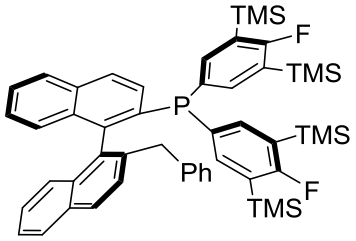
separated from the solution were filtered, washed with cold methanol, and dried to give a white crystalline material, mp 48-50 ℃. Yield: 12.5 g (78%).

Under N_2 atmosphere a heat-gun dried two-neck flask with a reflux condenser was charged with magnesium (1.6 g, 64.2 mmol, 2.5 eq) and THF (1 mL pro mmol bromide). Then the 1-Bromo-4-fluoro-3,5-bis(trimethylsilyl)benzene (20.4 g, 64.2 mmol, 2.5 eq) was added dropwise and the Grignard reagent formation started by heating with a heat gun. After the reaction had started, the reaction mixture was refluxed for four hours at 68 ℃. Under N_2 atmosphere a second heat-gun dried two-neck flask was charged with NaH (1.2 g, 30.8 mmol, 60% in mineral oil, 1.2 eq) and THF (0.5 mL pro mmol phosphite). Then this mixture was cooled in an ice bath and at 0 ℃ diethyl phosphite (3.3 mL, 25.7 mmol, 1.0 eq) was added dropwise over 15 minutes. Afterwards the reaction mixture was stirred for 30 minutes at 0 ℃ and then the freshly prepared Grignard reagent was added dropwise. After addition the mixture was stirred for 16 hours at room temperature and then quenched with saturated aqueous NH_4Cl solution (5 mL pro mmol phosphite). The aqueous layer was extracted with CH_2Cl_2 (3 × 5 mL pro mmol phosphite) and the combined organic layers were dried over Na_2SO_4. After concentration under vacuum the resulting crude product was purified by trituration with hexane/MTBE (3:1, 1 mL pro mmol phosphite) to afford the product (8.9 g, 16.4 mmol, 64%) as white solid. The synthesis of (*S*)-**B** was according to literature[3] and **L7** refered to previously reported literature.[3]

To a Schlenk flask charged with (*S*)-**B** (800 mg, 1.625 mmol, 1.0 eq), diarylphosphine oxide (1.7 g, 3.2 mmol, 2.0 eq), $Pd(OAc)_2$ (18.2 mg, 5 mol %) and DPPB (34.7 mg, 5 mol %) in DMSO (5 mL) was added DIPEA (420 mg, 3,2 mmol, 2.0 eq) under N_2. The resulting mixture was stirred at 100 ℃ for 60 h. Then the mixture was cooled to room temperature, diluted with EtOAc (20 mL), washed with water (5 mL × 3), brine (10 mL), successively. The organic phase was dried over anhydrous Na_2SO_4, filtered, concentrated, and the crude residue was filtrated through a short silica gel column and flushed with petroleum ether/ethyl acetate (3:1). The

filtrate was concentrated under reduce pressure, and a yellow solid (814 mg, 0.95 mmol, 59 % yield) was obtained and used for the next step without further purification. To a dried Schlenk flask charged with the above product (814 mg, 0.93 mmol, 1.0 eq) in dry toluene (10 mL), Et_3N (670 mg, 6.52 mmol, 7.0 eq) and $HSiCl_3$ (0.64 g, 4.65 mmol, 5.0 eq) were added successively under N_2 at 0 ℃. The resulting mixture was stirring at 100 ℃ for 18 h. After cooled to 0 ℃, diluted by Et_2O (20 mL), quenched with saturated Na_2CO_3 solution, the mixture was filtered by a short celite column, and washed with Et_2O (10 mL × 3). The filtrate was dried over anhydrous Na_2SO_4, filtered, concentrated, and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to afford the desired product 5a as a white solid (777 mg, 97 % yield).

(*R*)-(2'-benzyl-[1,1'-binaphthalen]-2-yl)bis(4-fluoro-3,5-bis(trimethylsilyl)phenyl) phosphane (L12)

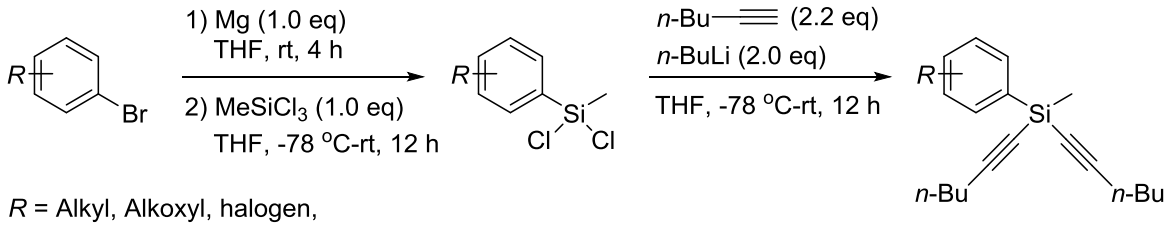


White solid. $[\alpha]_D^{25}$ =+22.586 (*c* 0.0068, $CHCl_3$, *l*=100 mm). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.5 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.51 (ddd, *J* = 8.1, 6.6, 1.3 Hz, 1H), 7.45 (dd, *J* = 8.5, 2.9 Hz, 1H), 7.38-7.31 (m, 4H), 7.25 (ddd, *J* = 8.1, 6.7, 1.3 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 1H), 7.15-7.08 (m, 5H), 6.99 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 6.87 (dd, *J* = 6.5, 2.9 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 1H), 3.61 (d, *J* = 16.5 Hz, 1H), 3.58 (d, *J* = 16.0 Hz, 1H), 0.23 (d, *J* = 2.4 Hz, 36H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5 (d, *J* = 239.0 Hz), 144.7 (d, *J* = 33.4 Hz), 143.3 (td, *J* = 21.5, 20.8, 12.0 Hz), 141.3, 139.1, 137.2 (d, *J* = 11.3 Hz), 136.3 (d, *J* = 8.1 Hz), 134.6, 134.2, 134.0 (d, *J* = 7.0 Hz), 132.9, 130.1, 130.5, 129.2, 129.1, 129.0, 128.9, 128.8, 128.4, 127.8, 127.7, 127.5, 126.7 (d, *J* = 13.8 Hz), 126.6 (d, *J* = 5.3 Hz), 126.1 (d, *J* = 2.7 Hz), 125.7 (d, *J* = 6.0 Hz), 40.7, 0.0. ^{29}Si NMR (99

MHz, $CDCl_3$) δ -4.0, -4.1, -4.2, -4.3. ^{31}P NMR (202 MHz, $CDCl_3$) δ -17.8 (t, *J* = 6.2 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -88.0, -88.2. HRMS (ESI): m/z: $[M + H]^+$ calculated for $C_{51}H_{60}F_2PSi_4$: 853.3472, Found: 853.3498.

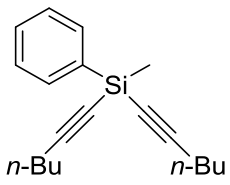
Ⅳ. Preparation of prochiral Si-linked bisakynes 1.

a) General synthesis procedure of 1a-1m.

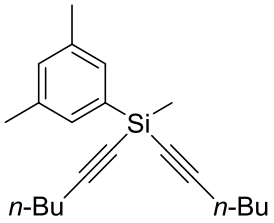


R = Alkyl, Alkoxyl, halogen,

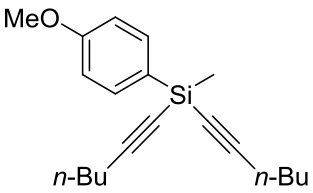
Under N_2 atmosphere a heat-gun dried two-neck flask with a reflux condenser was charged with magnesium (486 mg, 20.0 mmol, 1.0 eq) and THF. Then the Aryl halides (20.0 mmol, 1.0 eq) was added dropwise and the Grignard reagent formation started by heating with a heat gun. After the reaction had started, the reaction mixture was stirred for four hours at room temperature. Under N_2 atmosphere a Schlenk flask was charged with $MeSiCl_3$ (1.2 g, 20.0 mmol, 1.0 eq) and THF (1.0 mL pro mmol chlorosilane). Then this mixture was cooled at -78 ℃ and freshly prepared Grignard reagent (3.3 mL, 25.7 mmol, 1.0 eq) was added dropwise over 15 minutes and resultant solution was stirred for 12 h at room temperature, finally the white salt was filtered and hex-1-yn-1-yllithium was added dropwise at -78 ℃. The reaction mixture was brought to room temperature for 12h and quenched by saturated NH_4Cl. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel chromatography (petroleum ether) to afford the product.



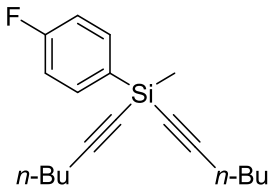
Di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a), Colorless oil, Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 6.7, 3.2 Hz, 2H), 7.38 (d, *J* = 2.4 Hz, 2H), 7.37 (d, *J* = 1.4 Hz, 1H), 2.28 (t, *J* = 7.1 Hz, 4H), 1.58-1.48 (m, 4H), 1.47-1.36 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 6H), 0.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 133.4, 129.1, 127.3, 109.5, 79.4, 29.9, 21.4, 19.2, 13.0, 0.00. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{19}H_{26}NaSi$: 305.1696, Found: 305.1709.



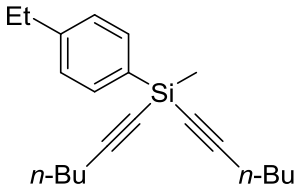
(3,5-dimethylphenyl)di(hex-1-yn-1-yl)(methyl)silane (1b), Colorless oil, Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (s, 2H), 7.00 (s, 1H), 2.32 (s, 6H), 2.26 (t, *J* = 7.0 Hz, 4H), 1.58-1.46 (m, 4H), 1.46-1.37 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 6H), 0.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 134.4, 131.1, 130.8, 109.1, 79.8, 29.9, 21.4, 20.7, 19.2, 13.0, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{21}H_{30}NaSi$: 333.2009, Found: 333.2024.



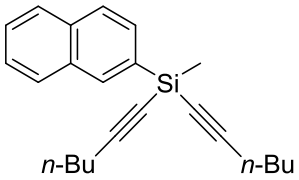
Di(hex-1-yn-1-yl)(4-methoxyphenyl)(methyl)silane (1c), Colorless oil, Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.7 Hz, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 3.78 (s, 3H), 2.27 (t, *J* = 7.1 Hz, 4H), 1.57-1.48 (m, 4H), 1.47-1.36 (m, 4H), 0.90 (t, *J* = 7.3 Hz, 6H), 0.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 134.7, 125.5, 112.9, 109.0, 79.6, 54.2, 29.8, 21.2, 19.0, 12.8, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{20}H_{28}NaOSi$: 335.1802, Found: 335.1815.



(4-fluorophenyl)di(hex-1-yn-1-yl)(methyl)silane (1d), Colorless oil, Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 8.6, 6.2 Hz, 2H), 7.07 (t, *J* = 9.0 Hz, 2H), 2.28 (t, *J* = 7.1 Hz, 4H), 1.58-1.49 (m, 4H), 1.47-1.37 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 6H), 0.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5 (d, $^{1}J_{FC}$ = 248.8 Hz, carbon of fluorine atom), 135.4 (d, $^{3}J_{FC}$ = 7.7 Hz, aromatic carbon *meta* to fluorine atom), 130.4 (d, $^{4}J_{FC}$ = 3.7 Hz, aromatic carbon *para* to fluorine atom), 114.3 (d, $^{2}J_{FC}$ = 19.9 Hz, aromatic carbon *ortho* to fluorine atom), 109.6, 79.2, 29.8, 21.3, 19.1, 12.9, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{19}H_{25}FNaSi$: 323.1602, Found: 323.1617.

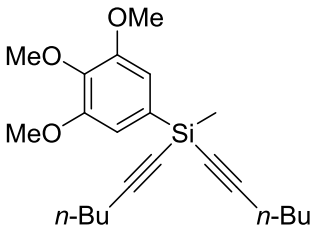


(4-ethylphenyl)di(hex-1-yn-1-yl)(methyl)silane (1e), Colorless oil, Yield: 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 2.64 (q, *J* = 7.6 Hz, 2H), 2.27 (t, *J* = 7.1 Hz, 4H), 1.63-1.48 (m, 4H), 1.46-1.36 (m, 4H), 1.23 (t, *J* = 7.6 Hz, 3H), 0.90 (t, *J* = 7.3 Hz, 6H), 0.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.2, 133.4, 131.5, 126.9, 109.2, 79.6, 29.9, 28.3, 21.3, 19.1, 14.8, 12.9, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{21}H_{30}NaSi$: 333.2193, Found: 333.2201.

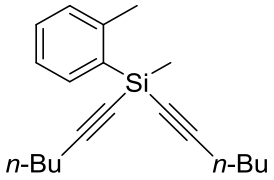


Di(hex-1-yn-1-yl)(methyl)(naphthalen-2-yl)silane (1f), Colorless oil, Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.76-7.71 (m, 2H), 7.68 (d, *J* = 7.3 Hz,

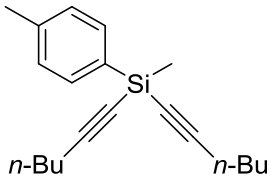
2H), 7.35 (d, *J* = 3.2 Hz, 1H), 7.33 (d, *J* = 3.4 Hz, 1H), 2.18 (t, *J* = 7.1 Hz, 4H), 1.51-1.38 (m, 4H), 1.37-1.26 (m, 4H), 0.79 (t, *J* = 7.3 Hz, 6H), 0.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.4, 133.5, 132.3, 132.2, 129.2, 127.6, 127.1, 126.6, 126.0, 125.3, 109.7, 79.5, 29.9, 21.4, 19.2, 13.0, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{23}H_{28}NaSi$: 355.1852, Found: 355.1864.



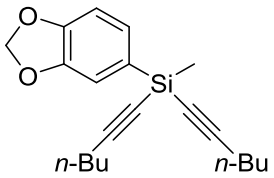
Di(hex-1-yn-1-yl)(methyl)(3,4,5-trimethoxyphenyl)silane (1g), Colorless oil, Yield: 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 2H), 3.90 (s, 6H), 3.87 (s, 3H), 2.31 (t, *J* = 7.0 Hz, 4H), 1.59-1.51 (m, 4H), 1.50-1.39 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 6H), 0.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 139.6, 130.3, 110.7, 110.16, 80.0, 60.7, 56.0, 30.4, 21.9, 19.7, 13.6, 0.7. MS (EI) m/z: 372, 357, 341, 327, 315, 299, 248.



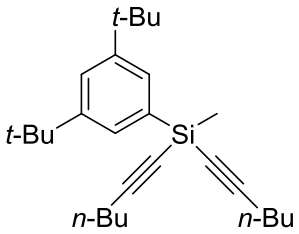
Di(hex-1-yn-1-yl)(methyl)(o-tolyl)silane (1h), Colorless oil, Yield: 77%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.27 (td, *J* = 7.5, 1.6 Hz, 1H), 7.17 (d, *J* = 7.3 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 1H), 2.60 (s, 3H), 2.24 (t, *J* = 7.1 Hz, 4H), 1.54-1.45 (m, 4H), 1.44-1.34 (m, 4H), 0.89 (t, *J* = 7.3 Hz, 6H), 0.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 134.5, 132.5, 129.4, 129.1, 124.3, 109.1, 79.9, 29.8, 21.9, 21.3, 19.1, 12.9, 0.0. MS (EI) m/z: 296, 281, 266, 251, 209, 205, 91.



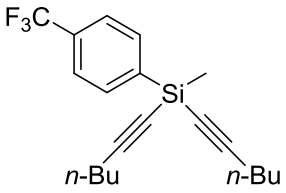
Di(hex-1-yn-1-yl)(methyl)(p-tolyl)silane (1i), Colorless oil, Yield: 79%. 1H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.8 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 2.35 (s, 3H), 2.27 (t, *J* = 7.1 Hz, 4H), 1.53 (p, *J* = 6.9 Hz, 4H), 1.42 (dq, *J* = 14.2, 7.0 Hz, 4H), 0.90 (t, *J* = 7.3 Hz, 6H), 0.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9, 133.4, 131.2, 128.0, 109.2, 79.6, 29.9, 21.3, 20.9, 19.1, 13.0, 0.00. MS (EI) m/z: 296, 281, 266, 251, 209, 205, 91.



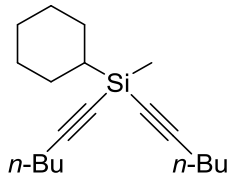
Benzo[d][1,3]dioxol-5-yldi(hex-1-yn-1-yl)(methyl)silane (1j), Colorless oil, Yield: 82%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 7.7 Hz, 1H), 7.17 (s, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 5.91 (s, 2H), 2.27 (t, *J* = 7.1 Hz, 4H), 1.57-1.48 (m, 4H), 1.47-1.36 (m, 4H), 0.90 (t, *J* = 7.3 Hz, 6H), 0.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3, 146.7, 127.6, 127.5, 112.6, 109.1, 107.8, 99.9, 79.4, 29.7, 21.2, 19.0, 12.8, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{20}H_{26}NaO_2Si$: 349.1594, Found: 349.1602.



(3,5-di-tert-butylphenyl)di(hex-1-yn-1-yl)(methyl)silane (1k), Colorless oil, Yield: 90%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 1.7 Hz, 2H), 7.48 (t, *J* = 2.1 Hz, 1H), 2.29 (t, *J* = 6.9 Hz, 4H), 1.59-1.49 (m, 4H), 1.48-1.40 (m, 4H), 1.35 (s, 18H), 0.91 (t, *J* = 7.2 Hz, 6H), 0.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.8, 133.2, 127.2, 123.0, 108.7, 79.6, 34.0, 30.6, 29.6, 21.0, 18.9, 12.7, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{27}H_{42}NaSi$: 417.2948, Found: 417.2950.

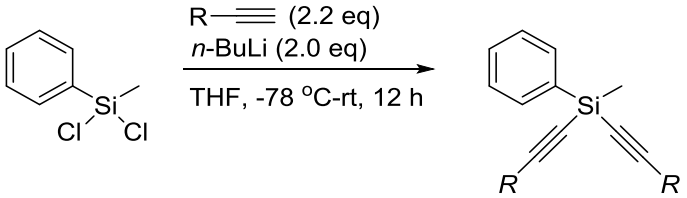


Di(hex-1-yn-1-yl)(methyl)(4-(trifluoromethyl)phenyl)silane (1l), Colorless oil, Yield: 65%. 1H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 1H), 2.29 (t, *J* = 7.1 Hz, 2H), 1.60-1.49 (m, 3H), 1.47-1.37 (m, 3H), 0.91 (t, *J* = 7.3 Hz, 3H), 0.52 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 134.0, 131.3 (d, $^2J_{FC}$ = 32.2 Hz, aromatic carbon bearing CF_3 group), 123.9 (q, $^1J_{FC}$=273.6 Hz, carbon of CF_3 group), 124.0 (d, $^3J_{FC}$ = 3.7 Hz, aromatic carbon *ortho* to CF_3 group), 110.5, 78.9, 30.1, 21.6, 19.4, 13.2, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{20}H_{25}F_3NaSi$: 373.1570, Found: 373.1572.



Cyclohexyldi(hex-1-yn-1-yl)(methyl)silane (1m), Colorless oil, Yield: 52%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.05 (t, *J* = 7.0 Hz, 4H), 1.66-1.50 (m, 5H), 1.38-1.28 (m, 4H), 1.27-1.18 (m, 4H), 1.11-0.97 (m, 5H), 0.73 (t, *J* = 7.3 Hz, 6H), 0.58-0.46 (m, 1H), 0.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 108.6, 80.0, 30.6, 27.7, 26.9, 26.8, 25.9, 21.8, 19.6, 13.5, -3.01. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{19}H_{32}NaSi$: 311.2165, Found: 311.2180.

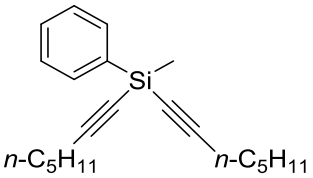
b) General synthesis procedure of 1n-1q.



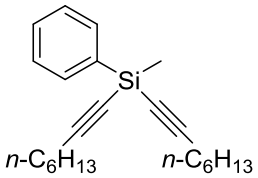
R = Alkyl, phenyl

To a solution of terminal alkyne in THF was added dropwise *n*-BuLi under nitrogen atmosphere at -78 ℃. The reaction mixture was be stirred for 30 min at

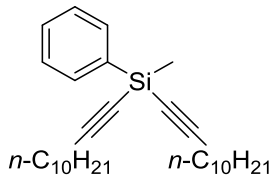
-78 ℃, then the $MePhSiCl_2$ was added dropwise into the above reaction mixture. The reaction mixture was brought to room temperature for 12 h and quenched by saturated NH_4Cl. The aqueous layer was extracted with diethyl ether, and the organic layer was washed with brine and dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel chromatography (petroleum ether) to afford the product.



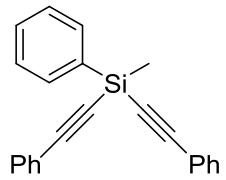
Di(hept-1-yn-1-yl)(methyl)(phenyl)silane (1n), Colorless oil, Yield: 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.36 (d, *J* = 2.2 Hz, 2H), 7.35 (d, *J* = 1.3 Hz, 1H), 2.32-2.18 (m, 4H), 1.65-1.47 (m, 4H), 1.44-1.24 (m, 8H), 0.89 (t, *J* = 7.3 Hz, 6H), 0.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 133.3, 129.0, 127.2, 109.4, 79.5, 30.5, 27.5, 21.6, 19.4, 13.4, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{21}H_{30}NaSi$: 333.2009, Found: 333.2011.



Methyldi(oct-1-yn-1-yl)(phenyl)silane (1o), Colorless oil, Yield: 99%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.36 (d, *J* = 2.1 Hz, 1H), 7.35 (d, *J* = 1.8 Hz, 1H), 2.26 (t, *J* = 7.1 Hz, 4H), 1.63-1.48 (m, 4H), 1.44-1.34 (m, 4H), 1.33-1.20 (m, 8H), 0.88 (t, *J* = 7.0 Hz, 6H), 0.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 133.4, 129.0, 127.2, 109.5, 79.5, 30.7, 27.9, 27.8, 22.0, 19.5, 13.4, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{23}H_{34}NaSi$: 361.2322, Found: 361.2337.

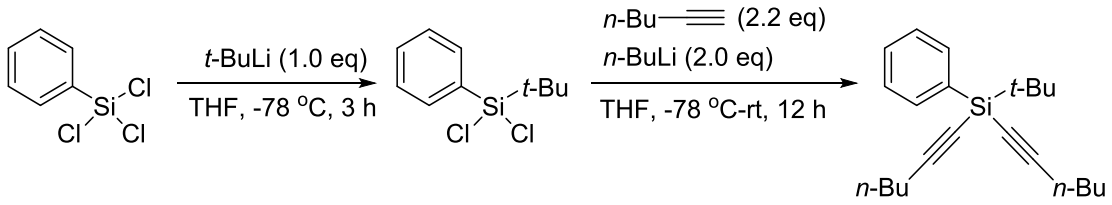


Di(dodec-1-yn-1-yl)(methyl)(phenyl)silane (1p), Colorless oil, Yield: 92%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.35 (d, *J* = 2.2 Hz, 1H), 7.34 (d, *J* = 1.4 Hz, 1H), 2.25 (t, *J* = 7.1 Hz, 3H), 1.59-1.47 (m, 2H), 1.43-1.34 (m, 2H), 1.33-1.20 (m, 24H), 0.88 (t, *J* = 6.8 Hz, 6H), 0.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 133.4, 129.0, 127.2, 109.4, 79.5, 31.4, 29.0, 29.0, 28.8, 28.6, 28.3, 27.9, 22.2, 19.5, 13.5, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{31}H_{50}NaSi$: 473.3574, Found: 473.3579.



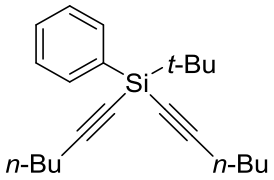
Methyl(phenyl)bis(phenylethynyl)silane (1q), Colorless oil, Yield: 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 6.4, 3.0 Hz, 2H), 7.53 (d, *J* = 2.2 Hz, 2H), 7.51 (d, *J* = 2.2 Hz, 2H), 7.45-7.39 (m, 3H), 7.39-7.21 (m, 6H), 0.72 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.0, 132.0, 129.9, 128.9, 128.0, 127.9, 122.3, 107.3, 88.9, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{23}H_{18}NaSi$: 345.1070, Found: 345.1075.

c) Synthesis of procedure of 1r



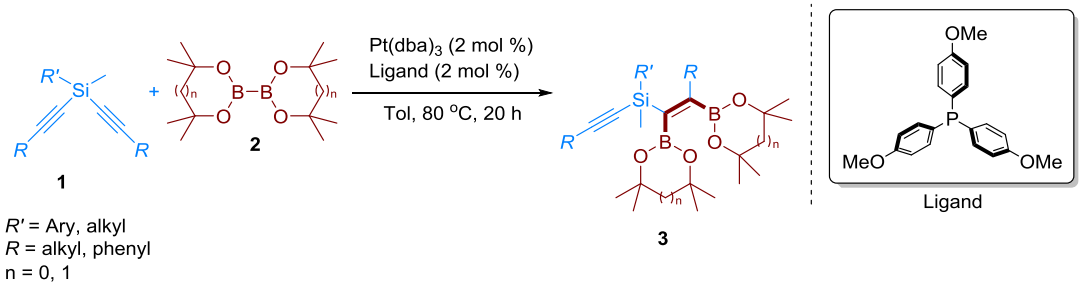
To a solution of $MeSiCl_3$ (1.5 g, 10.0 mmol, 1.0 eq) in THF (20 mL) was added dropwise *t*-BuLi (6.25 mL, 1.6 M in Hex, 1.0 eq) under nitrogen atmosphere at -78 ℃, then the reaction mixture was be stirred for 3 hours at the same temperature, finally

the white salt was filtered and hex-1-yn-1-yllithium was added dropwise at -78 ℃. The reaction mixture was brought to room temperature for 12h and quenched by saturated NH_4Cl (20 mL) was added. The aqueous layer was extracted with diethyl ether (3 x 20 mL), and the organic layer was washed with brine (20 mL), dried over $NaSO_4$, and concentrated under reduced pressure. Silica gel fresh column chromatography (petroleum ether) gave **1r** (2.5 g, 7.7 mmol, 77%) as colorless oil.



Tert-butyldi(hex-1-yn-1-yl)(phenyl)silane (1r), Colorless oil, Yield: 77%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 7.2, 2.0 Hz, 2H), 7.42-7.29 (m, 3H), 2.31 (t, *J* = 6.9 Hz, 4H), 1.60-1.51 (m, 4H), 1.51-1.41 (m, 4H), 0.99 (s, 9H), 0.92 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.1, 133.1, 129.6, 127.5, 110.5, 78.1, 30.6, 25.9, 22.0, 19.8, 18.1, 13.6. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{22}H_{32}NaSi$: 347.2165, Found: 347.2181.

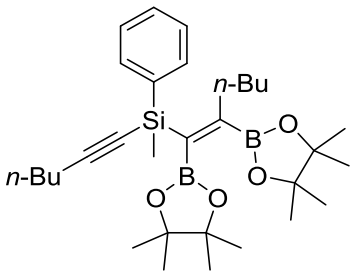
Ⅴ. General procedure for Pt(0)-catalyzed diboration of Si-linked bisalkynes (1) with Bis(pinacolato)diboron (2a)



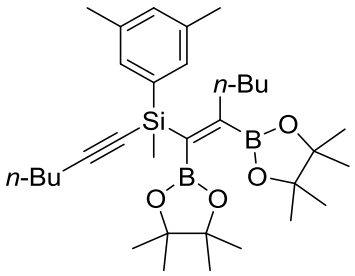
R′ = Ary, alkyl
R = alkyl, phenyl
n = 0, 1

To the $Pt(dba)_3$ (2.7 mg, 0.002 mmol, 2 mol %) catalysis in anhydrous Toluene (0.5 mL), Ligand (0.7 mg, 0.002 mmol, 2 mol %) was added. The mixture was stirred at room temperature for 30 minutes, then di(hex-1-yn-1-yl)(methyl)(phenyl)silane and derivates **1** (0.1 mmol, 1.0 eq) and Bis(pinacolato)diboron and derivates **2a** (0.12

mmol, 1.2 eq) was added. The reaction was allowed to proceed for 20h at 80 ℃ in a 25 mL of sealed tube. The reaction was dilute with Et_2O and the mixture was filterted through Celite. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel chromatography (petroleum ether: ethyl acetate= 50:1) to afford the product.

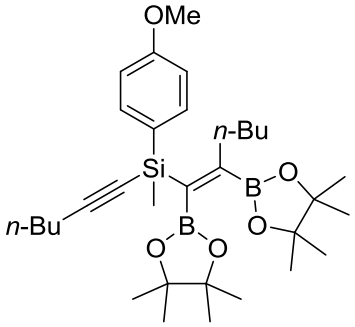


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(phenyl)silane (3a), Colorless oil, Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 6.1, 3.0 Hz, 2H), 7.31 (d, *J* = 2.3 Hz, 2H), 7.30 (d, *J* = 1.4 Hz, 1H), 2.43 (t, *J* = 7.4 Hz, 2H), 2.25 (t, *J* = 7.0 Hz, 2H), 1.56-1.47 (m, 2H), 1.45-1.37 (m, 2H), 1.27 (s, 12H), 1.22 (s, 6H), 1.19-1.10 (m, 10H), 0.90 (t, *J* = 7.2 Hz, 3H), 0.75 (t, J = 6.8 Hz, 3H), 0.54 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 134.1, 128.2, 126.8, 108.9, 83.0, 82.7, 82.0, 38.4, 31.0, 30.0, 24.8, 24.8, 24.2, 24.2, 22.4, 21.4, 19.3, 13.4, 13.0, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{31}H_{50}B_2NaO_4Si$: 559.3568, Found: 559.3567.

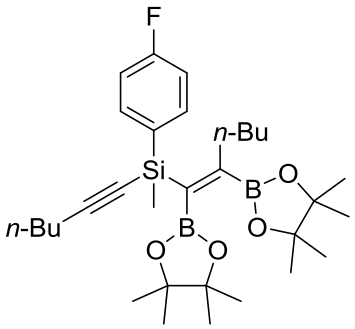


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(3,5-dimethylphenyl)(hex-1-yn-1-yl)(methyl)silane (3b), Colorless oil, Yield: 89%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 2H), 6.87 (s, 1H), 2.37 (t, *J* = 7.5 Hz, 2H), 2.21 (s, 6H), 2.17 (t, *J* = 8.0 Hz, 3H), 1.48-1.40 (m, 2H), 1.39-1.30 (m, 2H), 1.22-1.05 (m, 28H),

0.83 (t, *J* = 7.1 Hz, 3H), 0.70 (t, *J* = 6.8 Hz, 3H), 0.46 (s, 3H). 13C NMR (101 MHz, $CDCl_3$) δ 136.3, 135.3, 131.3, 129.3, 108.2, 82.4, 82.0, 81.7, 37.8, 30.5, 29.3, 24.2, 24.1, 23.6, 21.8, 20.7, 20.1, 18.7, 12.8, 12.4, -0.7. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{33}H_{54}B_2NaO_4Si$: 587.3882, Found: 587.3891.

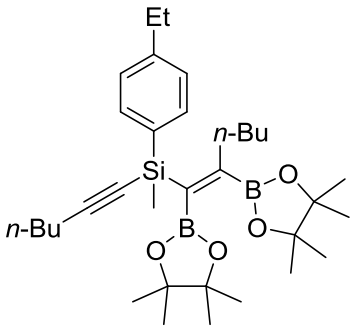


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(4-methoxyphenyl)(methyl)silane (3c), Colorless oil, Yield: 90%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 6.8 Hz, 2H), 6.78 (d, *J* = 6.9 Hz, 2H), 3.69 (s, 3H), 2.35 (t, *J* = 7.3 Hz, 2H), 2.16 (t, *J* = 6.9 Hz, 2H), 1.49-1.36 (m, 2H), 1.38-1.28 (m, 2H), 1.18 (s, 12H), 1.14 (s, 6H), 1.13-1.03 (m, 10H), 0.82 (t, *J* = 7.1 Hz, 3H), 0.69 (t, *J* = 6.7 Hz, 3H), 0.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 135.3, 128.1, 112.4, 108.4, 82.7, 82.4, 82.1, 54.1, 38.0, 30.8, 29.7, 24.6, 24.5, 24.0, 23.9, 22.2, 21.1, 19.0, 13.1, 12.7, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{32}H_{52}B_2NaO_5Si$: 589.3674, Found: 589.3691.

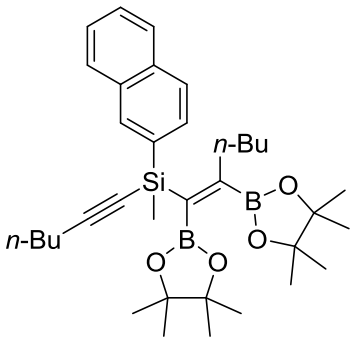


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(4-fluorophenyl)(hex-1-yn-1-yl)(methyl)silane (3d), Colorless oil, Yield: 90%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.7, 5.7 Hz, 2H), 6.92 (t, *J* = 8.2 Hz, 2H), 2.35 (t, *J* = 7.5

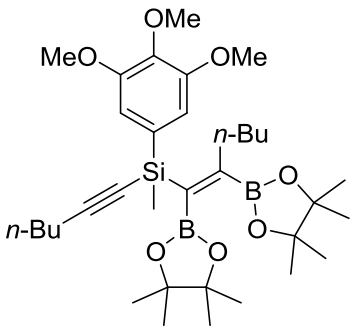
Hz, 2H), 2.17 (t, *J* = 7.1 Hz, 2H), 1.49-1.37 (m, 2H), 1.40-1.26 (m, 2H), 1.19 (s, 12H), 1.15 (s, 6H), 1.12-1.02 (m, 10H), 0.82 (t, *J* = 7.3 Hz, 3H), 0.69 (t, *J* = 7.0 Hz, 3H), 0.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9 (d, $^{1}J_{FC}$ = 247.5 Hz, carbon of fluorine atom), 135.9 (d, $^{3}J_{FC}$ = 7.4 Hz, aromatic carbon *meta* to fluorine atom), 132.9 (d, $^{4}J_{FC}$ = 3.6 Hz, aromatic carbon *para* to fluorine atom), 113.7 (d, $^{2}J_{FC}$ = 19.6 Hz, aromatic carbon *ortho* to fluorine atom), 109.0, 82.9, 82.6, 81.7, 38.2, 30.8, 29.8, 24.6, 24.6, 24.0, 24.0, 22.2, 21.2, 19.0, 13.1, 12.8, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{32}H_{52}B_2NaO_5Si$: 589.3674, Found: 589.3691.



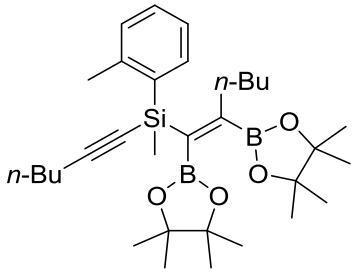
(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(4-ethylphenyl)(hex-1-yn-1-yl)(methyl)silane (3e), Colorless oil, Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.8 Hz, 2H), 7.06 (d, *J* = 7.7 Hz, 2H), 2.53 (q, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 7.6 Hz, 2H), 2.16 (t, *J* = 6.9 Hz, 2H), 1.47-1.38 (m, 2H), 1.37-1.29 (m, 2H)., 1.18 (s, 12H), 1.14-1.06 (m, 16H), 0.82 (t, *J* = 7.3 Hz, 3H), 0.68 (t, *J* = 7.1 Hz, 3H), 0.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.3, 134.2, 134.0, 126.4, 108.6, 82.9, 82.6, 82.2, 38.3, 31.0, 30.0, 28.3, 24.8, 24.7, 24.2, 24.2, 22.4, 21.3, 19.2, 15.0, 13.4, 12.9, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{33}H_{54}B_2NaO_4Si$: 587.3882, Found: 587.3896.



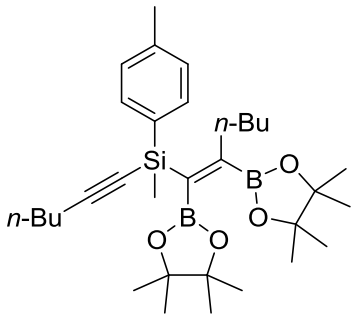
(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(naphthalen-2-yl)silane (3f), Colorless oil, Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.78-7.71 (m, 1H), 7.72-7.66 (m, 3H), 7.35 (d, *J* = 2.9 Hz, 1H), 7.34 (d, *J* = 3.5 Hz, 1H), 2.38 (t, *J* = 7.6 Hz, 2H), 2.20 (t, *J* = 6.9 Hz, 2H), 1.51-1.39 (m, 2H), 1.41-1.29 (m, 2H), 1.17 (s, 12H), 1.10 (s, 6H), 1.08-0.94 (m, 10H), 0.83 (t, *J* = 7.1 Hz, 3H), 0.57 (t, *J* = 6.9 Hz, 3H), 0.54 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.0, 134.6, 133.1, 132.2, 130.4, 127.5, 126.9, 125.9, 125.4, 124.8, 109.1, 82.9, 82.7, 82.0, 38.4, 30.9, 29.9, 24.7, 24.6, 24.2, 24.1, 22., 21.2, 19.2, 13.2, 12.9, 0.0. MS (EI) m/z: 586, 502, 487, 459, 445, 361, 127.



(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(3,4,5-trimethoxyphenyl)silane (3g), Colorless oil, Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (s, 2H), 3.79 (s, 6H), 3.76 (s, 3H), 2.42 (t, *J* = 7.9 Hz, 2H), 2.19 (t, *J* = 6.8 Hz, 2H), 1.50-1.38 (m, 2H), 1.41-1.31 (m, 2H), 1.25-1.13 (m, 16H), 1.09 (s, 6H), 1.05 (s, 6H), 0.82 (t, *J* = 7.1 Hz, 3H), 0.75 (t, *J* = 7.1 Hz, 3H), 0.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 138.3, 132.2, 111.1, 109.1, 83.0, 82.7, 82.0, 60.0, 55.4, 38.3, 31.2, 30.0, 24.8, 24.7, 24.2, 24.2, 22.5, 21.4, 19.2, 13.4, 13.0, 0.0. MS (EI) m/z: 626, 611, 569, 527, 459, 443, 167.

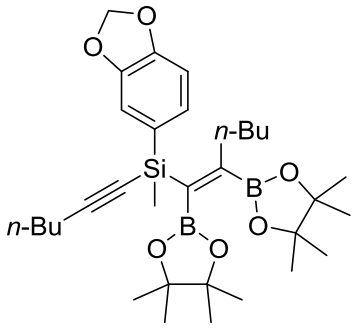


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(o-tolyl)silane (3h), Colorless oil, Yield: 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.14 (td, *J* = 8.1, 7.5, 1.6 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 2.42 (s, 3H), 2.32-2.26 (m, 2H), 2.14 (t, *J* = 7.0 Hz, 2H), 1.46-1.37 (m, 2H), 1.37-1.27 (m, 2H), 1.18 (s, 12H), 1.12 (s, 6H), 1.10 (s, 6H), 1.05-0.90 (m, 4H), 0.80 (t, *J* = 7.2 Hz, 3H), 0.63 (t, *J* = 7.1 Hz, 3H), 0.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 135.8, 134.7, 128.8, 128.6, 124.1, 108.6, 83.0, 82.7, 82.6, 38.1, 31.1, 29.9, 24.84, 24.7, 24.2, 24.2, 23.0, 22.4, 21.4, 19.4, 13.4, 13.0, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{32}H_{52}B_2NaO_4Si$: 573.3725, Found: 573.3739.

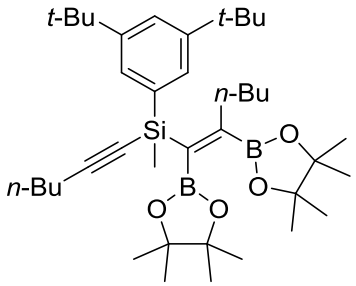


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(p-tolyl)silane (3i), Colorless oil, Yield: 90%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.3 Hz, 2H), 7.13 (d, *J* = 7.5 Hz, 2H), 2.41 (t, *J* = 7.6 Hz, 2H), 2.32 (s, 3H), 2.24 (t, *J* = 7.0 Hz, 2H), 1.56-1.45 (m, 2H), 1.45-1.35 (m, 2H), 1.26 (s, 12H), 1.23 (s, 6H), 1.21-1.12 (m, 10H), 0.90 (t, *J* = 7.0 Hz, 3H), 0.75 (t, *J* = 6.6 Hz, 3H), 0.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.9, 134.0, 133.7, 127.5, 108.8, 82.9, 82.6, 82.0, 38.3, 30.9, 29.9, 24.7, 24.7, 24.1, 24.1, 22.4, 21.3, 20.8, 19.2, 13.3,

12.9, 0.0. MS (EI) m/z: 550, 535, 451, 367, 352, 337, 91.

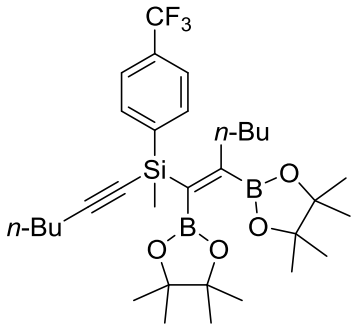


(*Z*)-benzo[d][1,3]dioxol-5-yl(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)silane (3j), Colorless oil, Yield: 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.14 (m, 2H), 6.81 (d, *J* = 7.4 Hz, 1H), 2.42 (t, *J* = 7.1 Hz, 2H), 2.24 (t, *J* = 6.9 Hz, 2H), 1.55-1.46 (m, 2H), 1.46-1.35 (m, 2H), 1.27 (s, 12H), 1.24 (s, 6H), 1.23-1.14 (m, 10H), 0.90 (t, *J* = 7.0 Hz, 3H), 0.78 (t, *J* = 6.5 Hz, 3H), 0.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 145.6, 129.6, 127.5, 112.9, 108.2, 106.8, 99.0, 82.3, 82.0, 81.2, 37.7, 30.3, 29.21, 24.1, 24.1, 23.5, 23.5, 21.7, 20.7, 18.5, 12.7, 12.3, 0.5. HRMS (ESI): m/z: [M + Na]+ calculated for $C_{32}H_{50}B_2NaO_6Si$: 603.3467, Found: 603.3483.

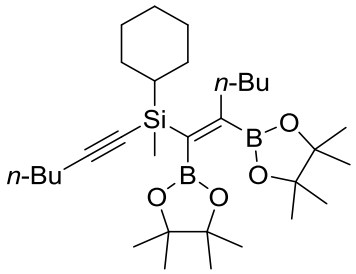


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(3,5-di-tert-butylphenyl)(hex-1-yn-1-yl)(methyl)silane (3k), Colorless oil, Yield: 81%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 2H), 7.39 (s, 1H), 2.53-2.42 (m, 2H), 2.25 (t, *J* = 6.7 Hz, 2H), 1.55-1.46 (m, 2H), 1.46-1.38 (m, 2H), 1.31 (s, 18H), 1.26 (s, 12H), 1.19-1.10 (m, 16H), 0.89 (t, *J* = 6.8 Hz, 3H), 0.76 (t, *J* = 7.0 Hz, 3H), 0.57 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.8, 134.3, 127.1, 121.7, 107.0, 81.5, 81.2, 81.1, 36.9, 32.8, 29.5, 28.6, 23.4, 23.4, 22.8, 22.8, 21.0, 20.0, 17.9, 12.0, 11.6, -1.5. HRMS (ESI):

m/z: [M + Na]+ calculated for $C_{39}H_{66}B_2NaO_4Si$: 671.4822, Found: 671.4838.

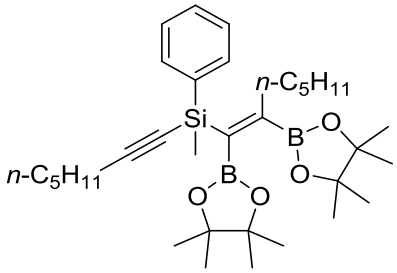


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(4-(trifluoromethyl)phenyl)silane (3l), Colorless oil, Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 7.8 Hz, 2H), 2.41 (t, *J* = 7.5 Hz, 2H), 2.26 (t, *J* = 7.1 Hz, 2H), 1.58-1.47 (m, 2H), 1.46-1.37 (m, 2H), 1.27 (s, 12H), 1.23 (s, 6H), 1.19 (s, 6H), 1.15-1.08 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 3H), 0.74 (t, *J* = 6.8 Hz, 3H), 0.55 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 134.5, 130.3 (d, $^2J_{FC}$ = 29.1 Hz, aromatic carbon bearing CF_3 group), 23.9 (q, $^1J_{FC}$=273.6 Hz, carbon of CF_3 group), 123.48 (d, $^3J_{FC}$ = 3.9 Hz, aromatic carbon *ortho* to CF_3 group), 109.9, 83.3, 83.0, 81.3, 38.8, 31.1, 30.0, 24.9, 24.9, 24.4, 24.4, 22.6, 21.5, 19.4, 13.5, 13.1, 0.0. HRMS (ESI): m/z: $[M + Na]^+$ calculated for $C_{32}H_{49}B_2F_3NaO_4Si$: 627.3442, Found: 627.3420.

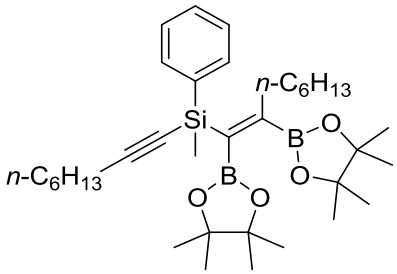


(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(cyclohexyl)(hex-1-yn-1-yl)(methyl)silane (3m), Colorless oil, Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.50-2.41 (m, 2H), 2.16 (t, *J* = 6.8 Hz, 2H), 1.84-1.61 (m, 5H), 1.50-1.20 (m, 38H), 0.87 (t, *J* = 7.0 Hz, 6H), 0.20 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 110.6, 85.8, 85.5, 85.5, 41.3, 34.5, 33.0, 30.5, 30.5, 30.1, 29.7, 29.3, 28.7, 27.8, 27.8, 27.2, 25.5, 24.3, 22.1, 16.5, 15.9, 0.0. HRMS (ESI): m/z: [M + Na]+ calculated for

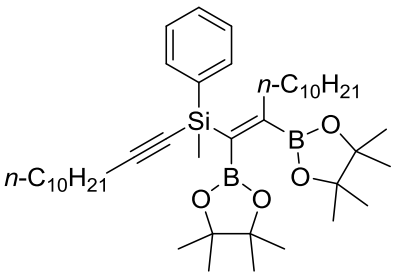
$C_{31}H_{56}B_2NaO_4Si$: 565.4037, Found: 565.4047.



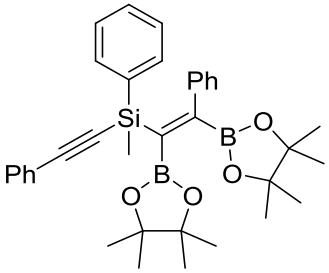
(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hept-1-en-1-yl)(hept-1-yn-1-yl)(methyl)(phenyl)silane (3n), Colorless oil, Yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 6.5, 3.2 Hz, 2H), 7.22 (d, *J* = 2.7 Hz, 2H), 7.21 (d, *J* = 1.3 Hz, 1H), 2.35 (t, *J* = 8.0 Hz, 2H), 2.15 (t, *J* = 7.1 Hz, 2H), 1.45 (p, *J* = 7.0 Hz, 2H), 1.33-1.01 (m, 34H), 0.81 (t, *J* = 7.1 Hz, 3H), 0.71 (t, *J* = 7.0 Hz, 3H), 0.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 134.1, 128.2, 126.8, 108.9, 83.0, 82.7, 82.0, 38.6, 31.5, 30.5, 28.5, 27.6, 24.8, 24.8, 24.2, 24.2, 21.94, 21.6, 19.5, 13.4, 0.0. HRMS (ESI): m/z: [M + Na]+ calculated for C33H54B2NaO4Si: 587.3882, Found: 587.3895.



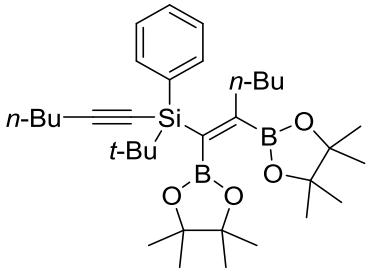
(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oct-1-en-1-yl)(methyl)(oct-1-yn-1-yl)(phenyl)silane (3o), Colorless oil, Yield: 84%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.22 (d, *J* = 2.5 Hz, 2H), 7.21 (d, *J* = 1.3 Hz, 1H), 2.34 (t, *J* = 7.8 Hz, 2H), 2.16 (t, *J* = 7.1 Hz, 2H), 1.49-1.39 (m, 2H), 1.36-1.27 (m, 2H), 1.25-1.06 (m, 32H), 0.81 (t, *J* = 6.9 Hz, 3H), 0.75 (t, *J* = 7.2 Hz, 3H), 0.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 134.1, 128.2, 126.8, 108.9, 83.0, 82.7, 82.0, 38.7, 31.2, 30.7, 29.0, 28.8, 28.0, 27.9, 24.8, 24.8, 24.2, 24.2, 22.0, 21.9, 19.6, 13.5, 13.4, 0.0. MS (EI) m/z: 592, 577, 535, 507, 478, 422, 338.



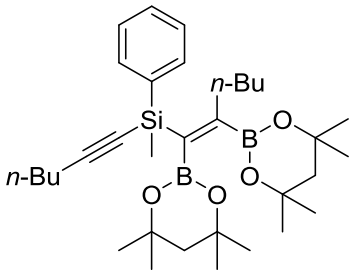
(Z)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)dodec-1-en-1-yl)(dodec-1-yn-1-yl)(methyl)(phenyl)silane (3p), Colorless oil, Yield: 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 6.3, 3.1 Hz, 2H), 7.23 (d, *J* = 2.4 Hz, 2H), 7.22 (d, *J* = 1.4 Hz, 1H), 2.33 (t, *J* = 8.2 Hz, 2H), 2.16 (t, *J* = 7.1 Hz, 2H), 1.51-1.39 (m, 2H), 1.36-1.27 (m, 2H), 1.24-1.02 (m, 56H), 0.81 (t, *J* = 6.8 Hz, 6H), 0.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6, 134.1, 128.1, 126.8, 108.9, 83.0, 82.7, 82.1, 38.7, 31.3, 29.4, 29.0, 29.0, 28.9, 28.85, 28.75, 28.7, 28.6, 28.3, 27.9, 24.82, 24.75, 24.2, 24.2, 22.1, 19.6, 13.5, 0.0.



(*Z*)-methyl(phenyl)(2-phenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) vinyl)(phenylethynyl)silane (3q), Colorless oil, Yield: 43%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 5.5 Hz, 2H), 7.39 (t, *J* = 6.0, 1.2 Hz, 2H), 7.25-7.15 (m, 11H), 0.96 (s, 6H), 0.93 (s, 6H), 0.79 (s, 12H), -0.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 137.0, 134.1, 131.3, 128.2, 127.6, 127.3, 127.0, 126.85, 126.77, 125.7, 122.9, 105.9, 93.4, 83.1, 82.7, 24.3, 24.2, 24.0, 23.8, -0.7. HRMS (ESI): m/z: [M + Na]+ calculated for $C_{35}H_{42}B_2NaO_4Si$: 599.2943, Found: 599.2955.



(*Z*)-(1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hex-1-en-1-yl)(tert-butyl)(hex-1-yn-1-yl)(phenyl)silane (3r), Colorless oil, Yield: 55%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 6.7, 2.5 Hz, 2H), 7.27 (d, *J* = 1.9 Hz, 2H), 7.26 (d, *J* = 2.3 Hz, 1H), 2.51-2.32 (m, 2H), 2.24 (t, *J* = 6.9 Hz, 2H), 1.57-1.46 (m, 2H), 1.46-1.36 (m, 2H), 1.27 (s, 12H), 1.26 (s, 6H), 1.19 (s, 6H), 1.14 (s, 9H), 1.06-0.94 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H), 0.67 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 135.8, 128.4, 127.0, 109.4, 83.5, 83.3, 82.7, 43.8, 40.2, 31.3, 30.7, 27.9, 26.2, 25.6, 25.2, 25.0, 24.9, 23.0, 22.0, 19.9, 19.1, 13.6. HRMS (ESI): m/z: [M + Na]+ calculated for $C_{34}H_{56}B_2NaO_4Si$: 601.4038, Found: 601.4025.



(Z)-(1,2-bis(4,4,6,6-tetramethyl-1,3,2-dioxaborinan-2-yl)hex-1-en-1-yl)(hex-1-yn-1-yl)(methyl)(phenyl)silane (3s), Colorless oil, Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (t, *J* = 3.6, 1.2 Hz, 2H), 7.31-7.28 (m, 3H), 2.38 (d, *J* = 7.7 Hz, 2H), 2.24 (t, *J* = 7.0 Hz, 2H), 1.78 (s, 2H), 1.71 (s, 2H), 1.60-1.47 (m, 2H), 1.46-1.37 (m, 2H), 1.34 (s, 12H), 1.33 (s, 6H), 1.30 (s, 6H), 1.22-1.07 (m, 4H), 0.90 (t, *J* = 7.3 Hz, 3H), 0.75 (t, *J* = 7.1 Hz, 3H), 0.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 132.6, 126.4, 125.1, 68.5, 68.4, 46.9, 46.1, 36.7, 29.8, 29.7, 29.7, 29.6, 28.5, 21.0, 19.9, 17.8, 11.8, 11.5, -1.2. MS (EI) m/z: 564, 549, 521, 492, 394, 296, 77.

Reference

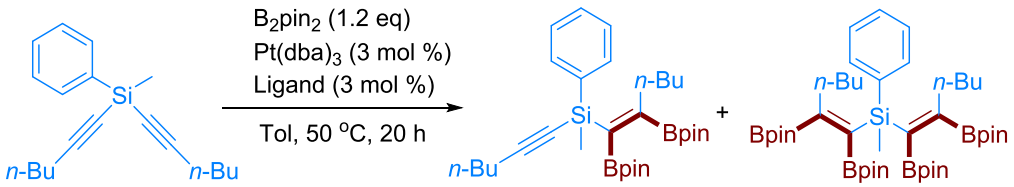
[1]. L. T. Kilman, S. N. Mlynarski, J. P. Morken, *J. Am. Chem. Soc*. **2009**, 131, 13210-13211.

[2]. L. Sergiusz, S. Janusz, *J. Org. Chem*. **2003**, 68, 9384-9388.

[3]. F. Li, Z-J. Zheng, L-W. Xu, *Chem. Asian J*. **2012**, 7, 2008–2013.

[4]. L-S. Zheng, L. Li, K-F. Yang, Z-J. Zheng, X-Q. Xiao, L-W. Xu, *Tetrahedron*. **2013**, 69, 8777-8784.

Table S1. Screening of phosphine ligands for Pt(0)-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pinacolato)diboron (2a) in Toluene.[a]

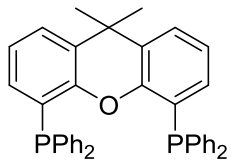


1a **3a** **4a**

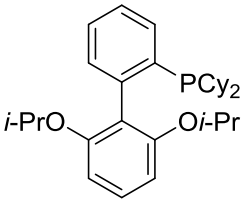
Entry	Ligand of Scheme S1	**3a**/**4a**	Yield(%)[b]	*Z*/*E*[c]
1	**XantPhos**	-	n.r	-
2	**RuPhos**	-	n.r	-
3	***t*-Bu$_3$P ·HBF$_4$**	-	n.r	-
4	**JohnPhos**	-	n.r	-
5	**XPhos**	-	n.r	-
6	**DPEPhos**	-	n.r	-
7	**Cy$_3$P ·HBF$_4$**	-	n.r	-
8	**SPhos**	-	n.r	-
9	**PPh$_3$**	>99:1	78	97/3
10	**L1**	-	n.r	-
11	**L2**	>99:1	72	98/2
12	**L3**	>99:1	83	99/1

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Platinum complex (3 mol %), Ligand shown in Scheme S1(3 mol %), Solvent (1 mL). Reaction time is 20 hours for every case. n.r. is no reaction. [b]The yield was determined by GC. [c]Determined by GC.

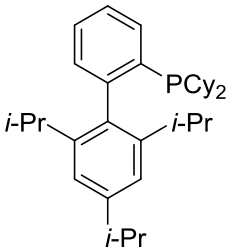
Scheme S1. The ligands evaluated in Pt(0)-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pin-acolato)diboron (2a).



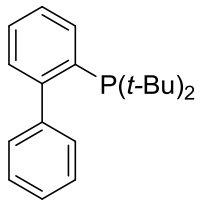
XantPhos



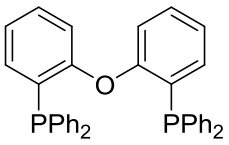
RuPhos



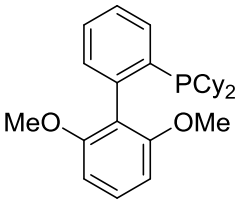
XPhos



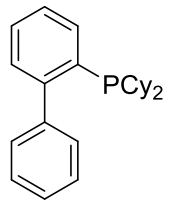
JohnPhos



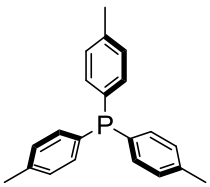
DPEPhos



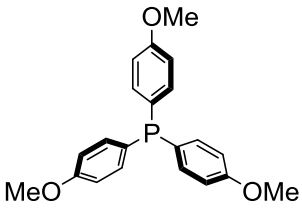
SPhos



L1

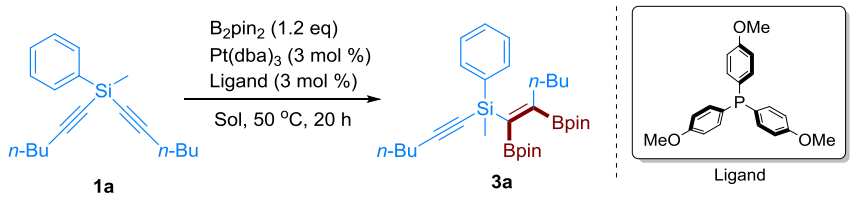


L2



L3

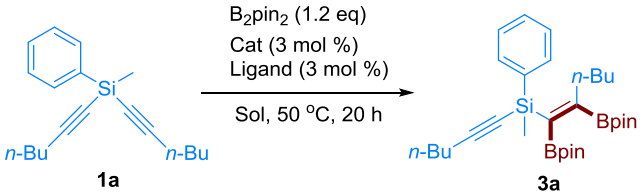
Table S2. Screening of Solvent for Pt(0)-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with Bis(pi-nacolato)di boron (2a) in toluene.[a]



Entry	Solvent	Yield(%)[b]	*Z*/*E*[c]
1	EA	63	99/1
2	DCM	n.r	-
3	THF	32	99/1
4	Et_2O	n.r	-
6	DME	43	99/1
7	CH_3CN	trace	-
8	EtOH	n.r	-
9	Hex	n.r	-

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Platinum complex (3 mol %), Ligand (3 mol %), Solvent (1 mL). Reaction time is 20 hours for every case. n.r. is no reaction. [b]The yield was determined by GC. [c]Determined by GC.

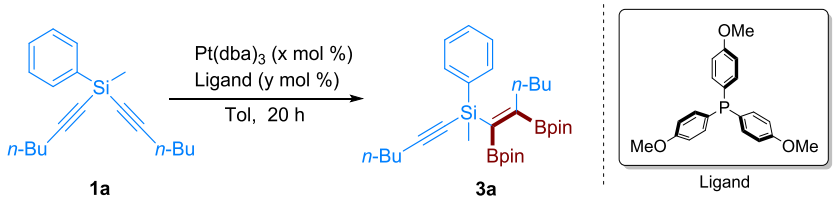
Table S3. Screening of catalysts for Pt(0)-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pi-nacolato)diboron (2a) in toluene.[a]



Entry	Metal salt	Ligand	Solvent	Yield (%)[b]	*Z*/*E*[c]
1	CuCl (10 mol %)	XantPhos (10 mol %)	MeOH	n.r	-
2	CuCl (10 mol %)	DPPP (10 mol %)	EtOH	n.r	-
3	CuCl (10 mol %)	DPPP (10 mol %)	Tol	n.r	-
4	$Cu(OAc)_2$ (10 mol %)	PCy_3	Tol	n.r	-
5	$Pt_2(dba)_3$ (3 mol %)	PPh_3	Tol	75	90/10
6	$Pt(dba)_3$ (3 mol %)	PPh_3	Tol	78	97/3
7	$[Rh(COD)Cl]_2$	PPh_3	Tol	n.r	-
8	$Pd_2(dba)_3$	PPh_3	Tol	n.r	-
9	$[Pd(\eta^3\text{-}C3H5)Cl]_2$	PPh_3	Tol	n.r	-
10	$[Ir(COD)Cl]_2$	PPh_3	Tol	n.r	-
11	[Ru(*p*-cymene)Cl]$_2$	PPh_3	Tol	n.r	-

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), catalysts (3 mol %), Ligand (3 mol %), Solvent (1 mL). Reaction time is 20 hours for every case. n.r. is no reaction. [b]The yield was determined by GC. [c]Determined by GC.

Table S4. Optimization for Pt(0)-catalyzed diboration of di-(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pi-nacola-to)diboron (2a) in toluene.[a]

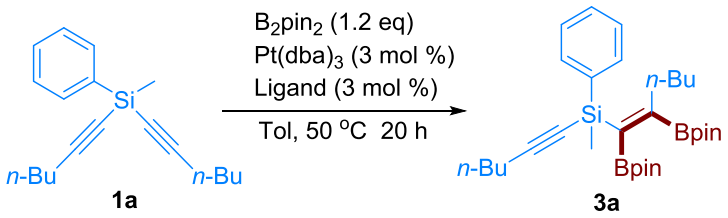


1a 3a Ligand

Entry	x/y	Concentration(M)	T (^{o}C)	Yield of 5a (%)[b]	*Z*/*E*[c]
1	3/3	0.1	60	73	99/1
2	3/3	0.1	80	91	98/2
3	3/3	0.1	100	90	97/3
4	3/3	0.5	80	93	97/3
5	3/3	1	80	55	97/3
6	3/3	0.05	80	90	97/3
7	2/2	0.5	80	95(88)[d]	>99/1
8	1/1	0.5	80	88	>99/1
9	0.5/0.5	0.5	80	70	97/3

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Reaction time is 20 hours for every case. n.r. is no reaction. [b]The yield was determined by GC. [c]Determined by GC. [d]The isolated yield in brackets.

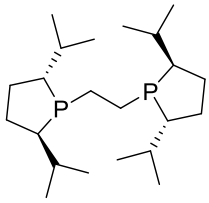
Table S5. Screening of chiral ligands for Pt(0)-catalyzed diborati on of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pinac-o lato)diboron (2a) in toluene.[a]



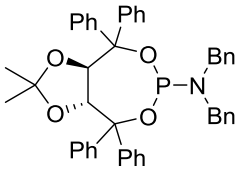
Entry	Ligand of Scheme S2	Yield (%)[b]	er (%)[c]	*Z*/*E*[d]
1	**(*R*)-FeiPhos**	-	-	
2	**(*R*)-DTBM-SegPhos**	-	-	
3	**(*S*)-DIOP**	-	-	
4	**(*S*)-BINAP**	-	-	
5	**(*2S, 5S*)-MeDuPhos**	-	-	
6	**(*R*)-DIPAMP**	-	-	
7	**(*R*)-BDPP**	-	-	
8	**L1**	-	-	
9	**L2**	-	-	
10	**L3**	-	-	
11	**L4**	57	50/50	95/5
12	**L5**	-	-	
13	**L6**	-	-	
14	**L7**	-	-	
15	**L8**	-	-	
16	**L9**	-	-	
17	**L10**	-	-	

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Platinum complex (3 mol %), Ligand shown in Scheme S2 (3 mol %), Toluene (1 mL). Reaction time is 20 hours for every case. [b]The yield was determined by GC. [c]Determined by HPLC. [d]Determined by GC.

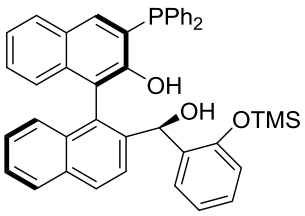
Scheme S2. The chiral ligands evaluated in Pt(0)-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pinacolato)diboron (2a).



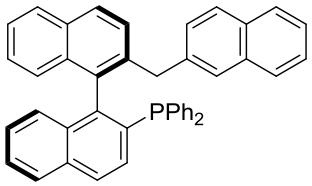
L1 (*R*, *R*)



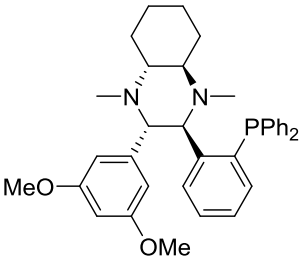
L2 (*R*, *R*)



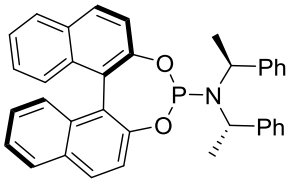
L3 (*R, S*)



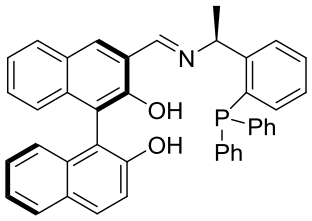
L4 (*R*)



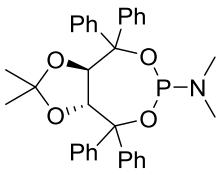
L5 (*R, R*)



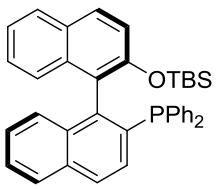
L6 (*R, S, S*)



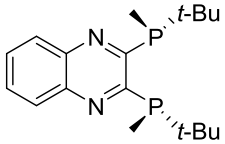
L7 (*R, S*)



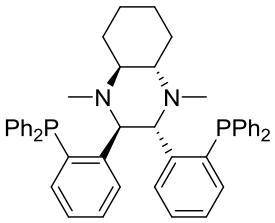
L8 (*R, R*)



L9 (*R*)

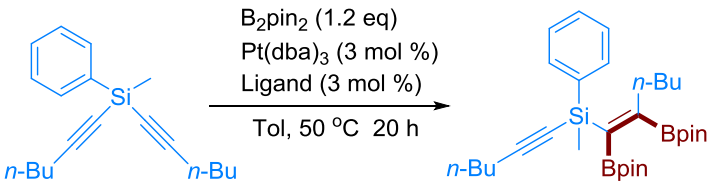


L10



(*R*)-**FeiPhos**

Table S6. Screening of chiral ligands for Pt(0)-catalyzed diborati on of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pinacol ato)diboron (2a) in toluene.[a]



1a **3a**

Entry	Ligand of Scheme S3	Yield (%)[b]	er (%)[c]		*Z*/*E*[d]
			Z	*E*	
1	**L1**	n.r	-		-
2	**L2**	n.r	-		-
3	**L3**	n.r	-		-
4	**L4**	n.r	-		-
5	**L5**	n.r	-		-
6	**L6**	66	50/50	53/47	93/7
7	**L7**	73	50/50	66/34	68/32
8	**L8**	32	55.5/44.5	64/36	84/16
9	**L9**	20	53/47	56/44	91/9
10	**L10**	76	54/46	61/39	94/6
11	**L11**	n.r	-		-
12	**L12**	46	50/50	59/41	84/16
13	**L13**	n.r	-		-
14	**L14**	42	56/44	42/58	88/12
15	**L15**	trace	-		-
16	**L16**	n.r	-		-

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Platinum complex (3 mol %), Ligand shown in Scheme S3 (3 mol %), Toluene (1 mL). Reaction time is 20 hours for every case. n.r. is no reaction. [b]The yield was determined by GC. [c]Determined by HPLC. [d]Determined by GC.

Scheme S3. The chiral ligands evaluated in Pt(0)-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pin-acolato)diboron (2a).

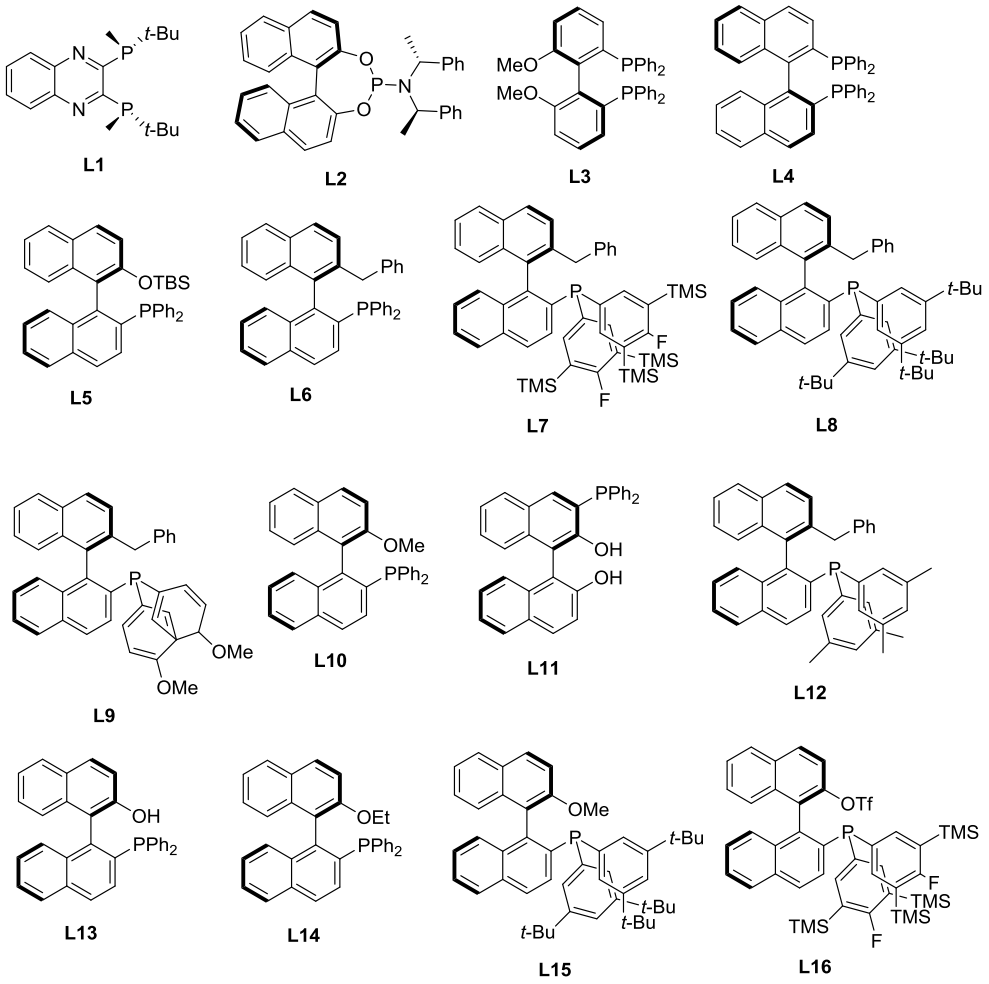
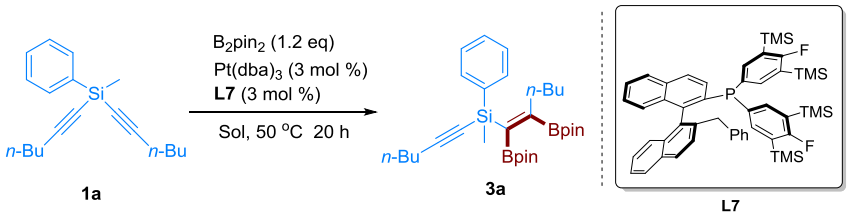


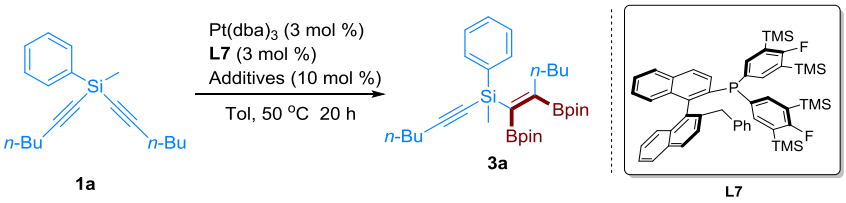
Table S7. Screening of solvent for Pt(0)/L7-catalyzed diboration of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with bis(pinacolato) diboron (2a) in toluene.[a]



Entry	Solvent	Yield (%)[b]	ee (%)[c]	*Z*/*E*[d]
1	THF	45	race/38	66/34
2	Et_2O	92	race/38	59/41
2-2	Et_2O (rt)	82	3/38	55/45
2-3	Et_2O (-20 °C)	n.r	-	-
3	DCM	<5	-	-
4	DCE	n.r	-	-
5	Dioxane	51	4/35	68/32
6	EtOH	22	-	65/35
7	MeCN	n.r	-	-
8	Hex	90	race/37	63/37
9	*i*-PrOH	67	10/40	73/27
10	Hex/*i*-PrOH (1:1)	82	race/40	68/32
11	Cyclohexane	83	race/36	68/32
12	MTBE	93	race/38	60/40
13	Benzene	64	race/38	67/33
14	$PhCF_3$	43	6/50	65/35
15	EA	84	nd/42	60/40
16	Hexafluorobenzene	72	race/44	53/47
17	2,2-Difluoroethanol	n.r	-	-
18	Octafluorotoluene	85	race/30	53/47
19	Hexafluoroisopropanol	n.r	-	-
20	2,2,2-Trifluoroethanol	n.r	-	-
21	DMF	n.r	-	-

[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Platinum complex (3 mol %), Ligand (3 mol %), Solvent (1 mL). Reaction time is 20 hours for every case. [b]The yield was determined by GC. [c]Determined by HPLC. [d]Determined by GC.

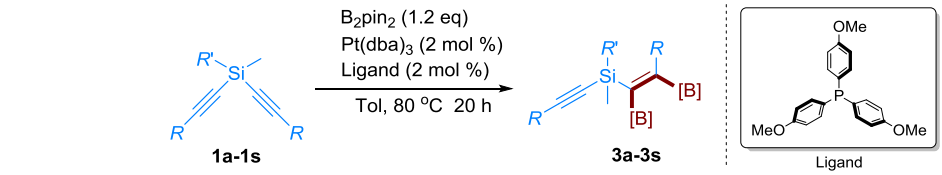
Table S8. Screening of additives for Pt(0)/L7-catalyzed diborati on of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) with Bis(pinacol ato)diboron (2a) in toluene.[a]

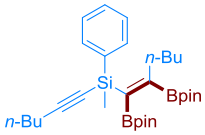


Entry	Additives	Yield (%)[b]	ee (%)[c]	*Z*/*E*[d]
1	$NaBAr_4$ (Ar=3,5-Bis(trifluoromethyl)phenyl)	-	-	-
2	2,2',4'-Trichloroacetophenone	93	race/40	45/55
3	$NaPF_6$	40	race/35	31/69
4	$PhB(OH)_2$	95	race/47	44/56
5	$NaBF_4$	92	race/46	45/55
6	NaF	76	race/34	35/65
7	$NaOOCCF_3$	71	race/34	35/65
8	$NaBH_3CN$	-	-	-
9	tris(pentafluorophenyl)borane	-	-	-
10	$Cu(BF_4)_2$ $6H_2O$	-	-	-

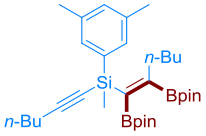
[a]Unless otherwise noted, the reaction conditions were as follows: Di(hex-1-yn-1-yl)(methyl)(phenyl)silane **1a** (0.1 mmol), Bis(pinacolato)diboron **2a** (0.12 mmol), Platinum complex (3 mol %), Ligand (3 mol %), Toluene (1 mL). Reaction time is 20 hours for every case. [b]The yield was determined by GC. [c] Determined by HPLC. [d]Determined by GC.

Scheme S4. Substrate scope for Pt(0)-catalyzed diboration of Si-bisakynes 1 with bis(pinacolato)diboron (2a).

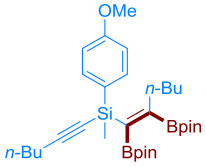




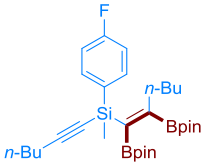
3a
88% yield



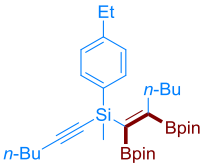
3b
89% yield



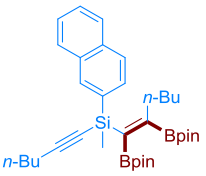
3c
90% yield



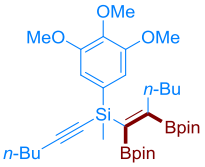
3d
84% yield



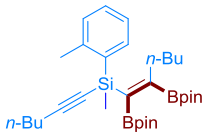
3e
88% yield



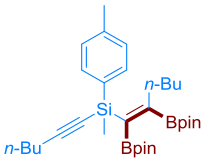
3f
80% yield



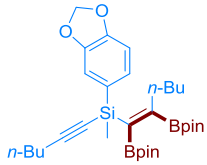
3g
76% yield



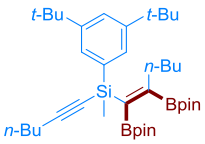
3h
90% yield



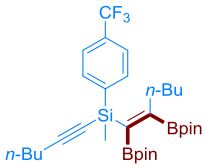
3i
86% yield



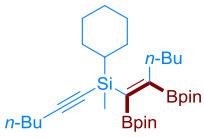
3j
85% yield



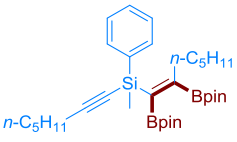
3k
81% yield



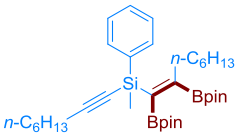
3l
76% yield



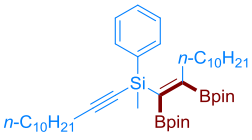
3m
70% yield



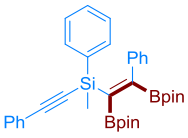
3n
81% yield



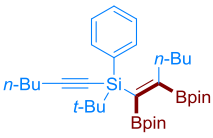
3o
84% yield



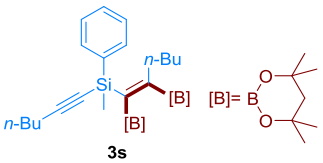
3p
88% yield



3q
43% yield

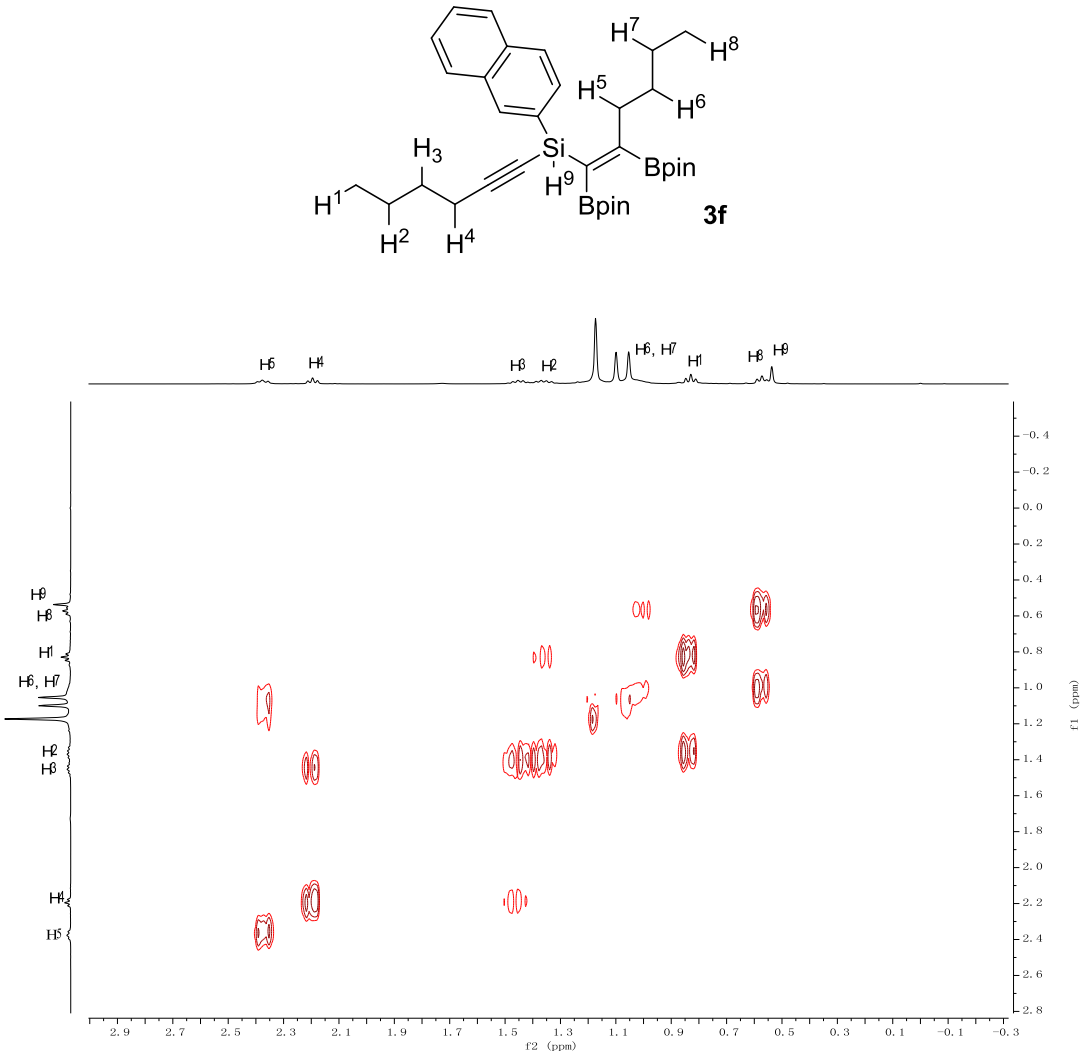


3r
55% yield

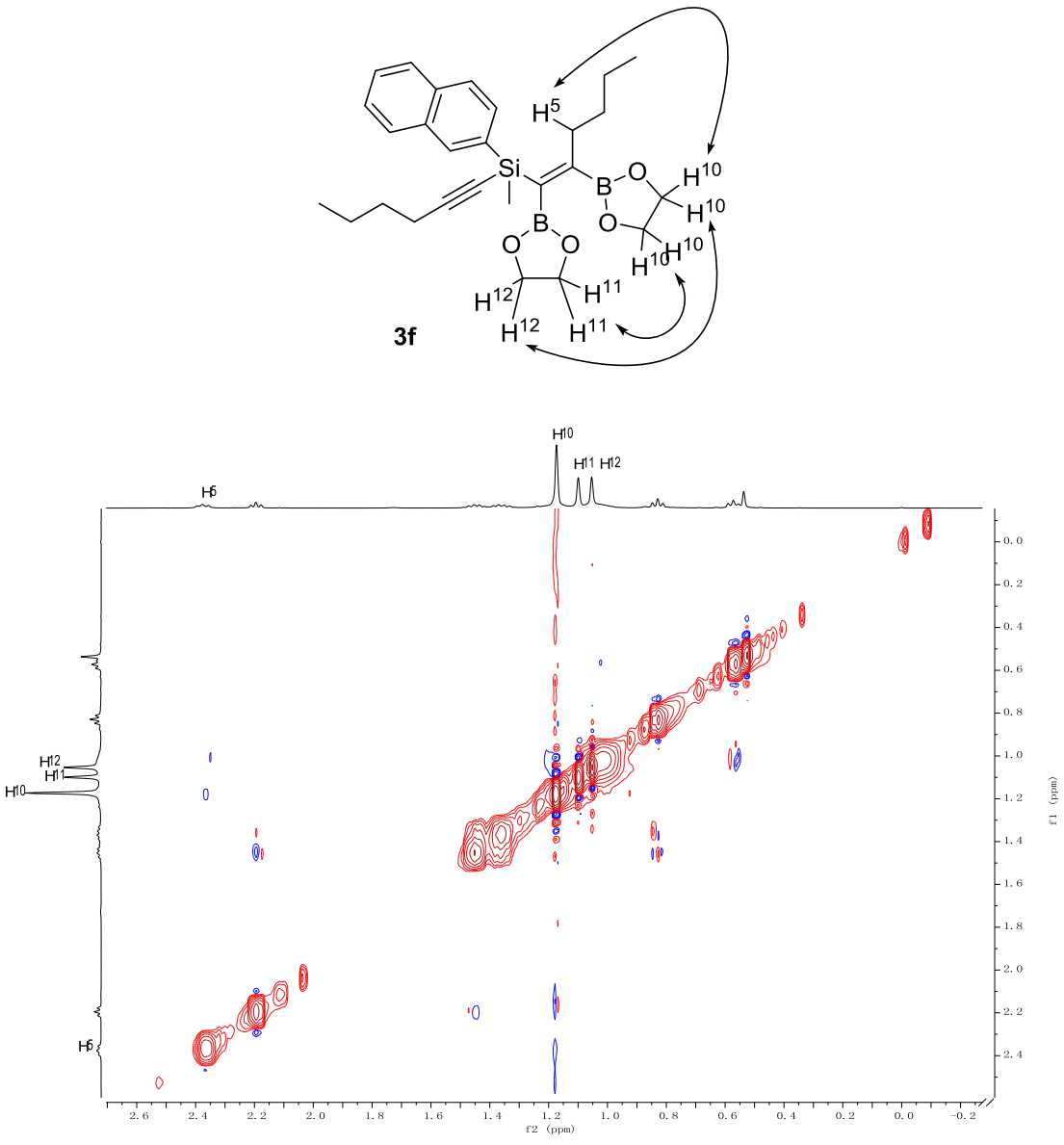


3s
65% yield

The COSY and NOESY spectra of 3f



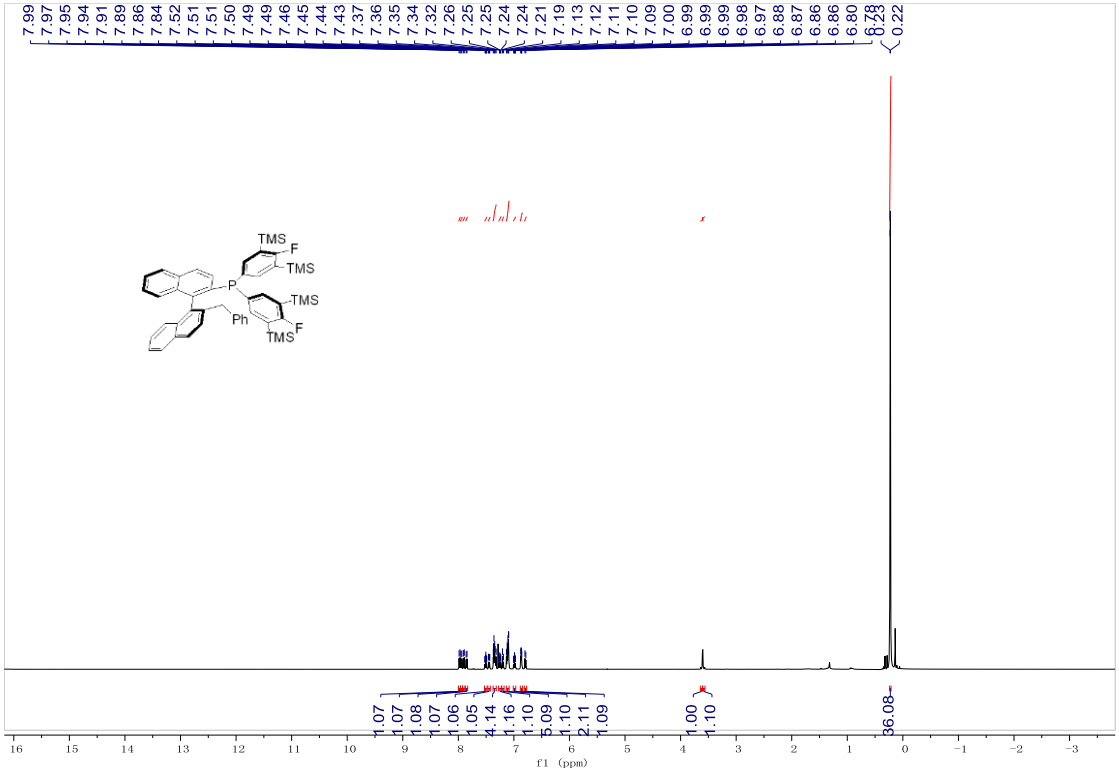
COSY spectra of **3f**



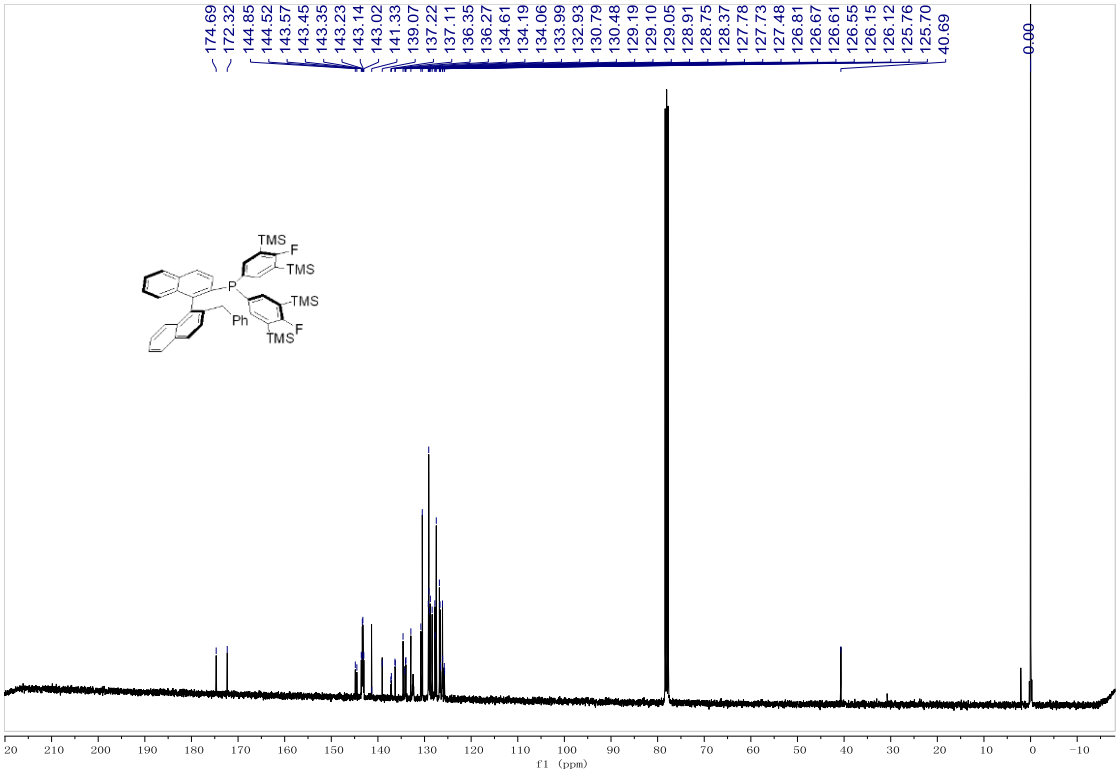
NOESY spectra of **3f**

NMR Spectra

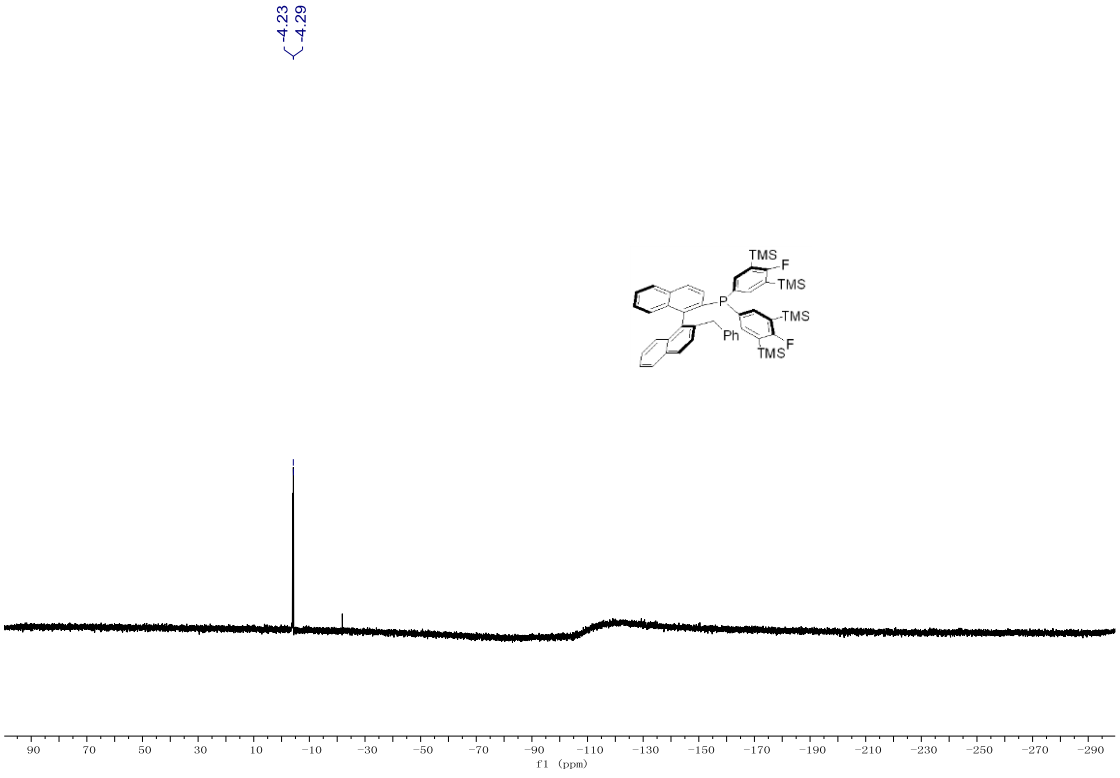
^{1}H NMR of **L12**



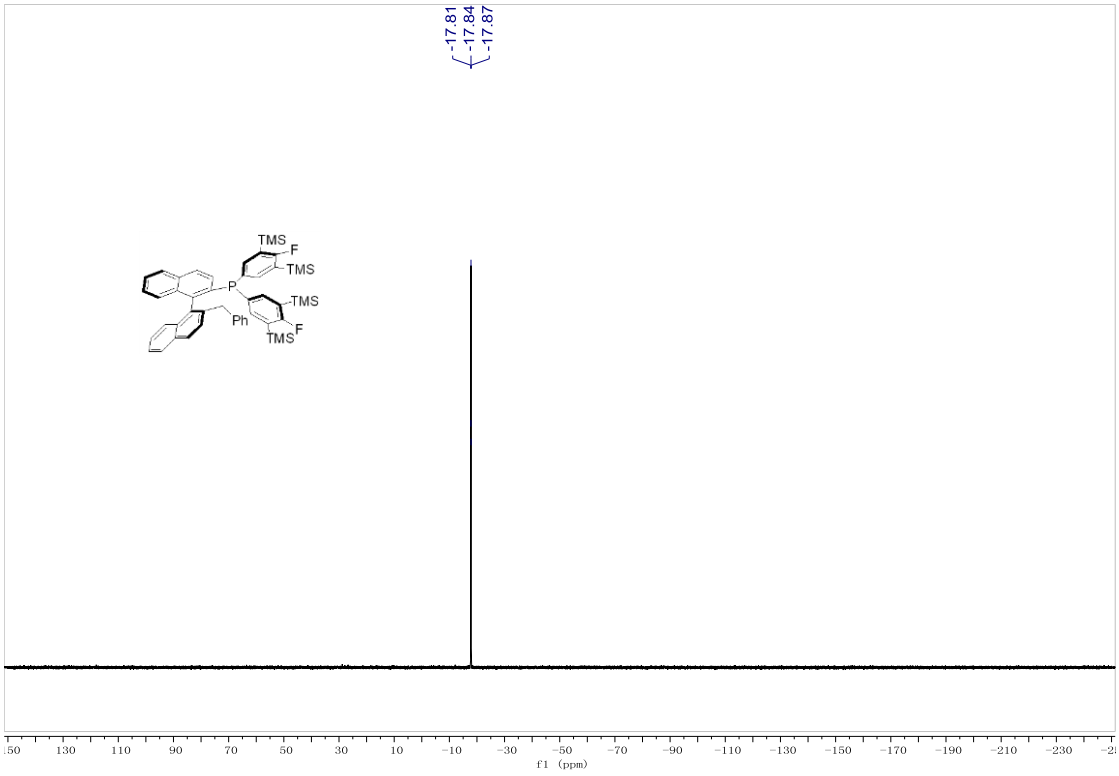
^{13}C NMR of **L12**



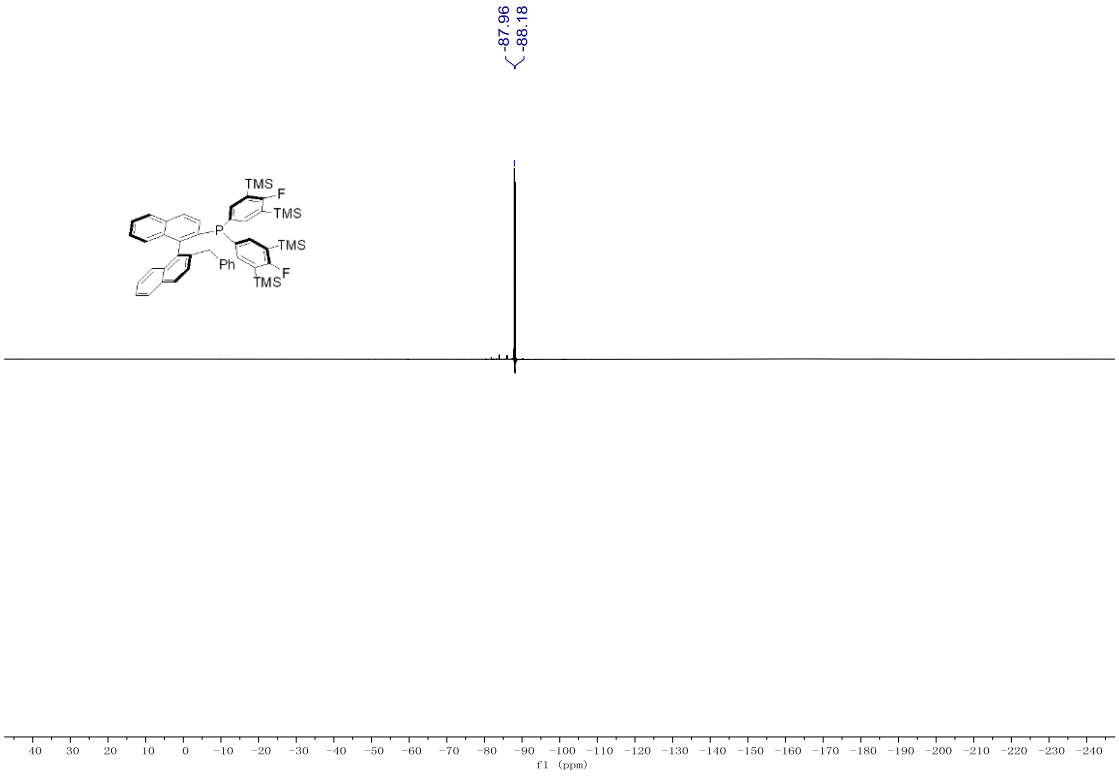
^{29}Si NMR of **L12**



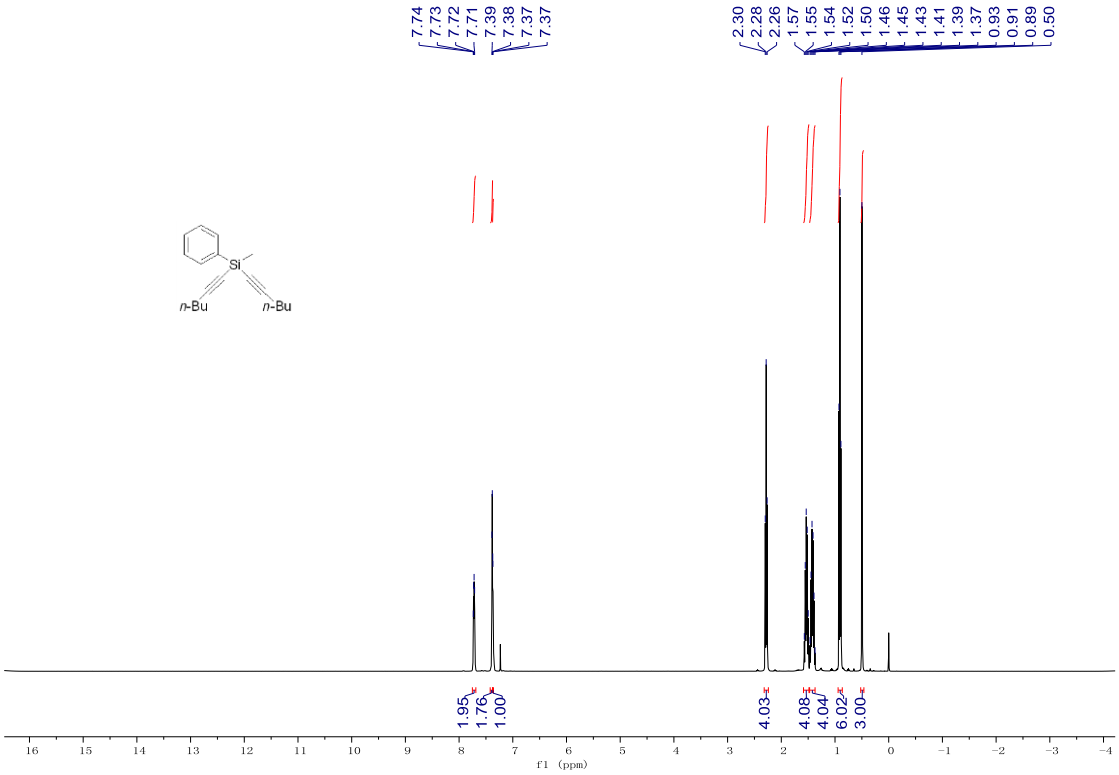
^{31}P NMR of **L12**



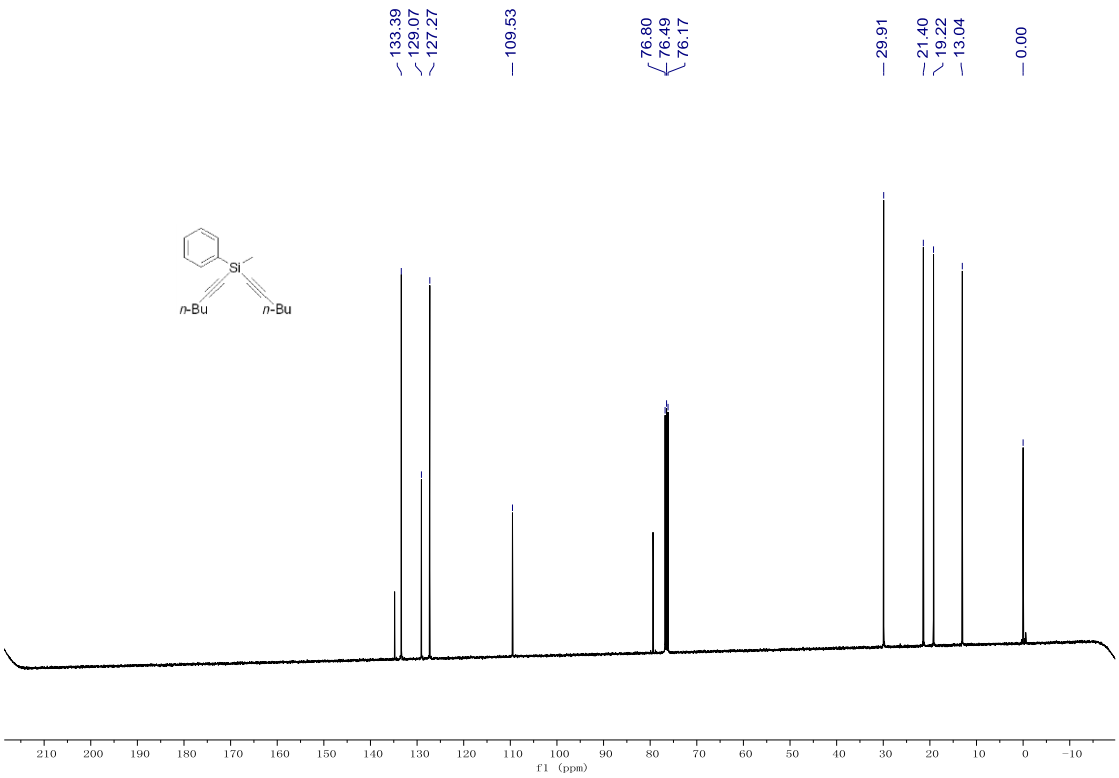
^{19}F NMR of **L12**



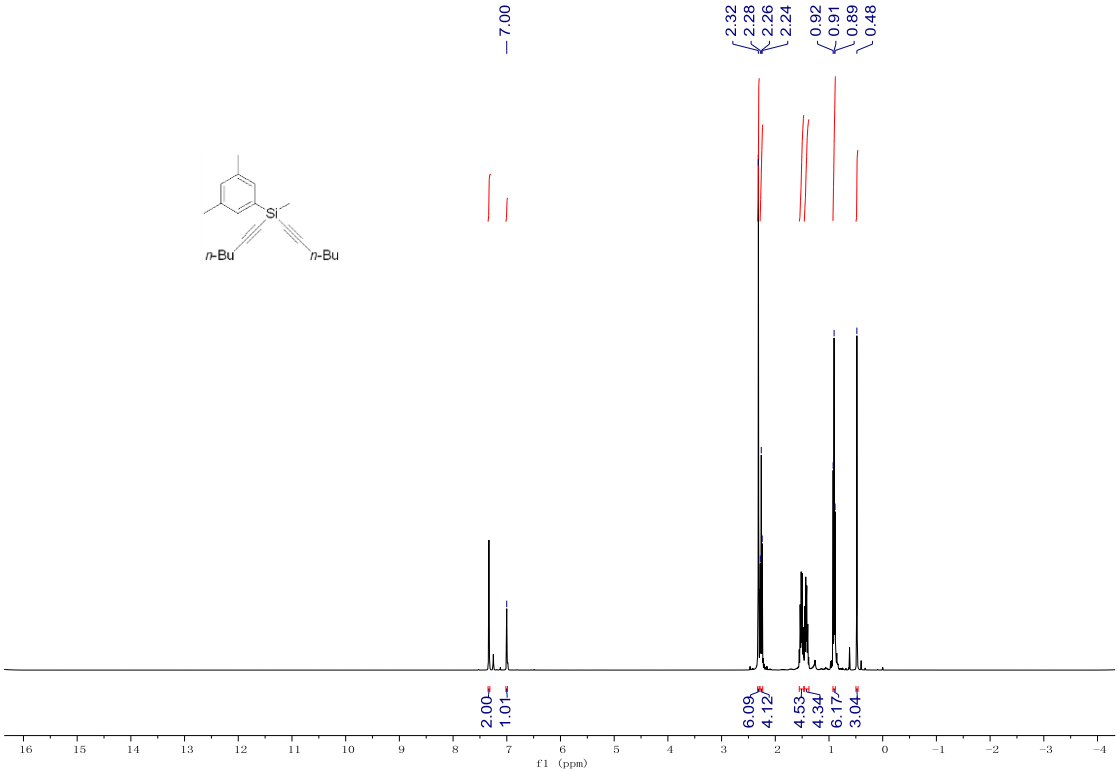
^{1}H NMR of **1a**



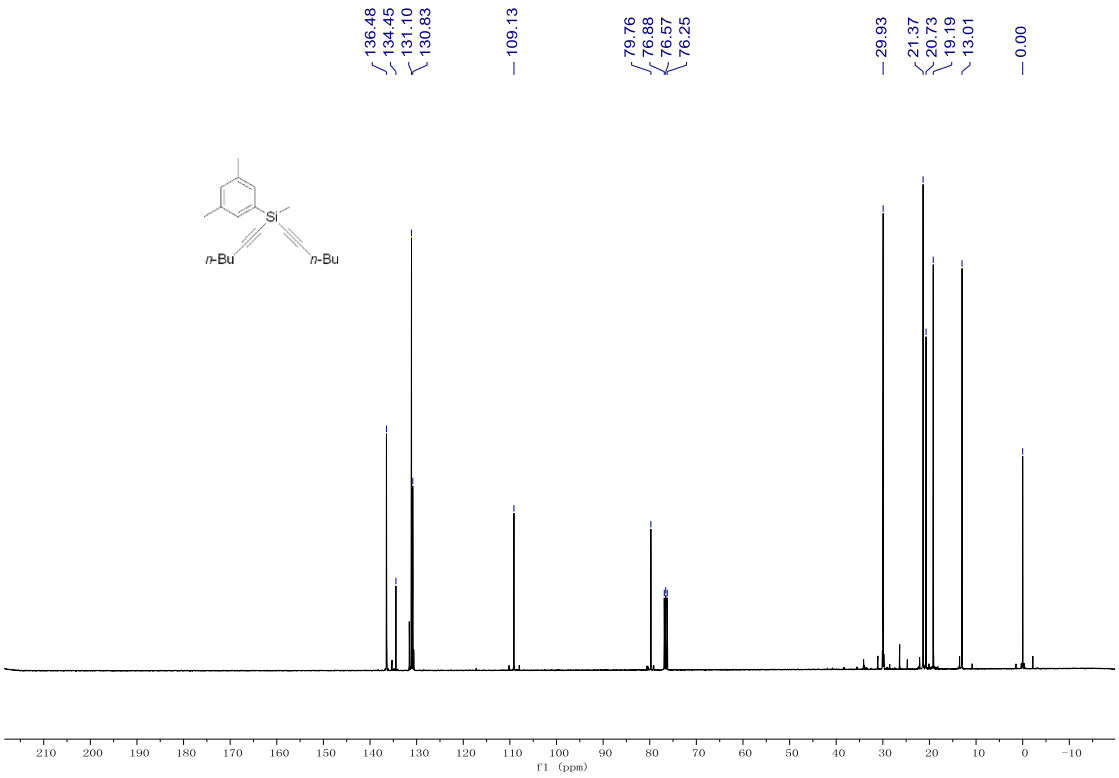
^{13}C NMR of **1a**



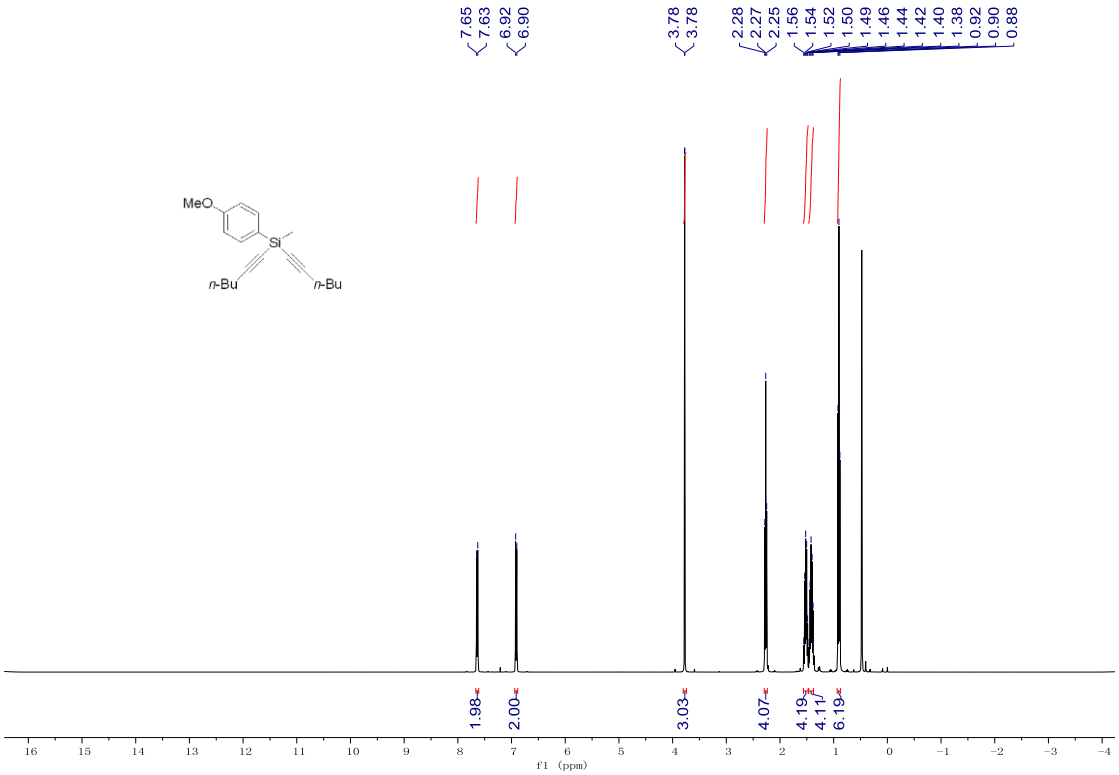
^{1}H NMR of **1b**



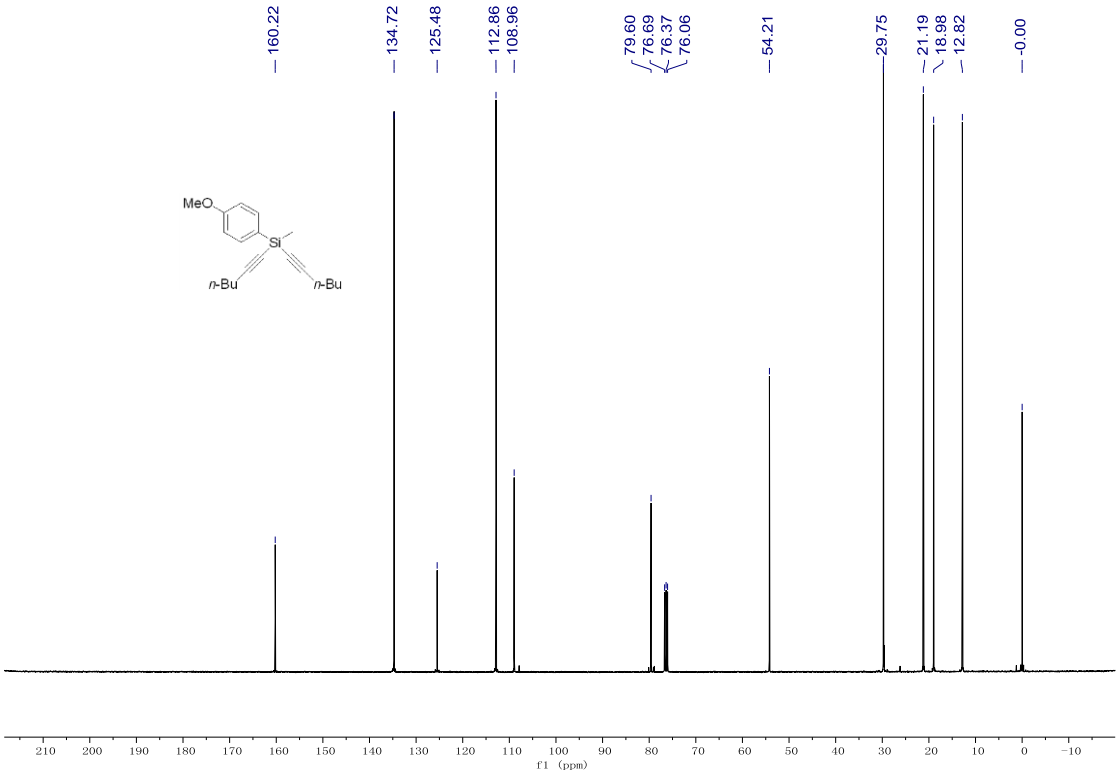
^{13}C NMR of **1b**



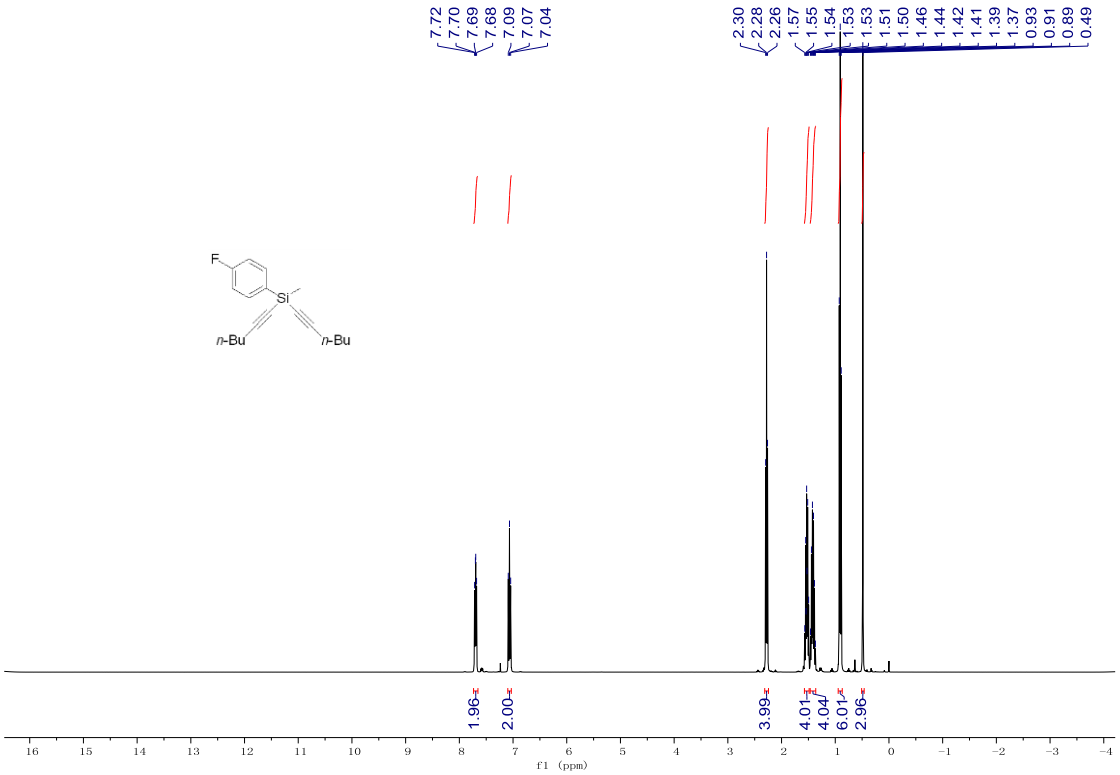
^{1}H NMR of **1c**



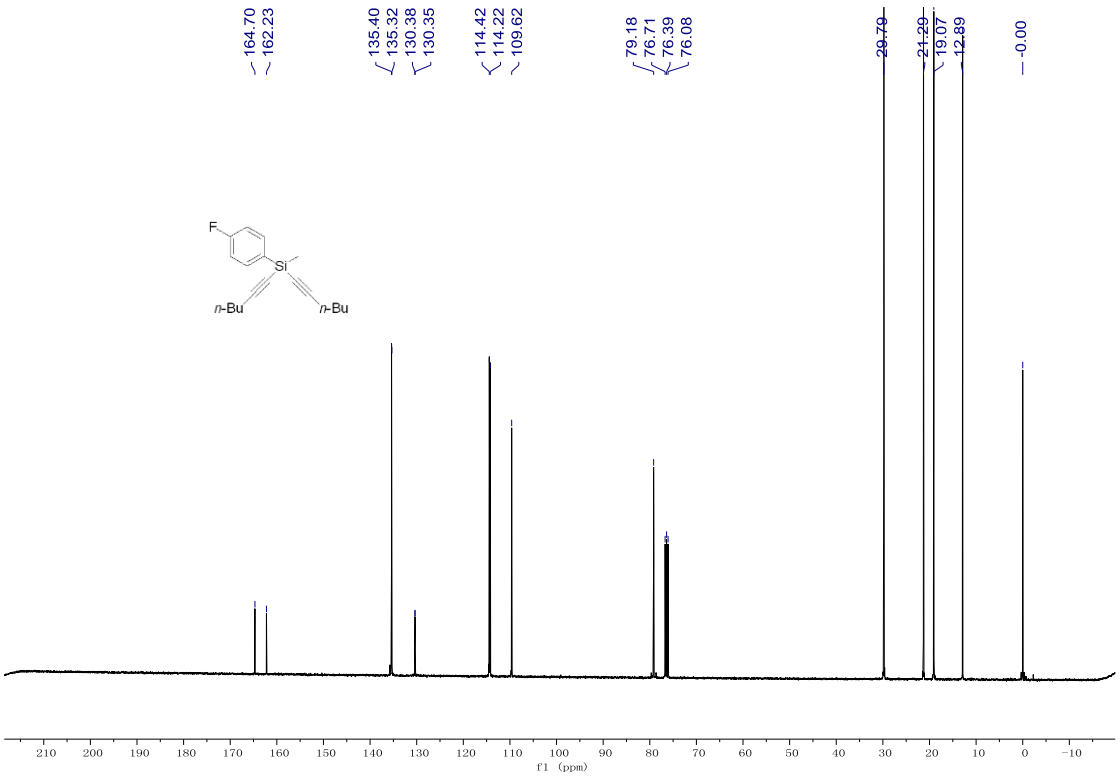
^{13}C NMR of **1c**



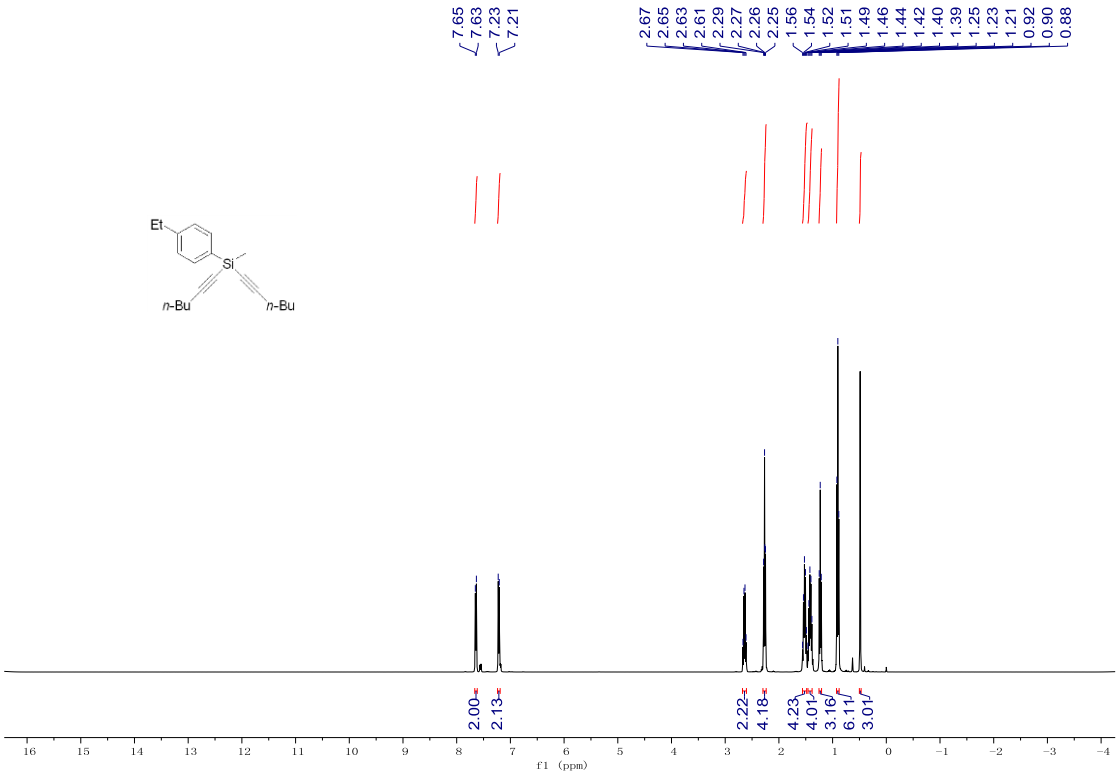
^{1}H NMR of **1d**



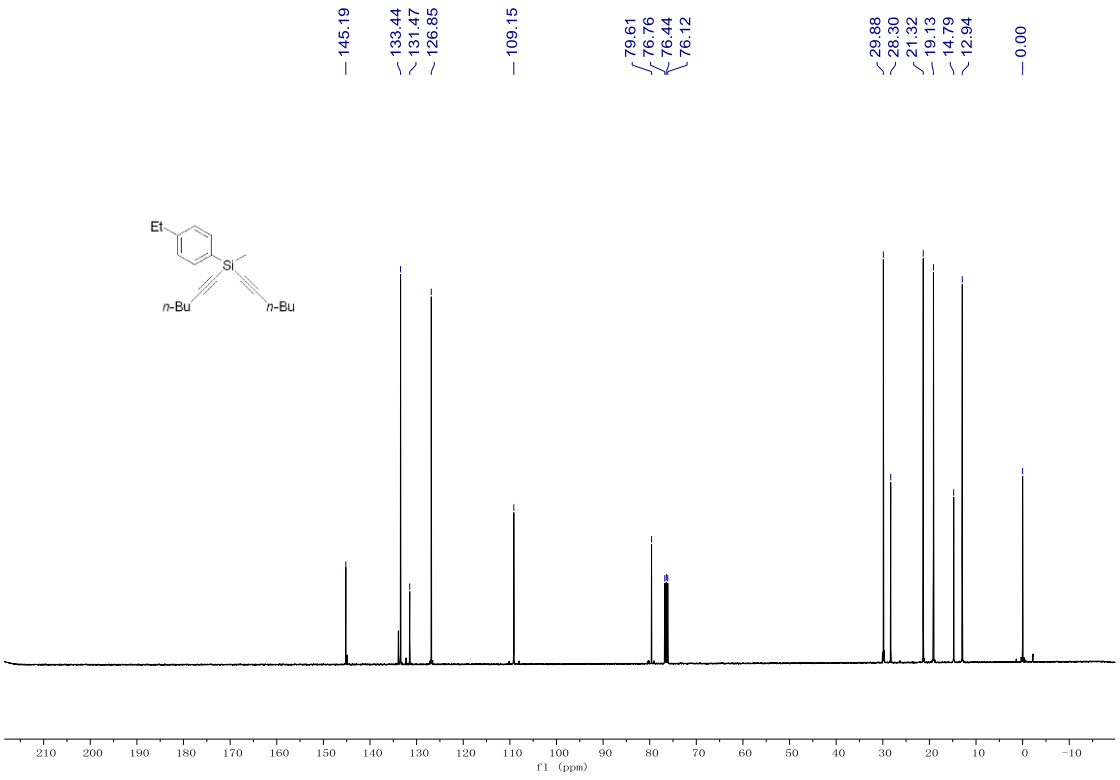
^{13}C NMR of **1d**



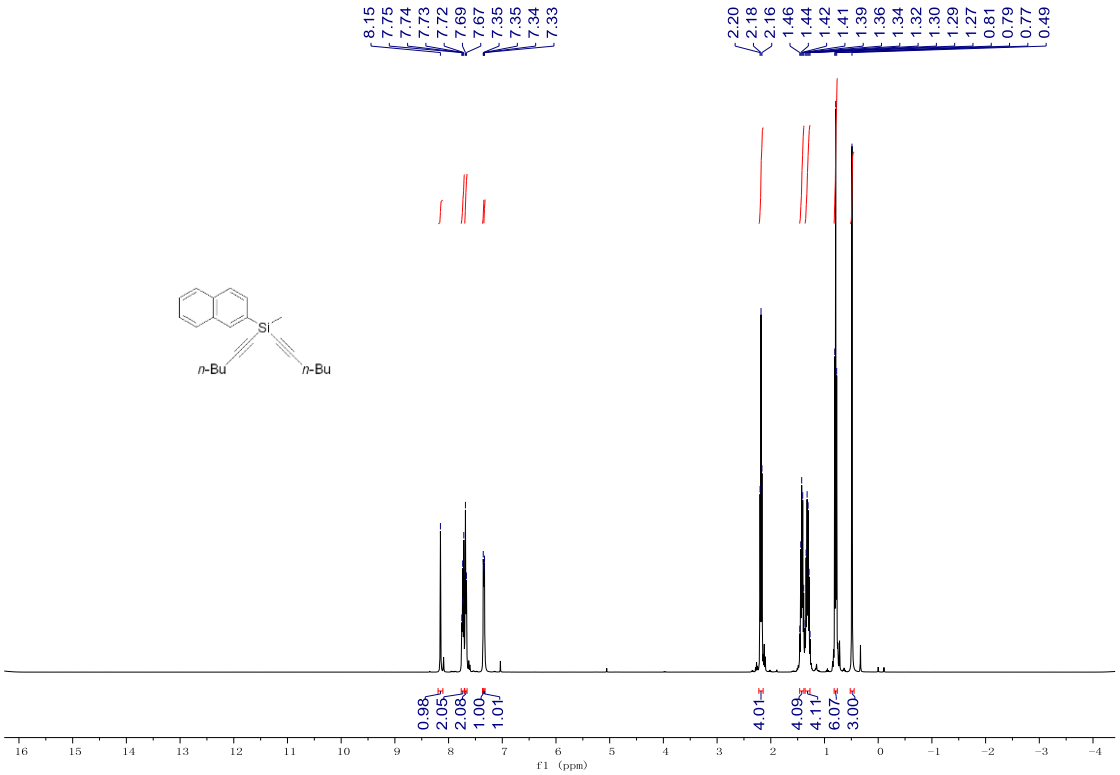
^{1}H NMR of **1e**



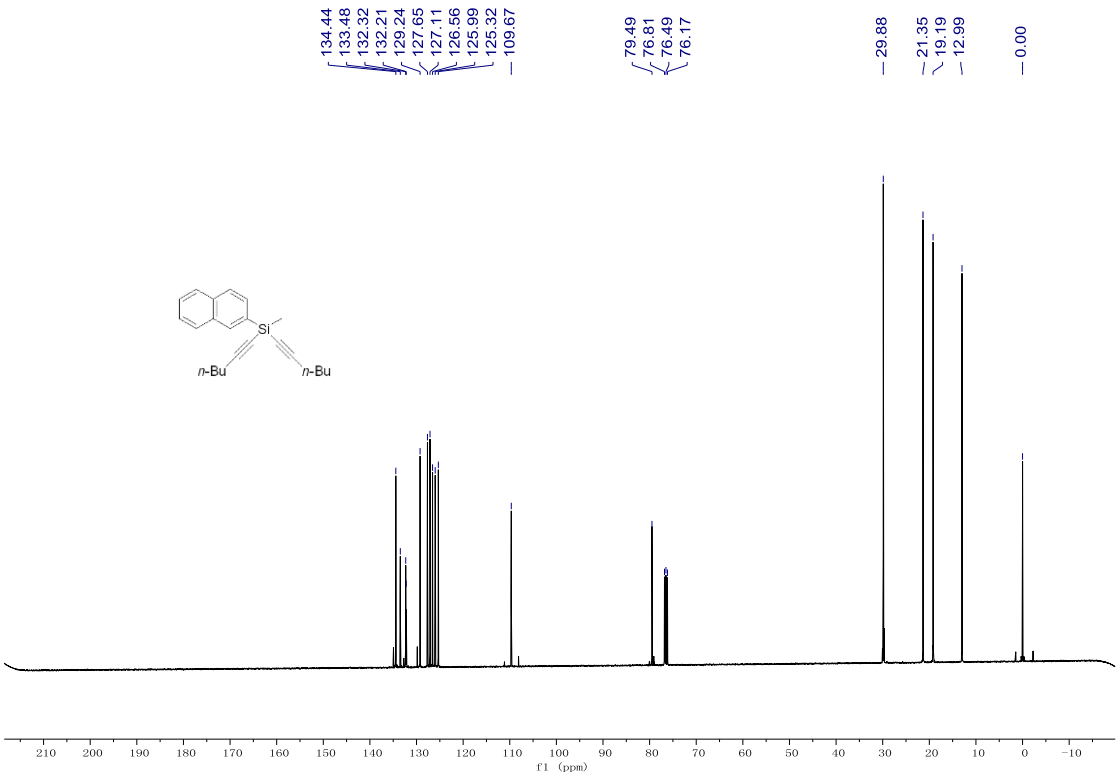
^{13}C NMR of **1e**



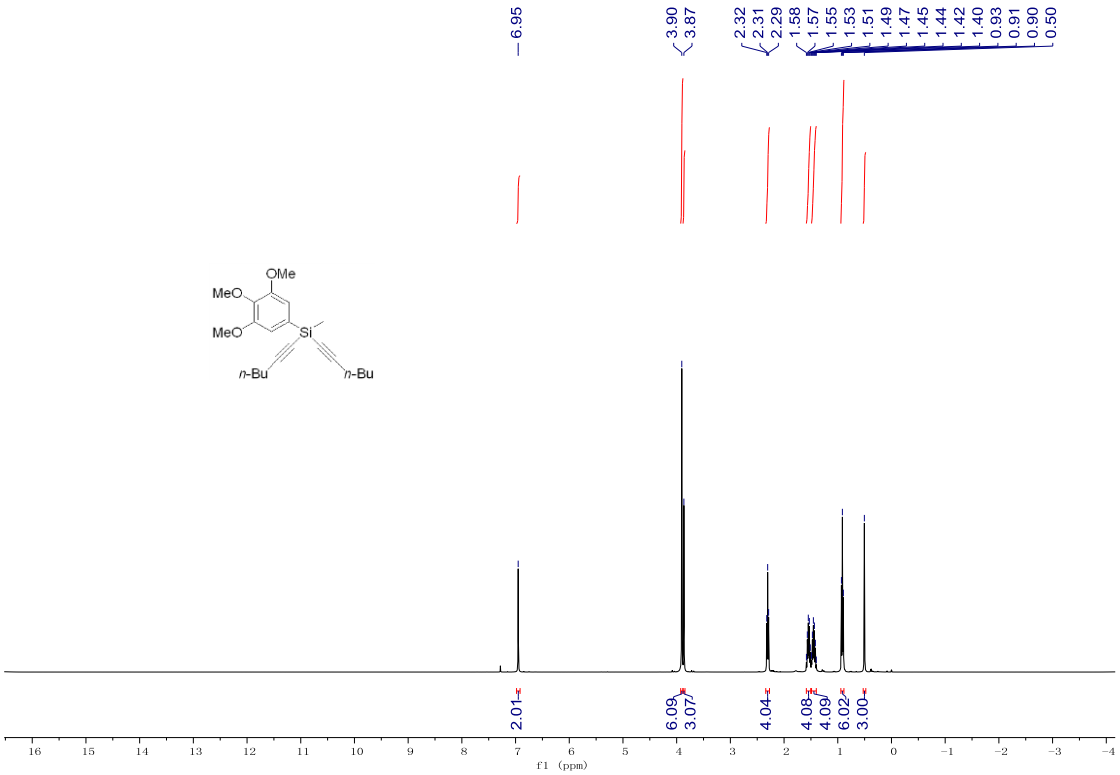
^{1}H NMR of **1f**



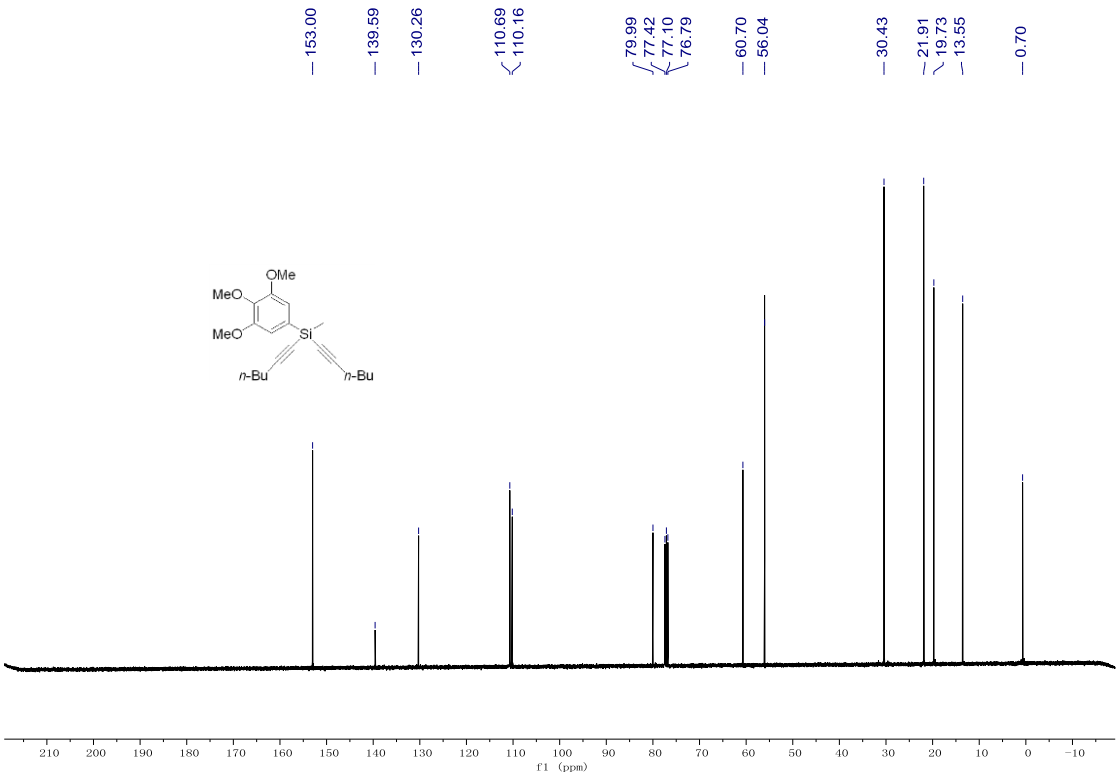
^{13}C NMR of **1f**



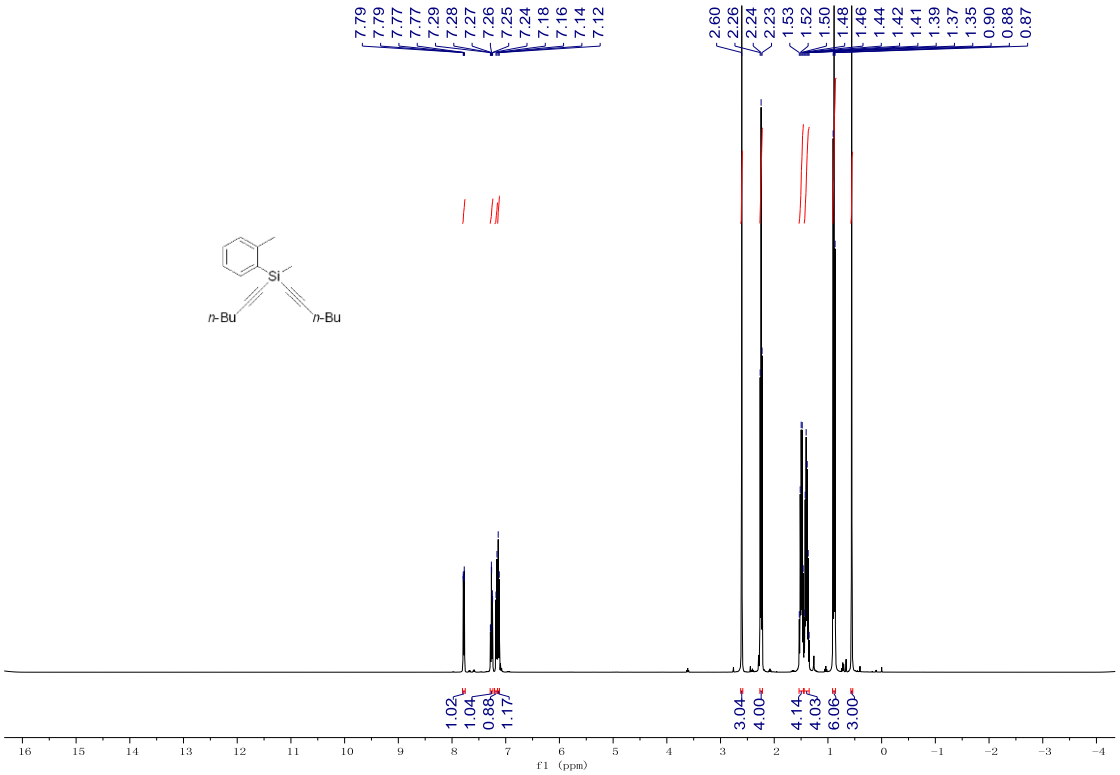
^{1}H NMR of **1g**



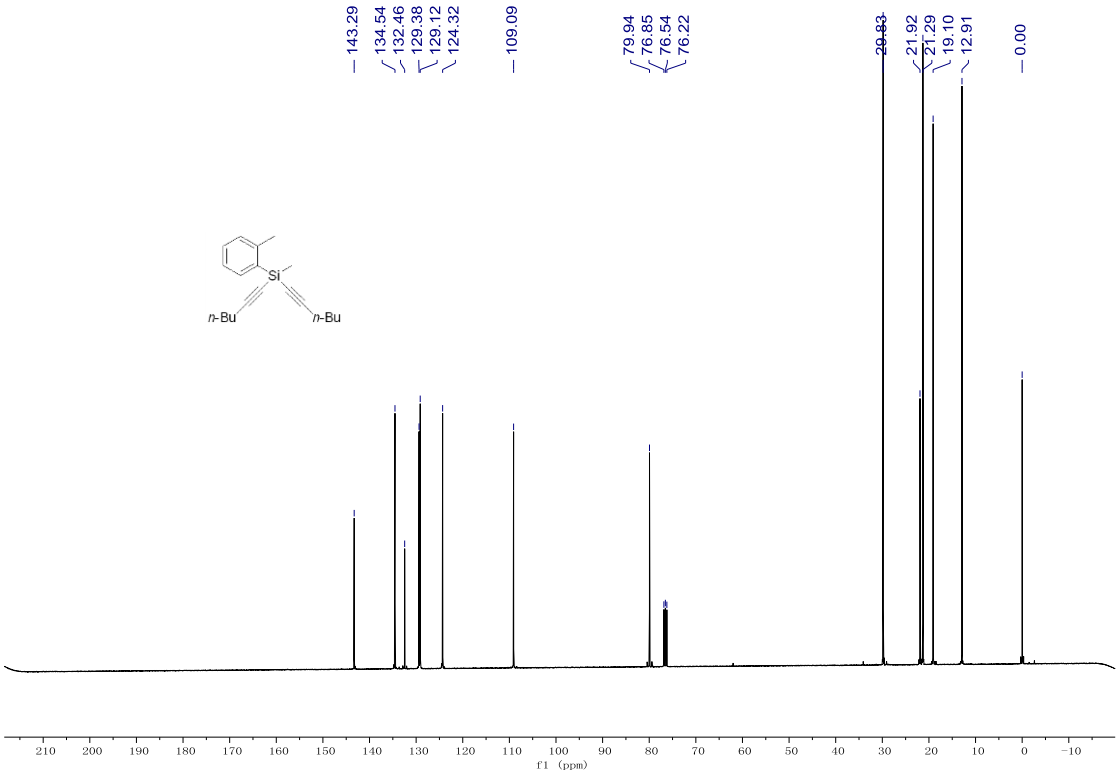
^{13}C NMR of **1g**



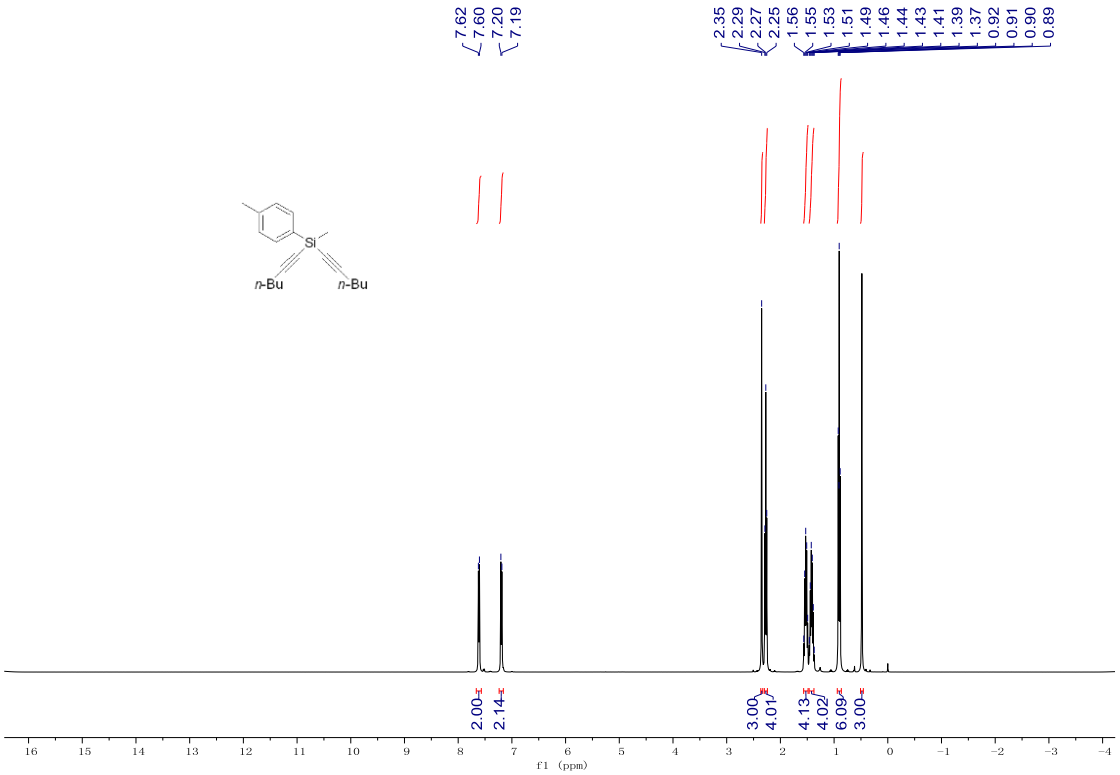
^{1}H NMR of **1h**



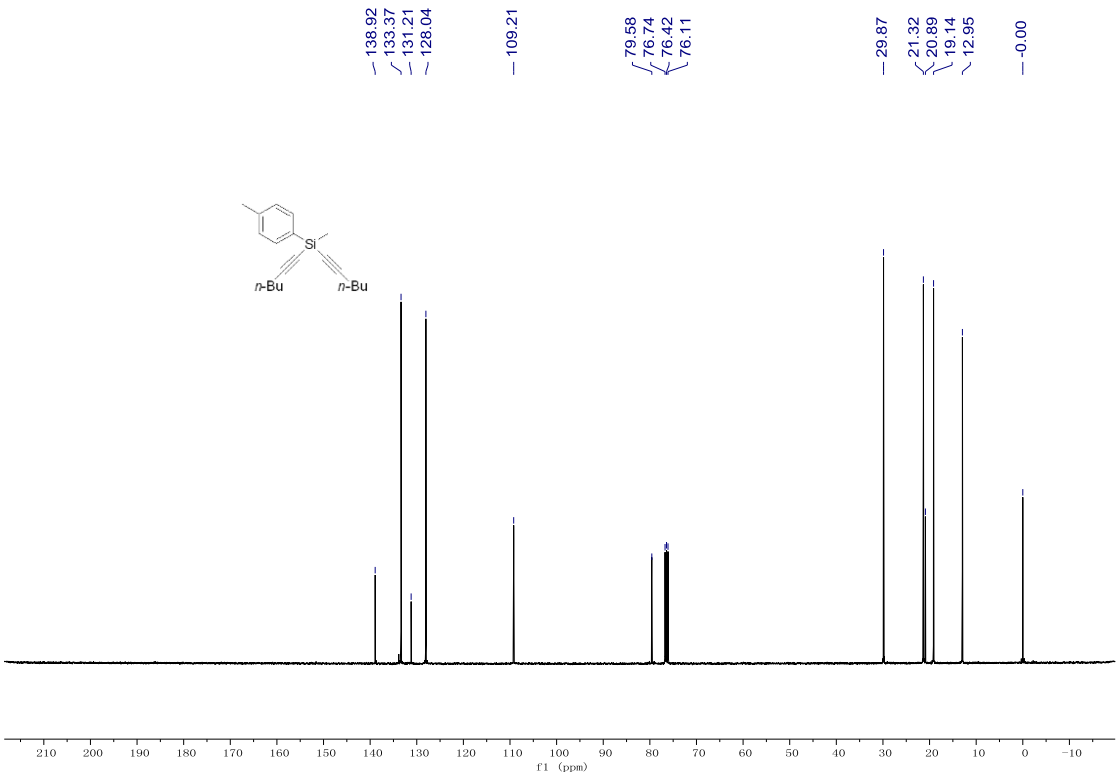
^{13}C NMR of **1h**



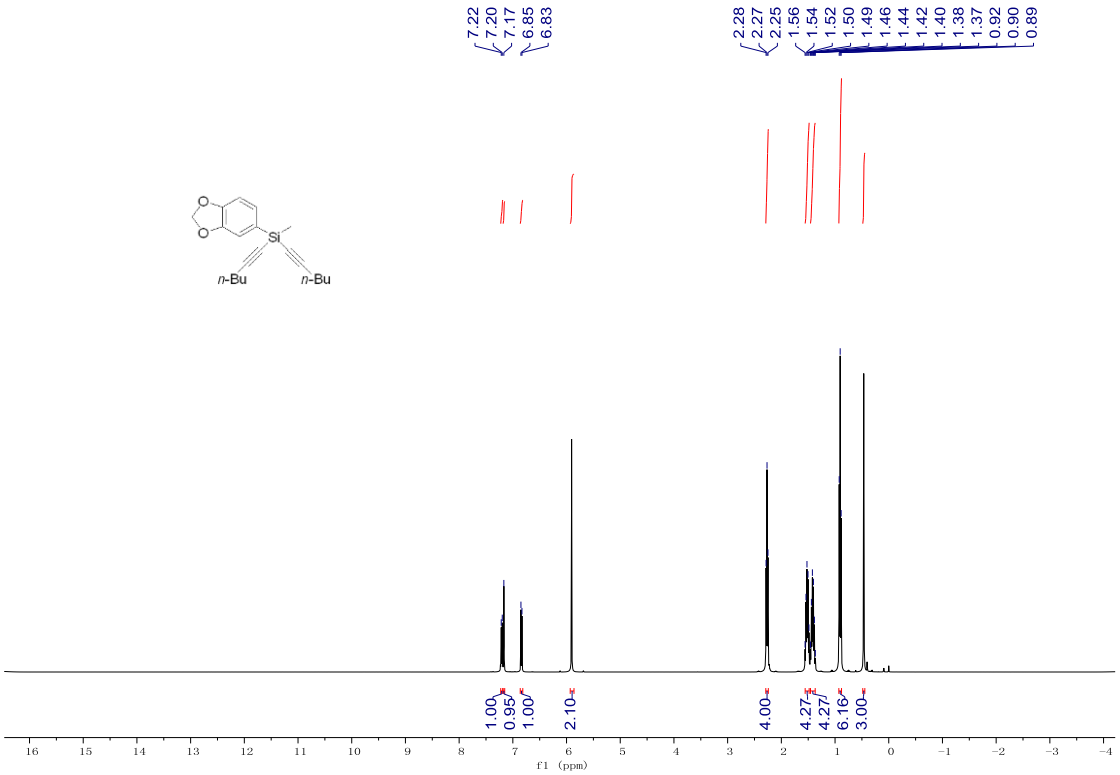
^{1}H NMR of **1i**



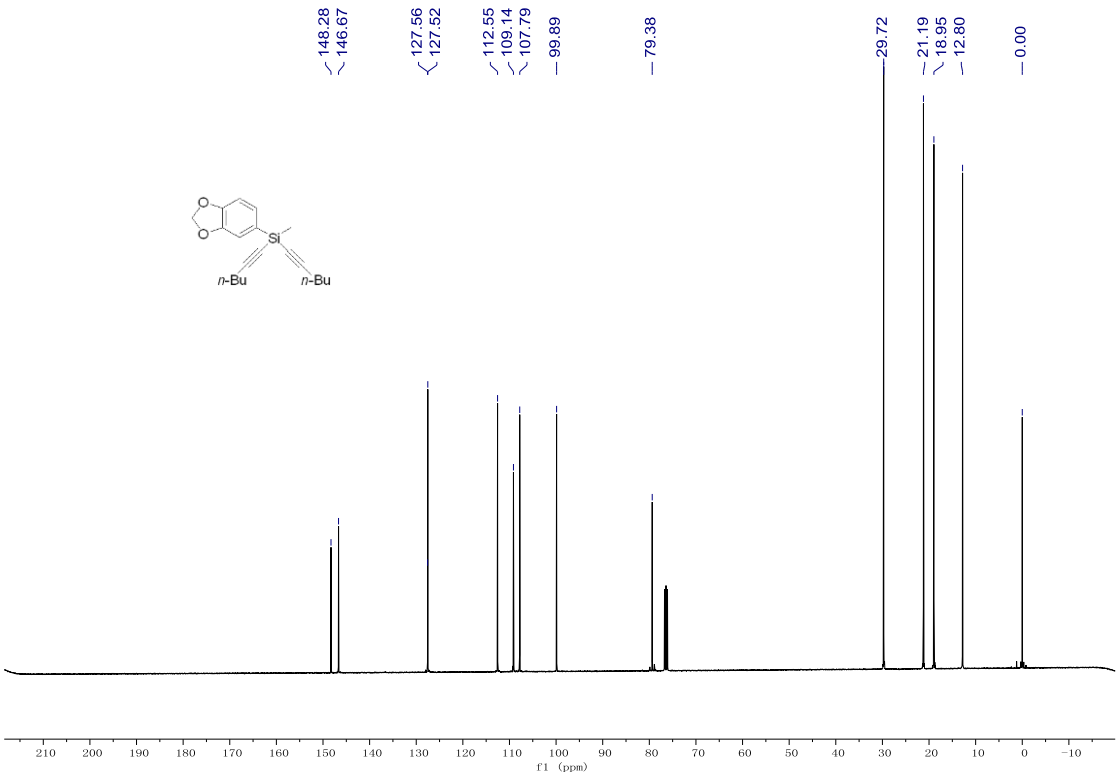
^{13}C NMR of **1i**



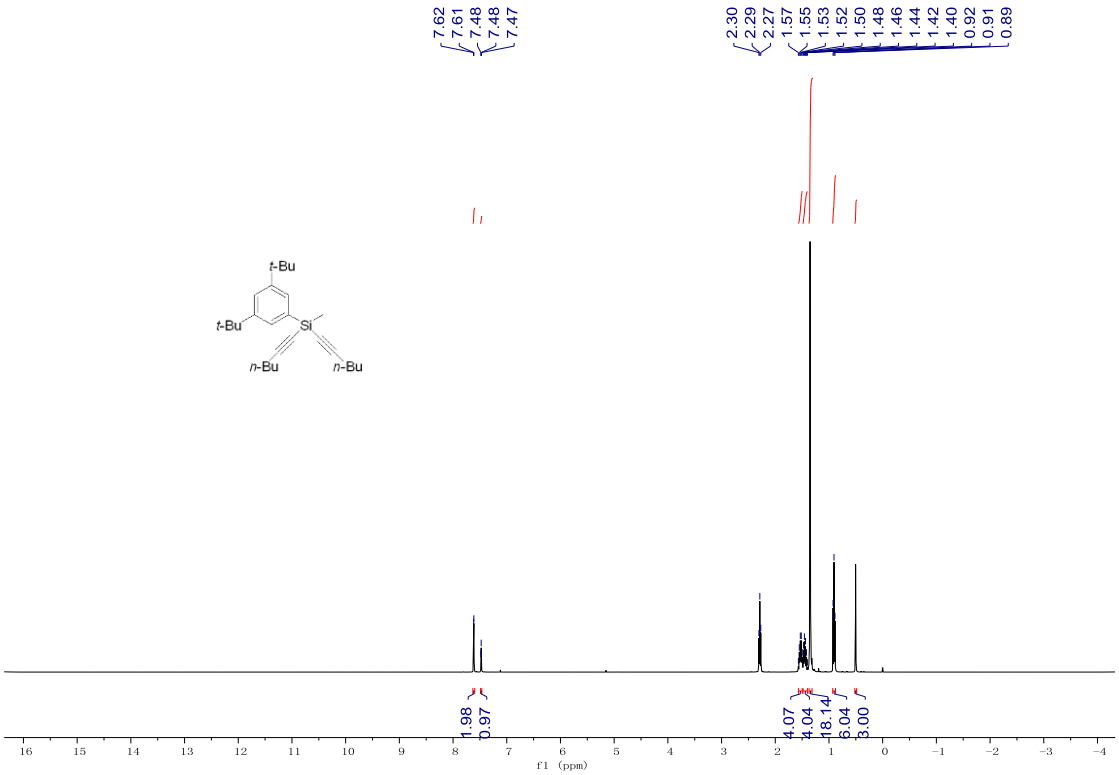
^{1}H NMR of **1j**



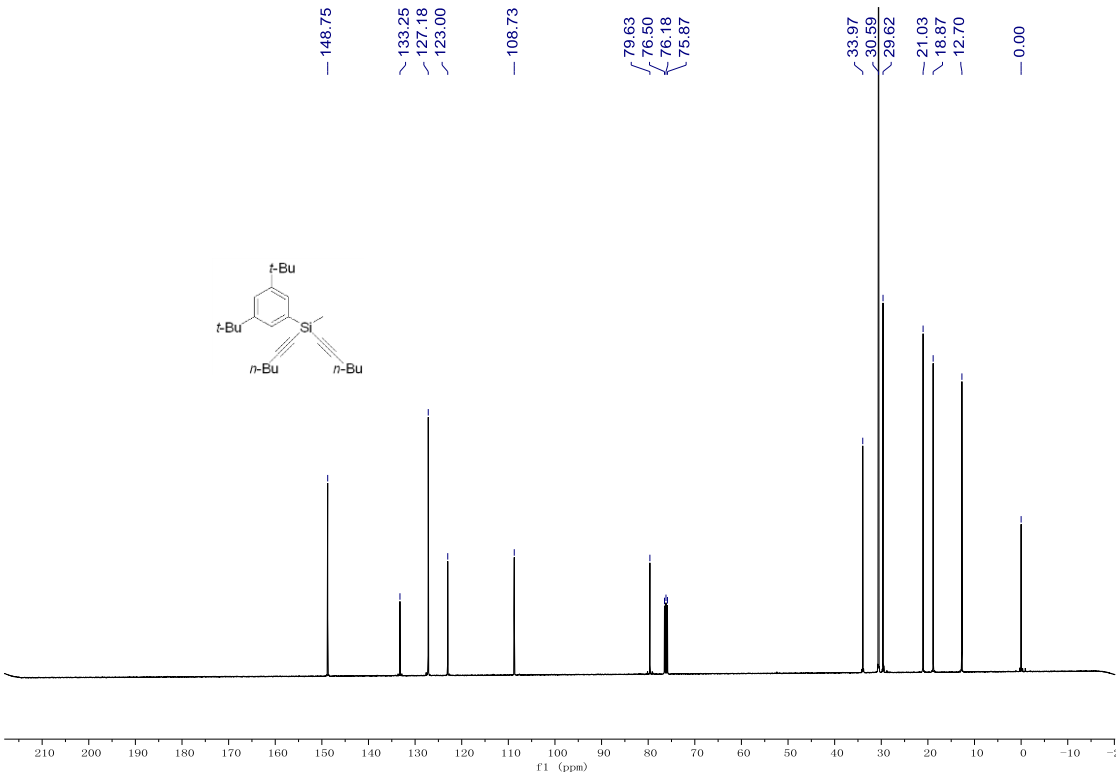
^{13}C NMR of **1j**



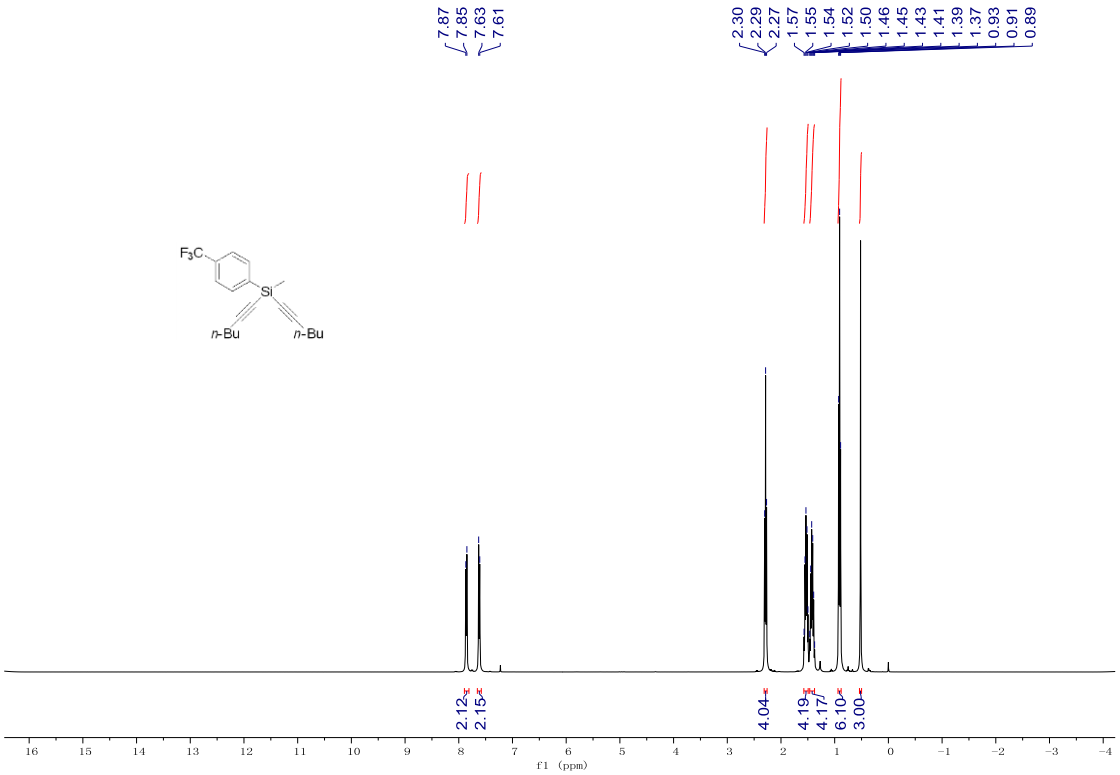
^{1}H NMR of **1k**



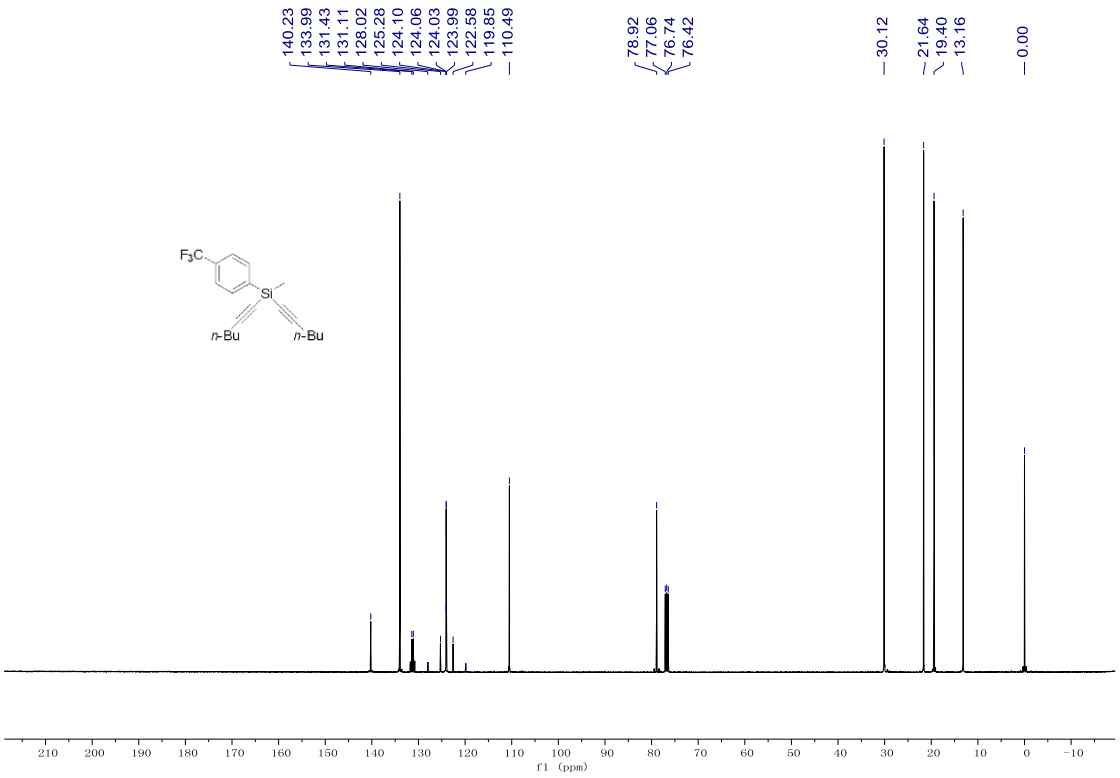
^{13}C NMR of **1k**



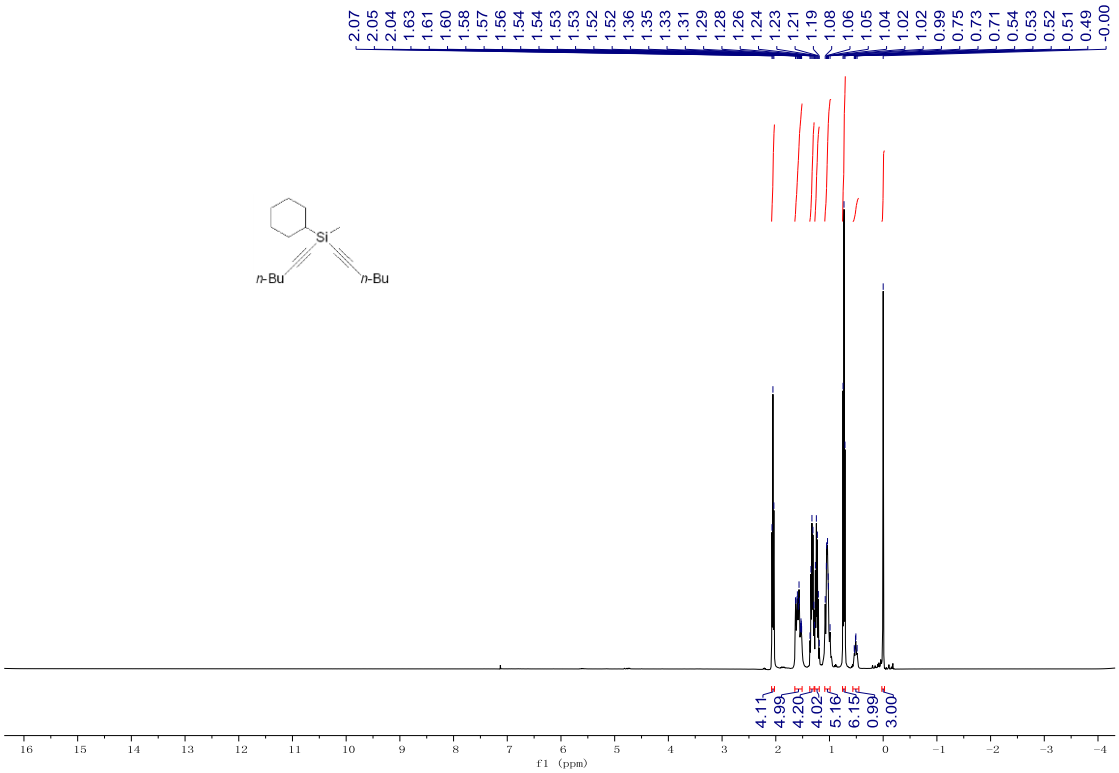
^{1}H NMR of **1l**



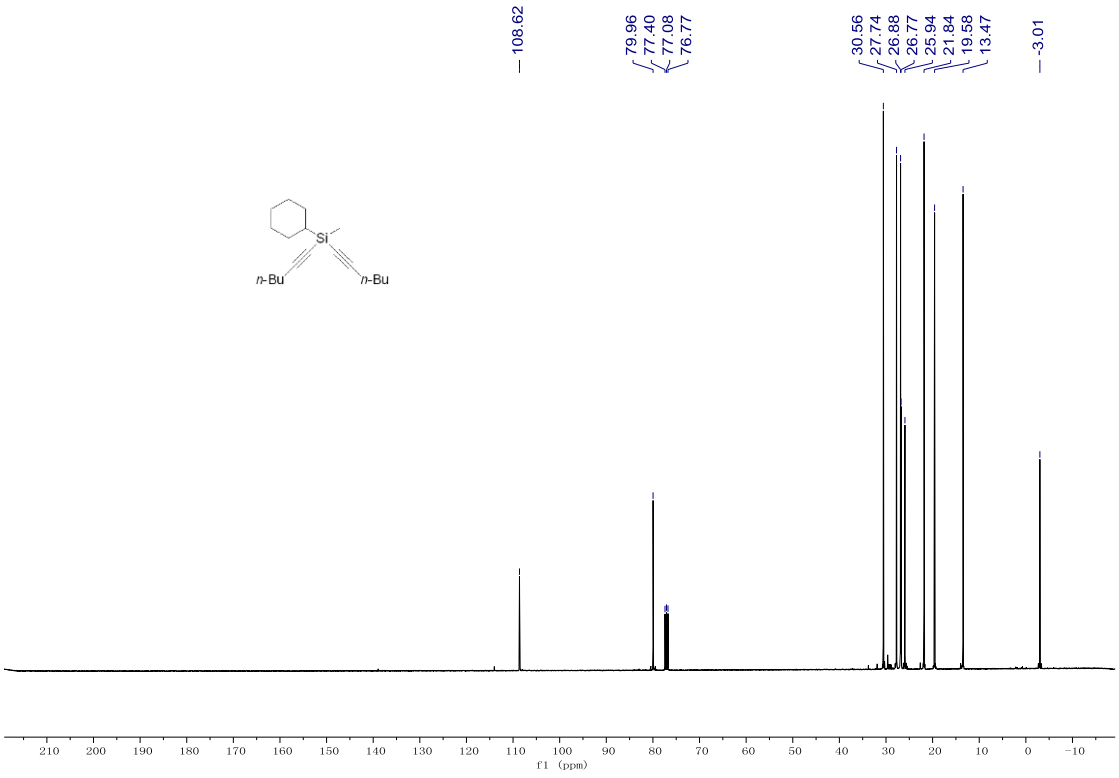
^{13}C NMR of **1l**



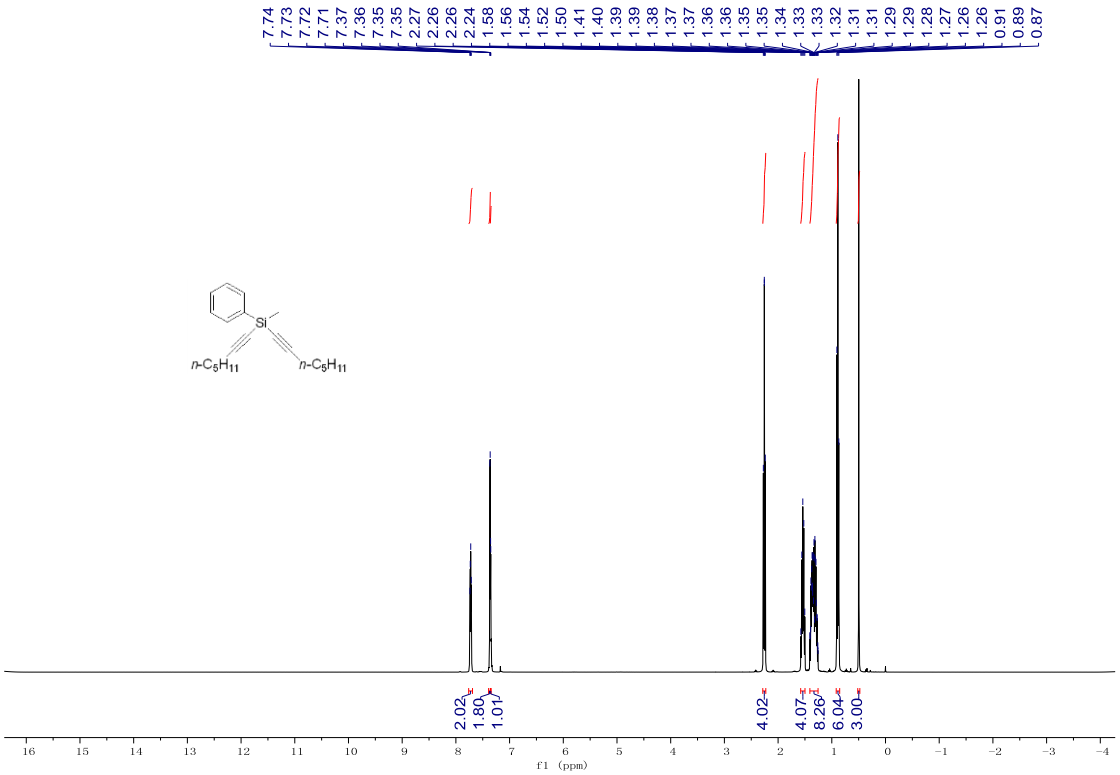
^{1}H NMR of **1m**



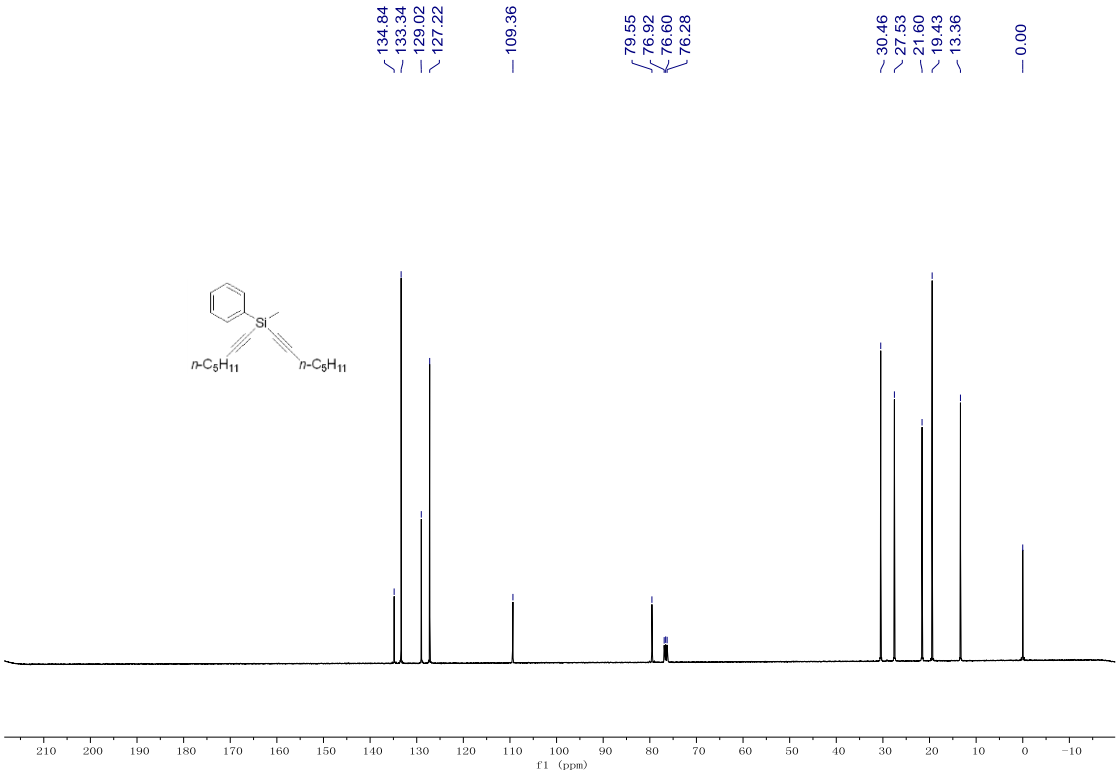
^{13}C NMR of **1m**



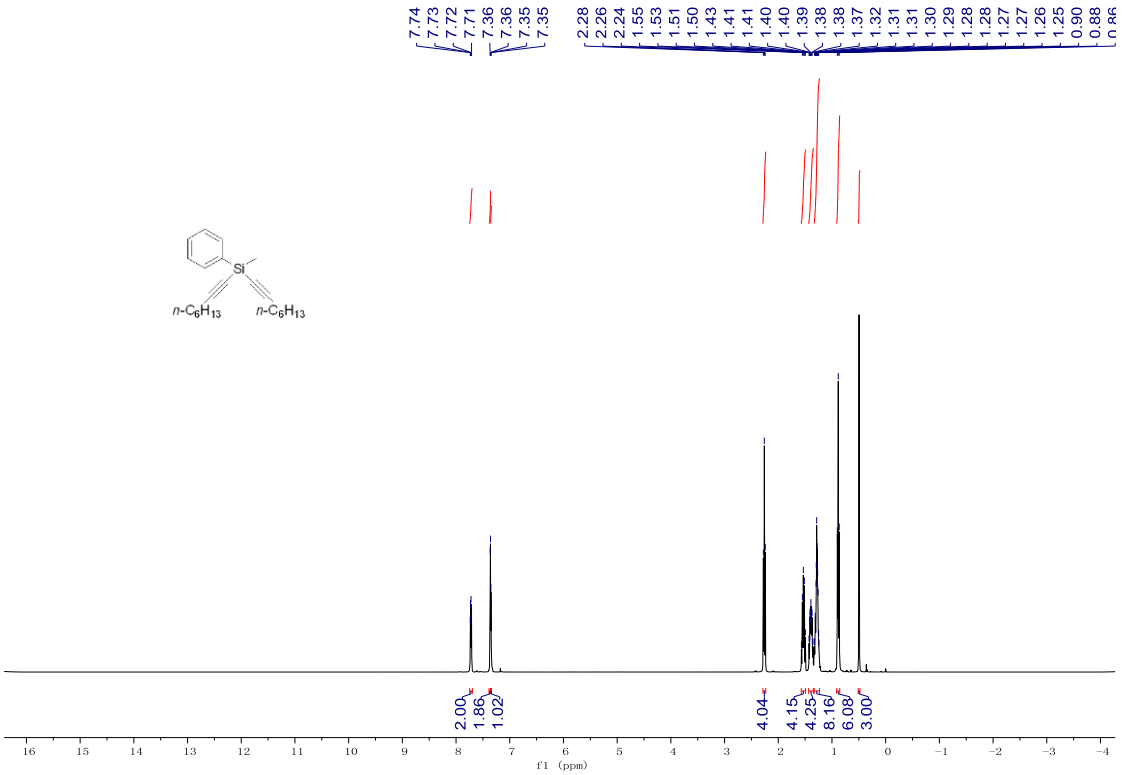
^{1}H NMR of **1n**



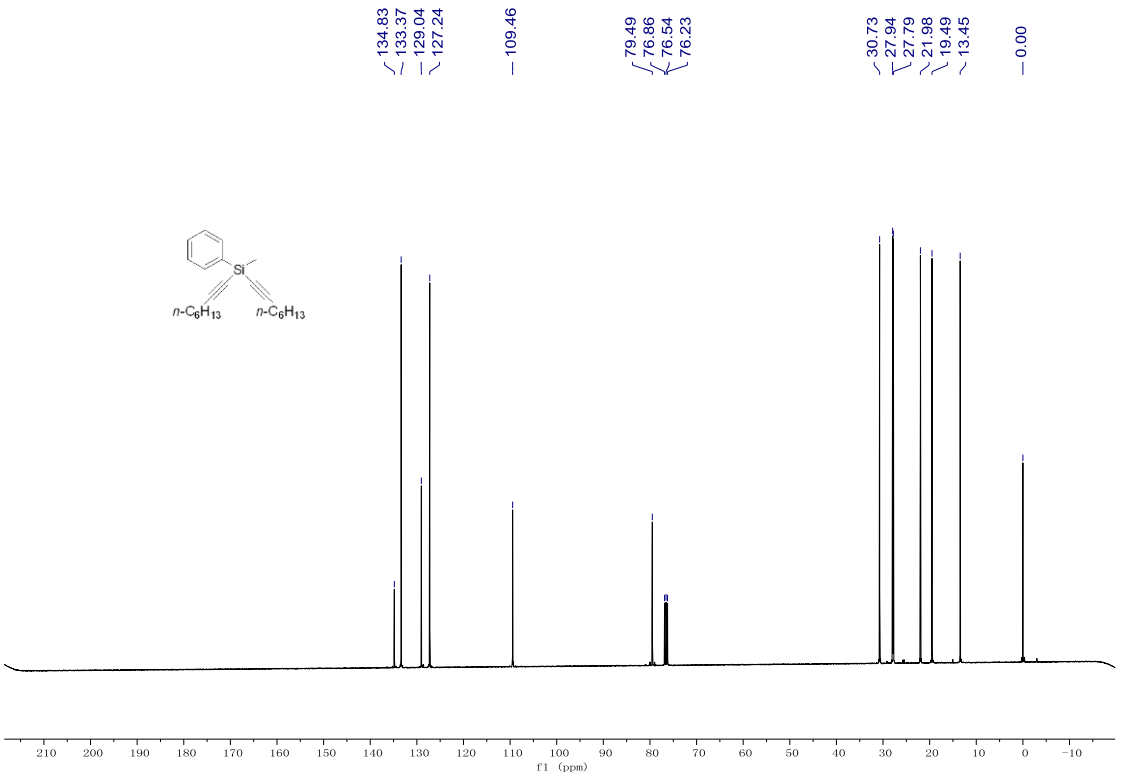
^{13}C NMR of **1n**



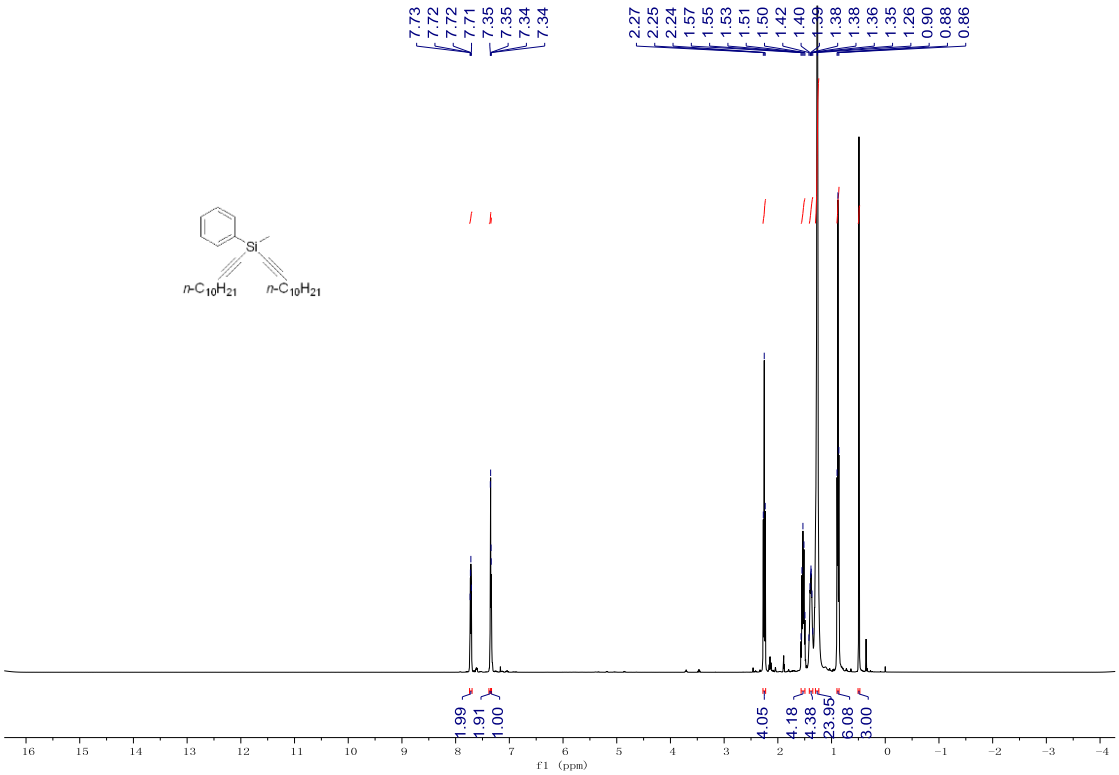
^{1}H NMR of **1o**



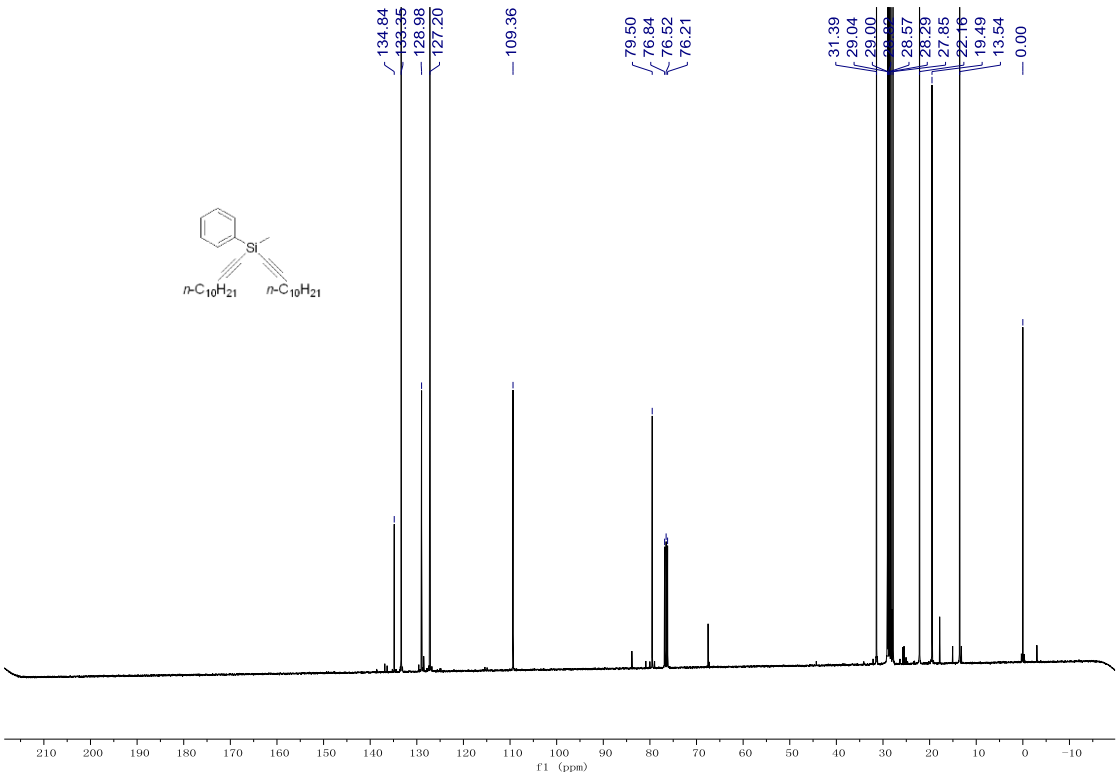
^{13}C NMR of **1o**



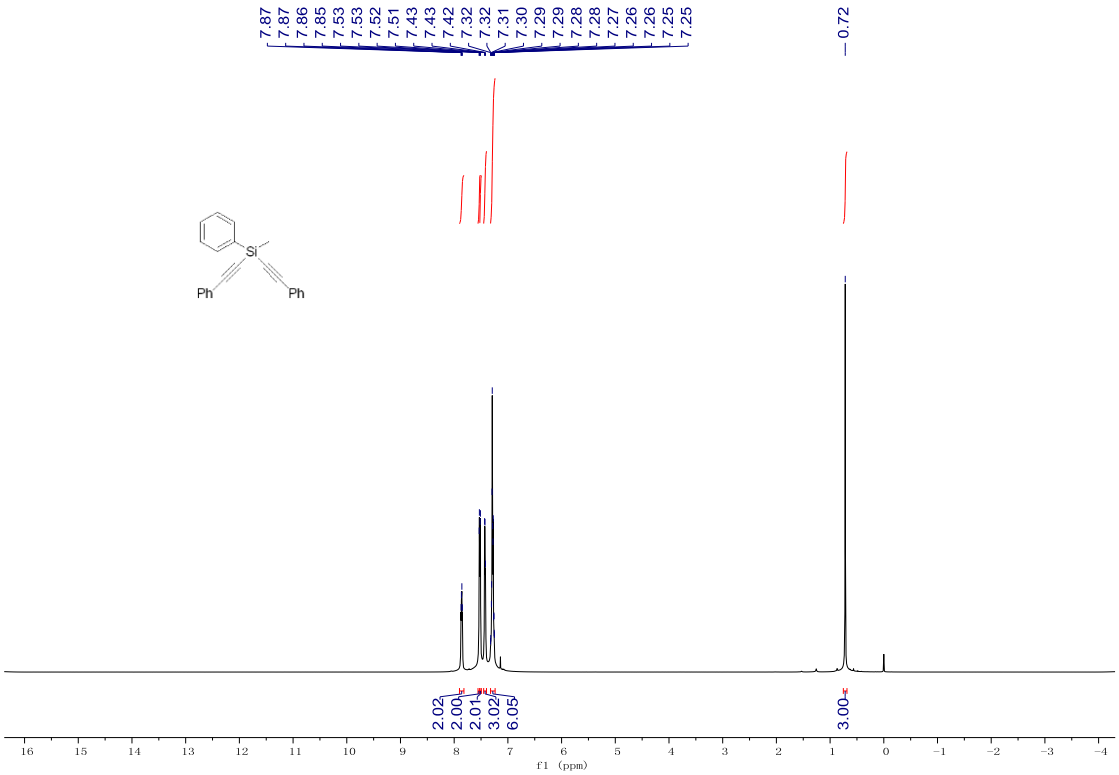
^{1}H NMR of **1p**



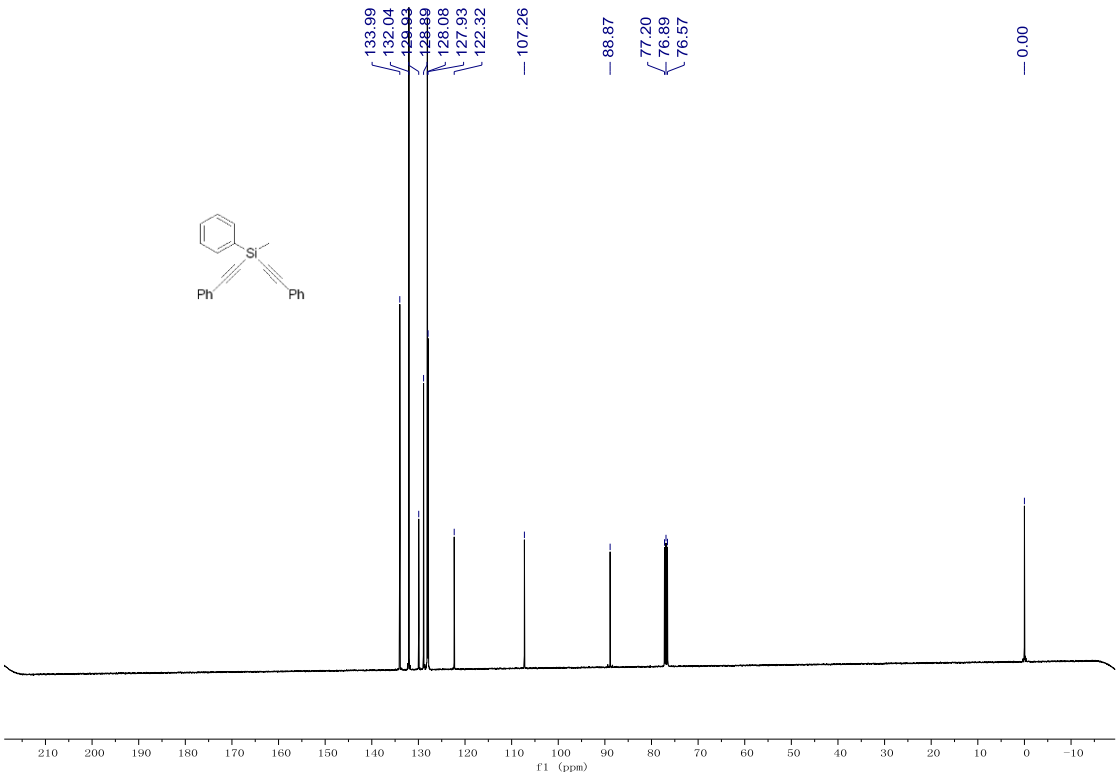
^{13}C NMR of **1p**



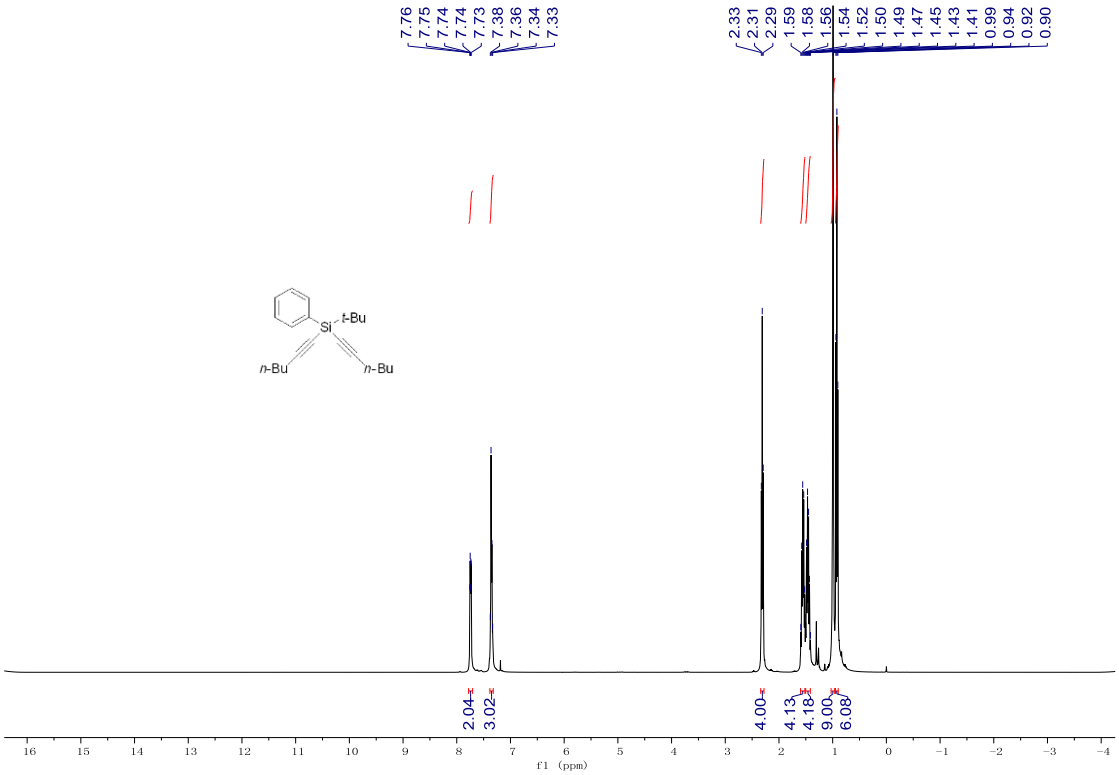
^{1}H NMR of **1q**



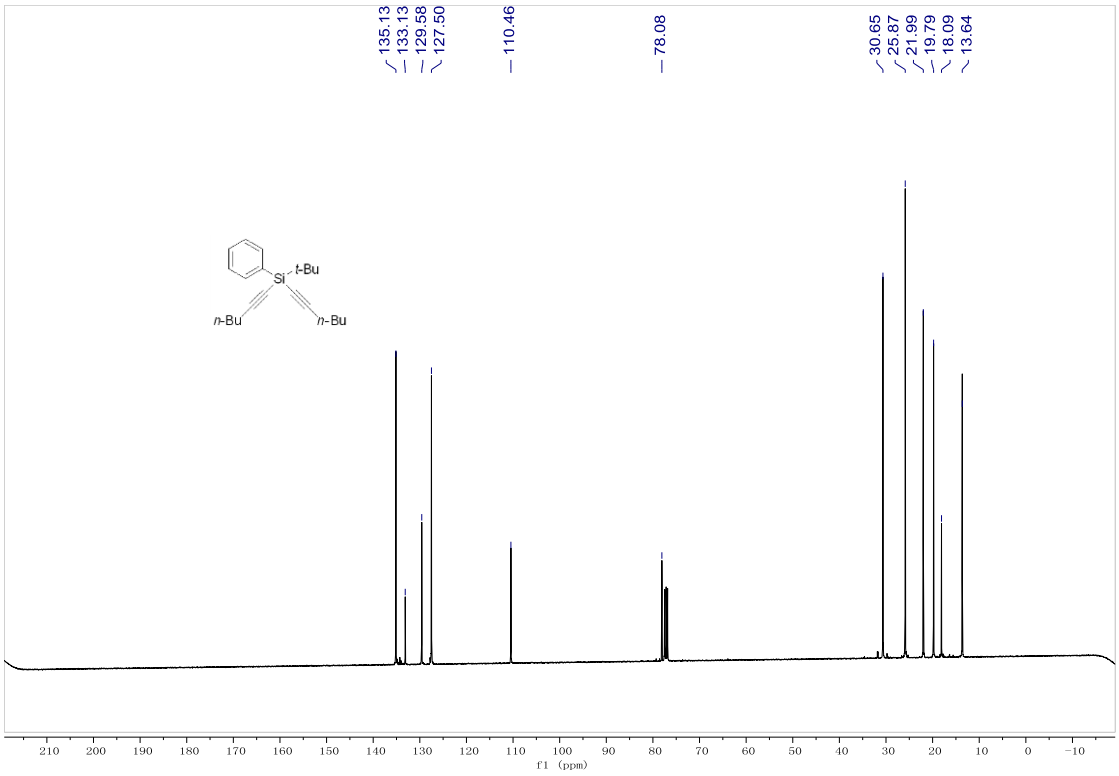
^{13}C NMR of **1q**



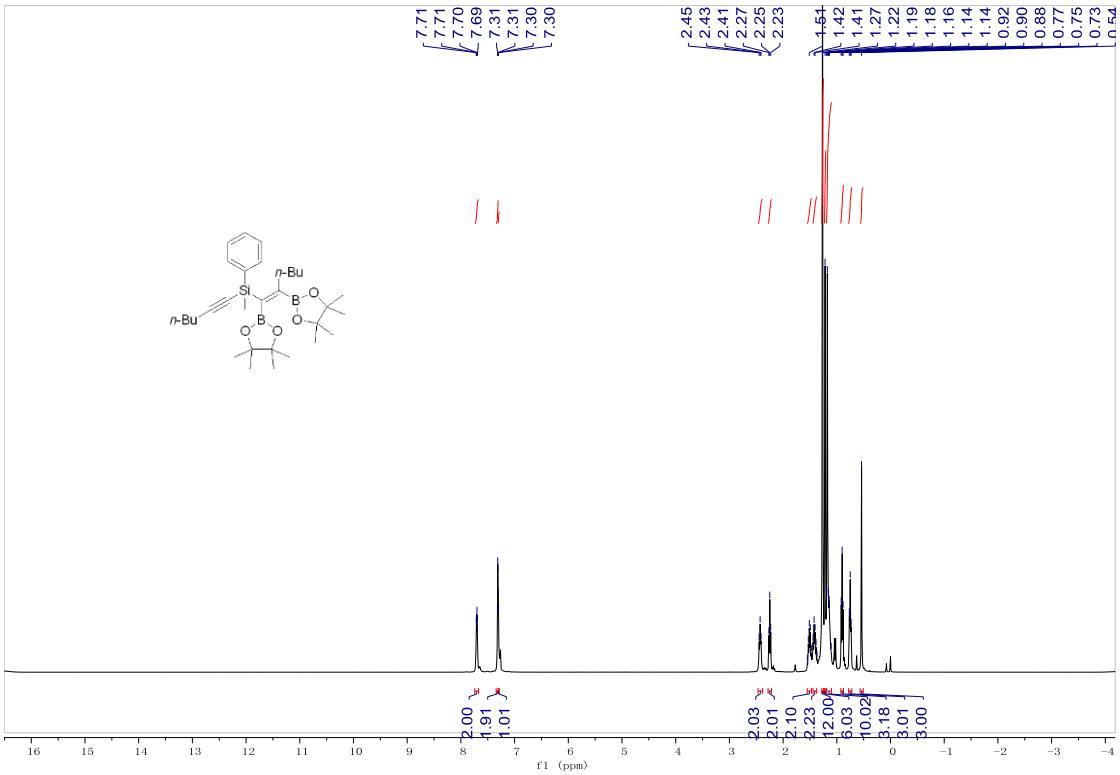
^{1}H NMR of **1r**



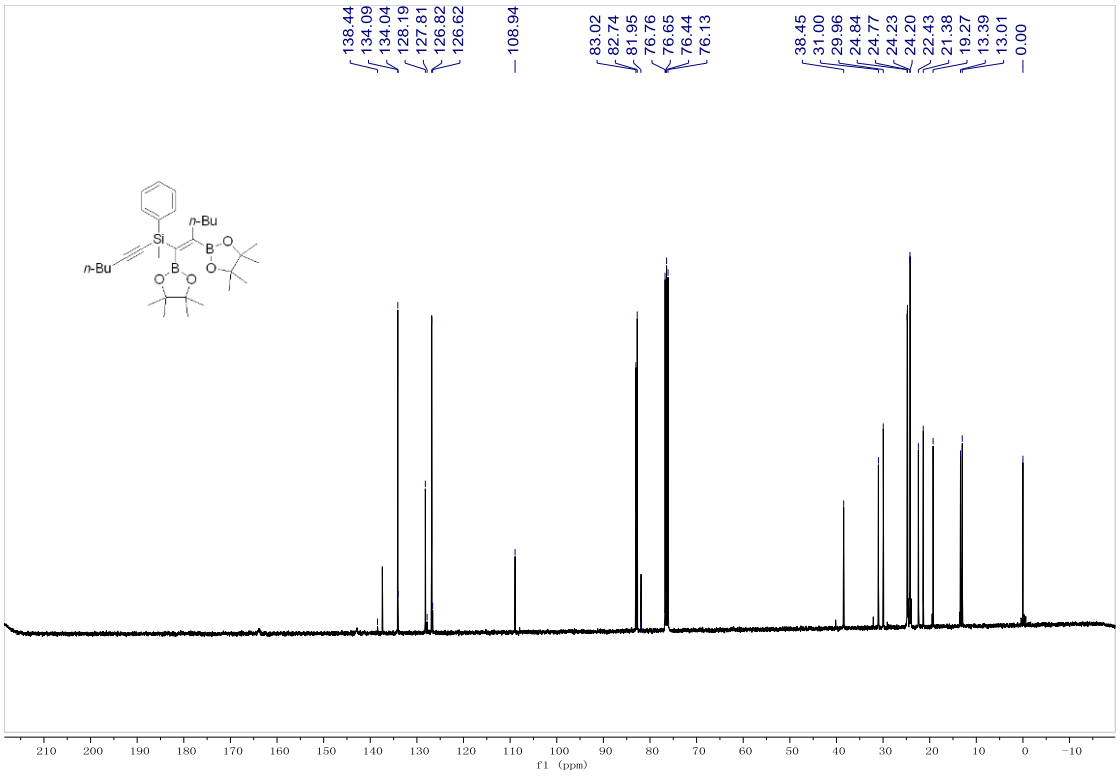
^{13}C NMR of **1q**



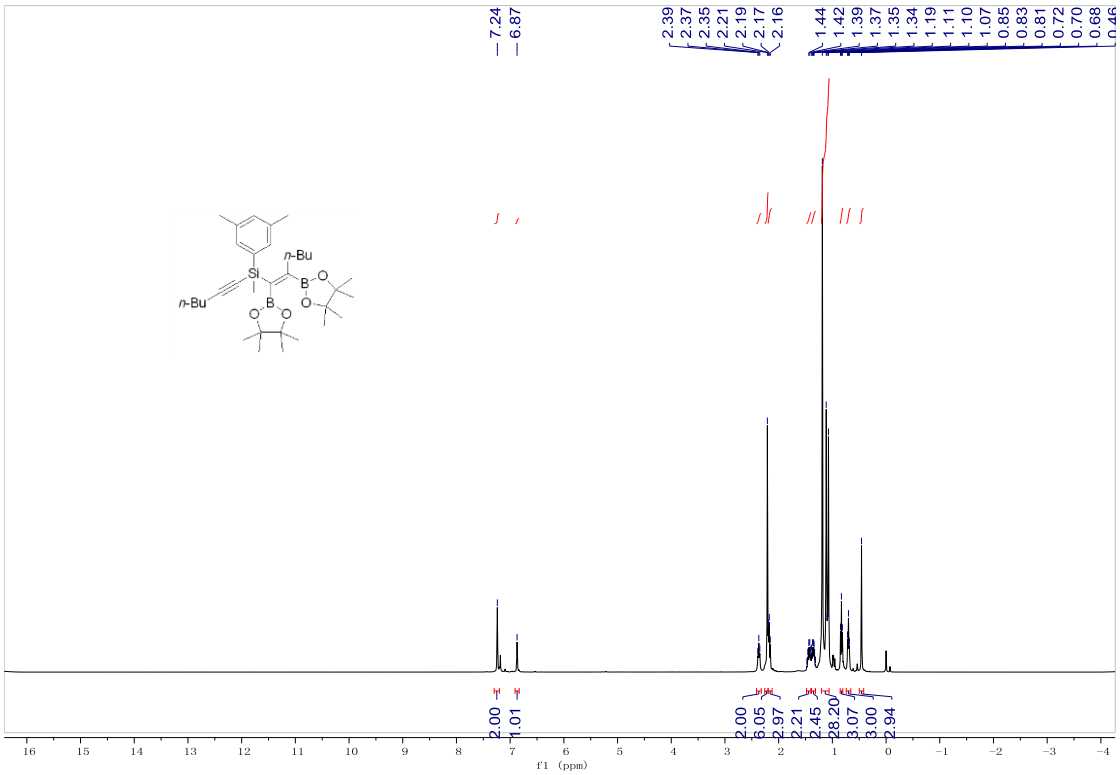
^{1}H NMR of **3a**



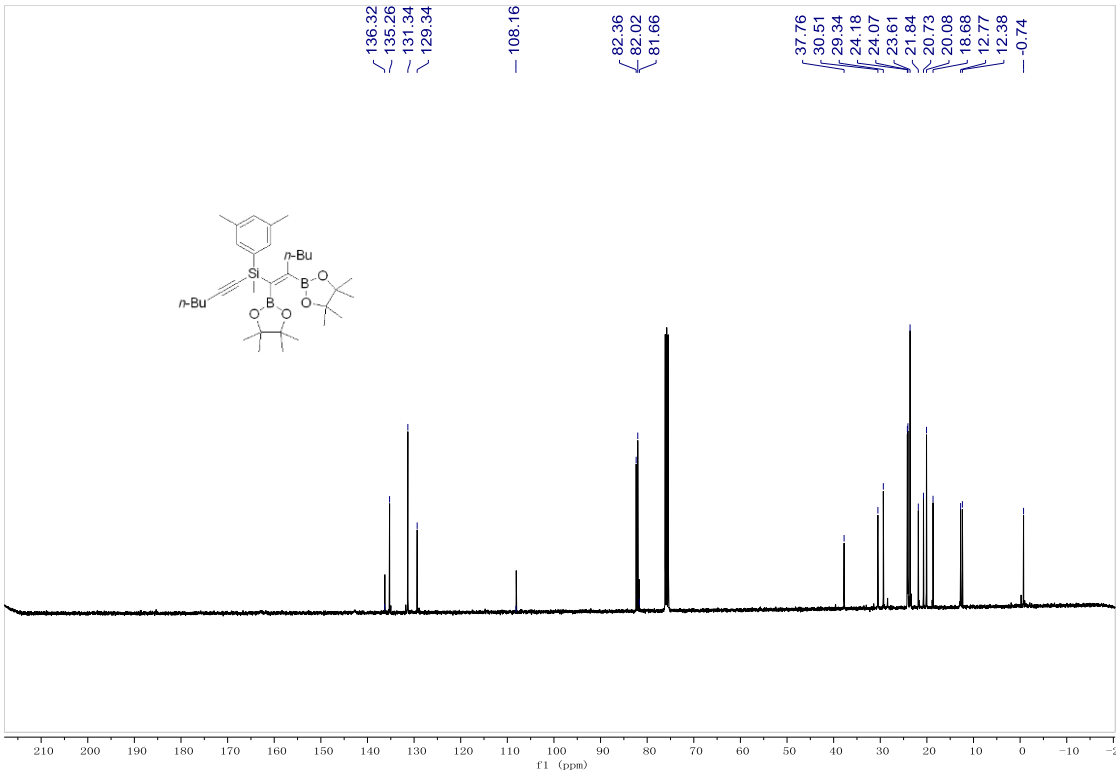
^{13}C NMR of **3a**



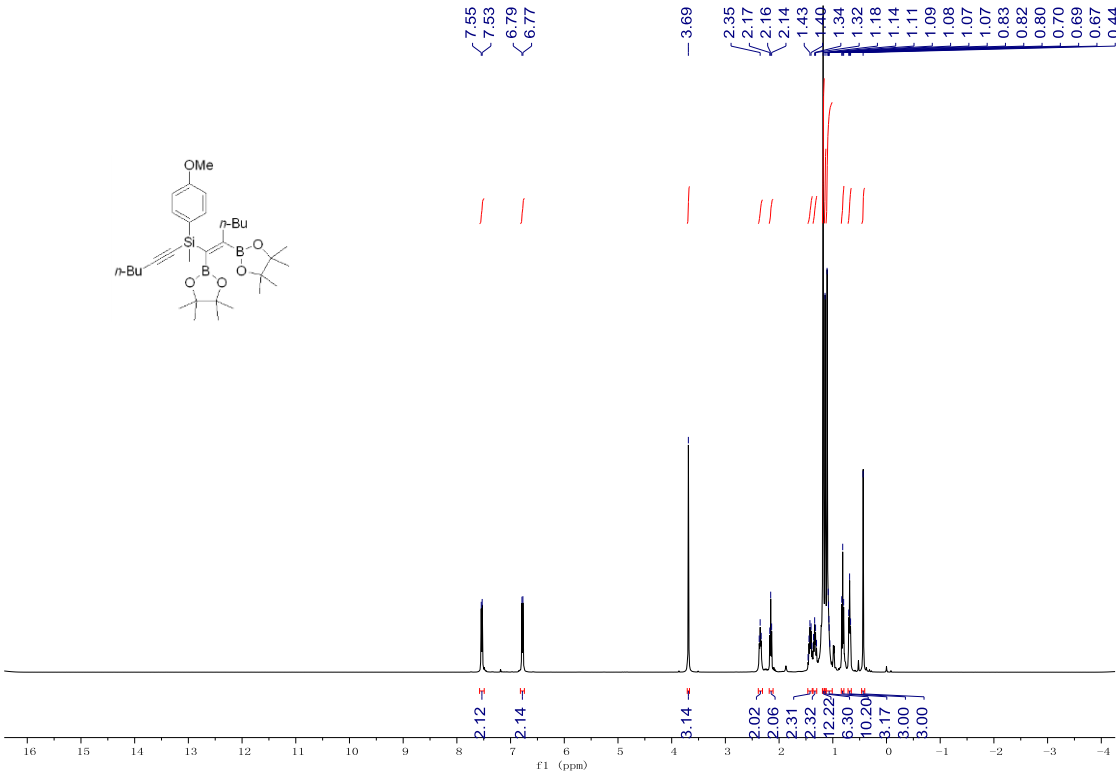
^{1}H NMR of **3b**



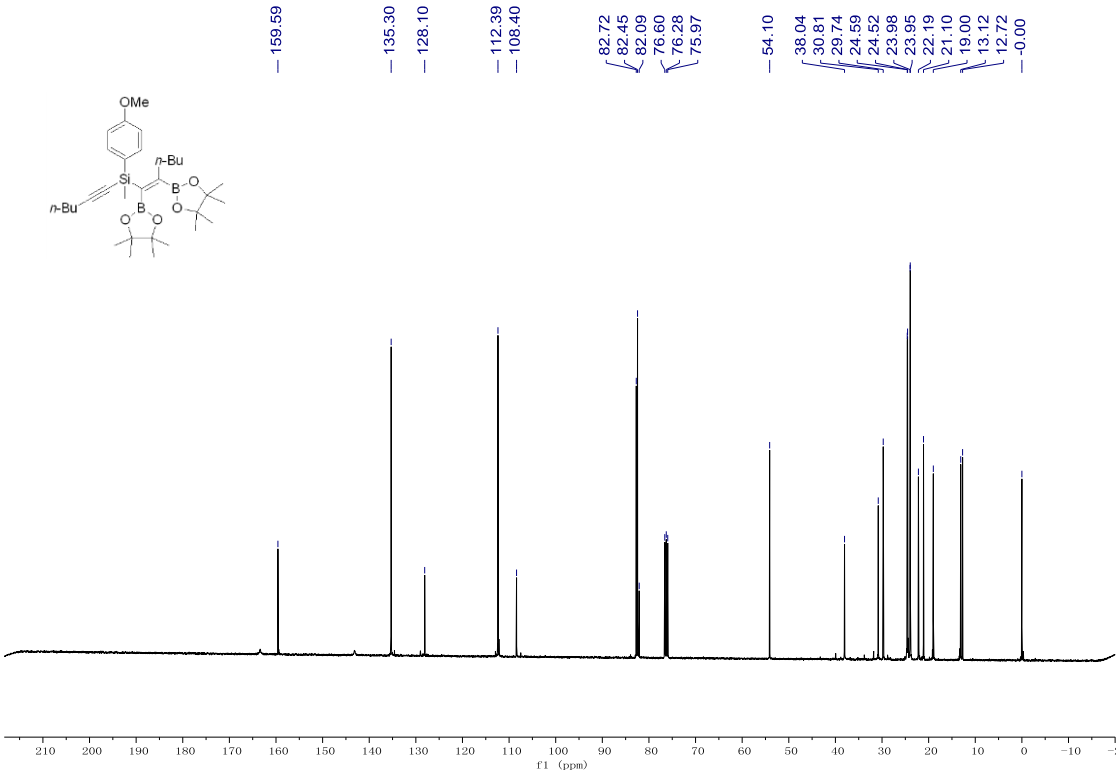
^{13}C NMR of **3b**



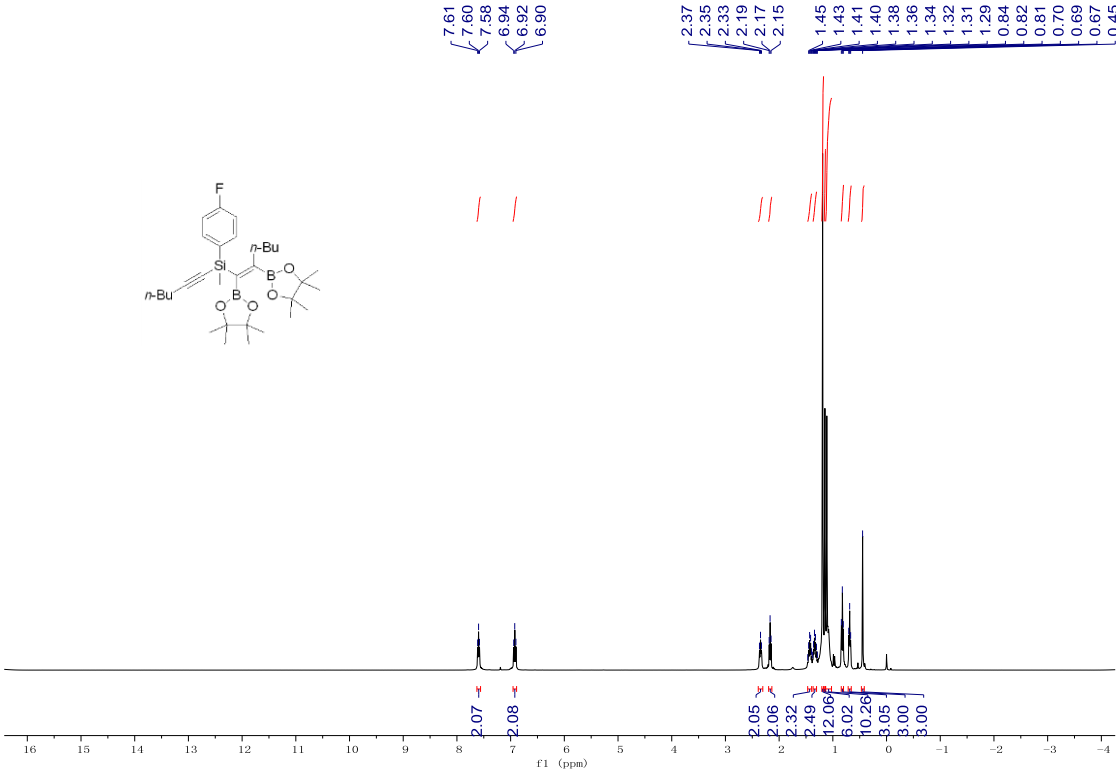
^{1}H NMR of **3c**



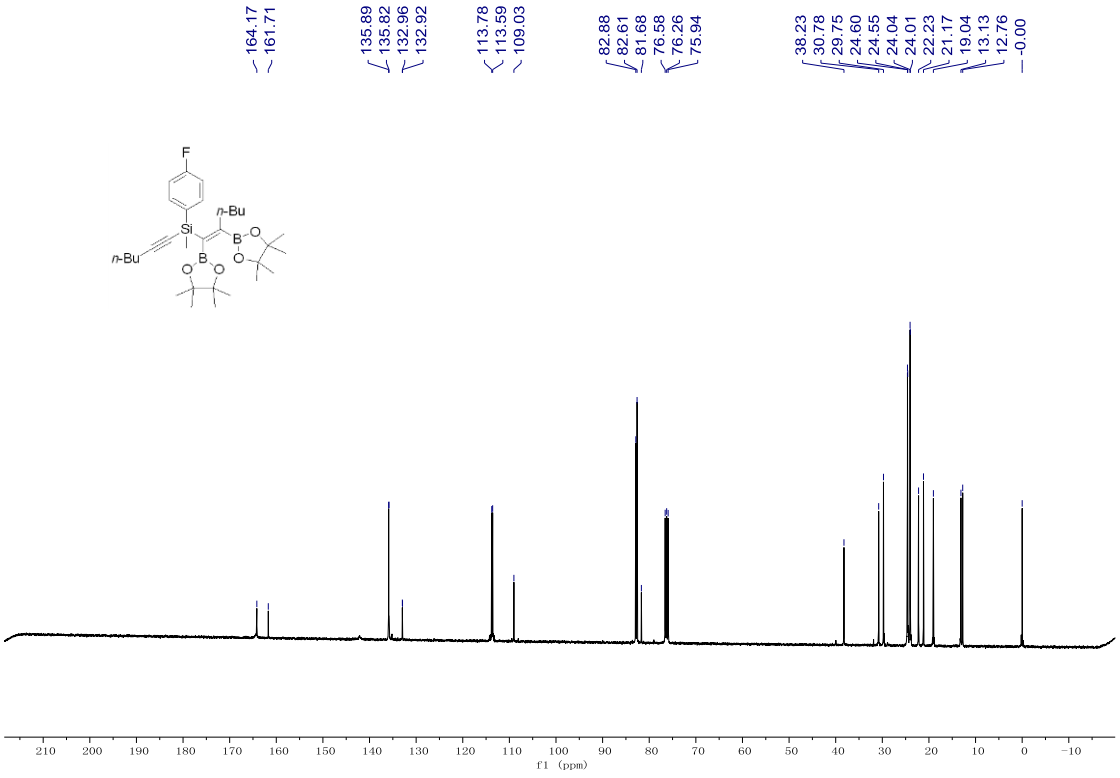
^{13}C NMR of **3c**



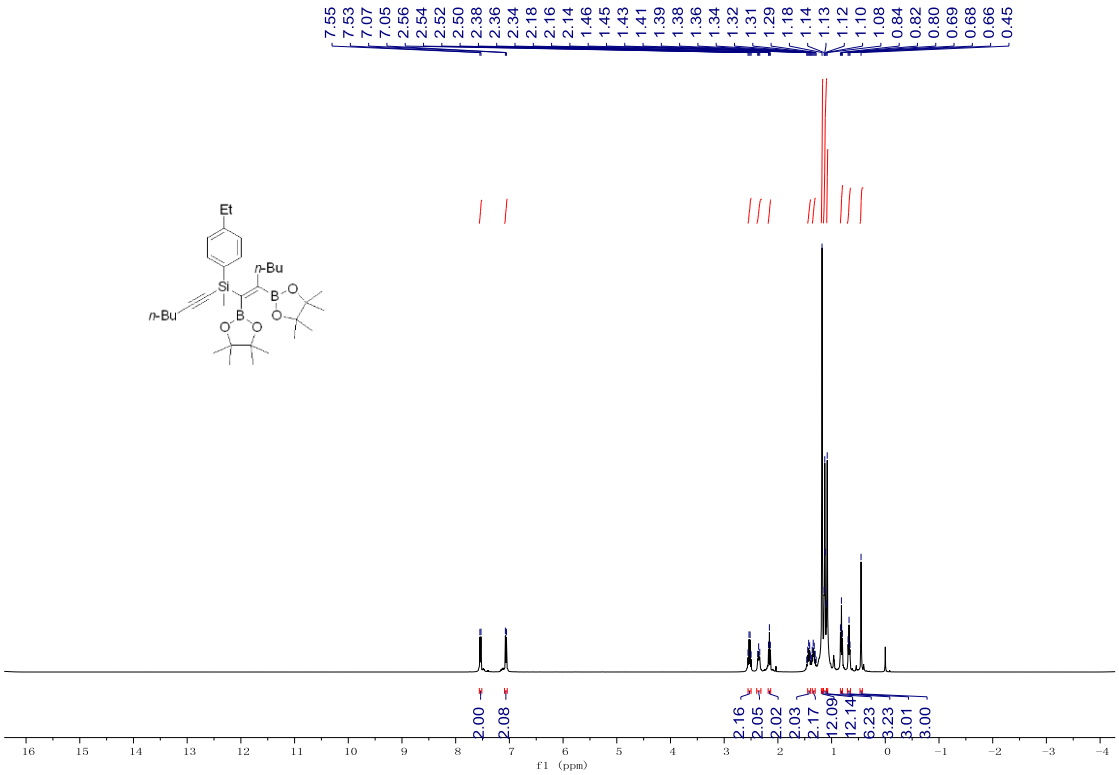
^{1}H NMR of **3d**



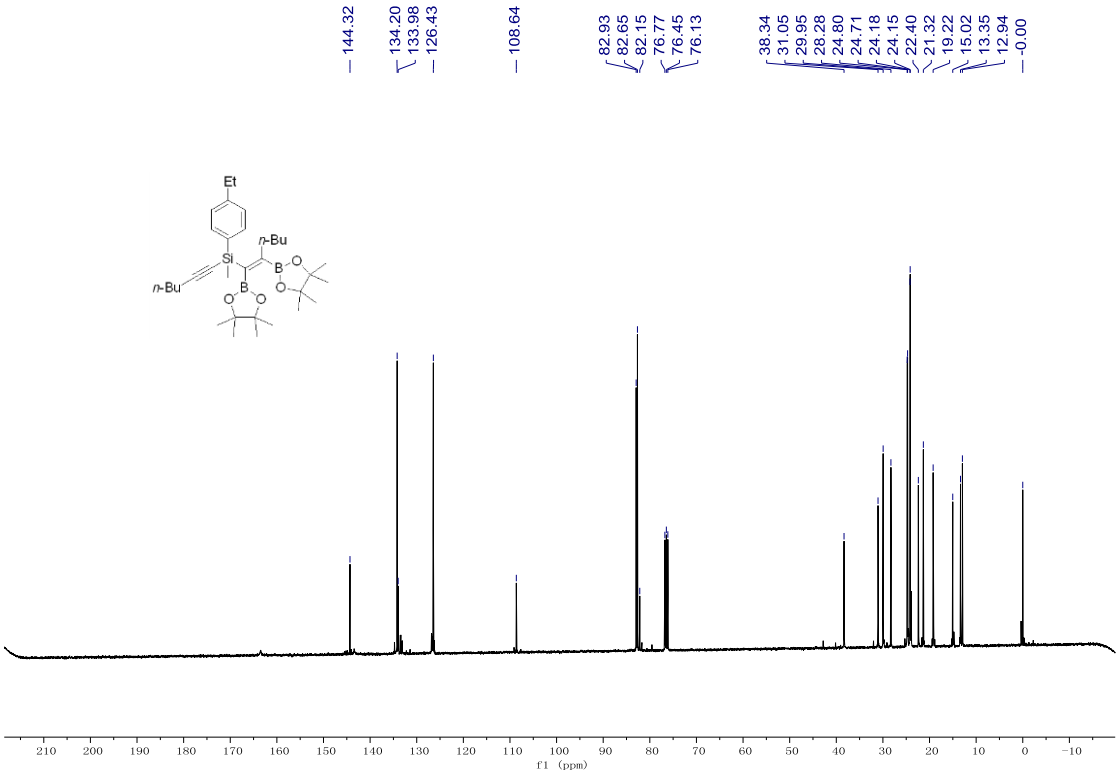
^{13}C NMR of **3d**



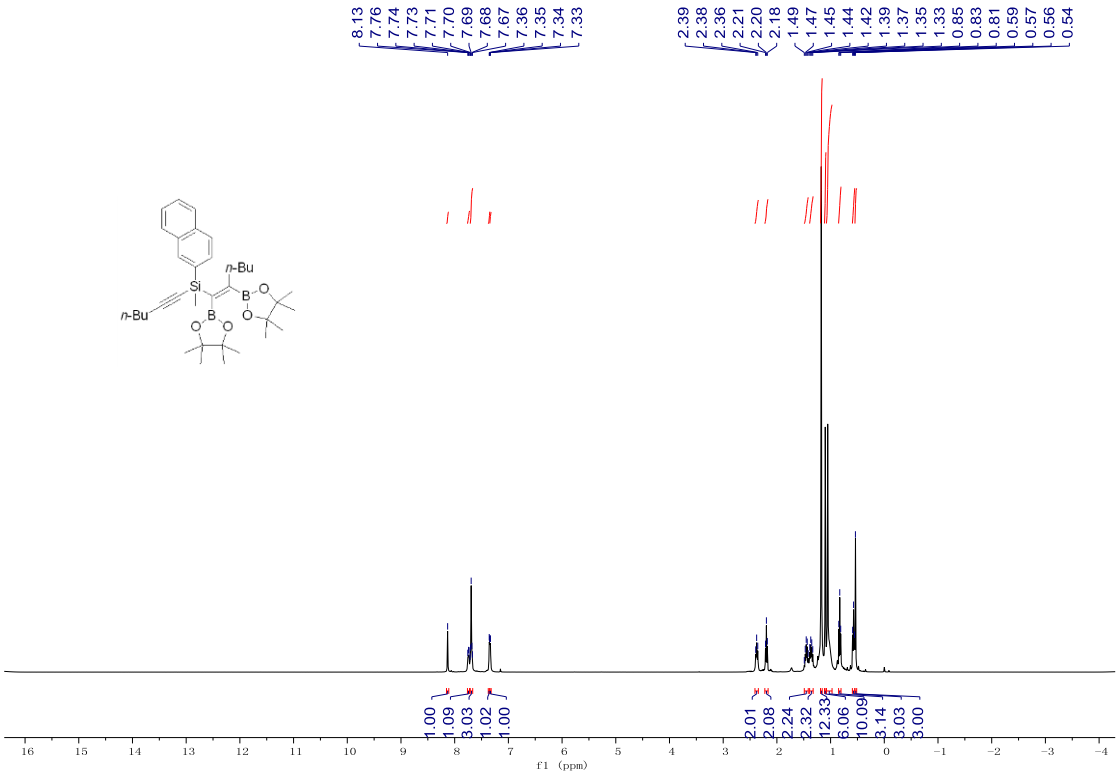
^{1}H NMR of **3e**



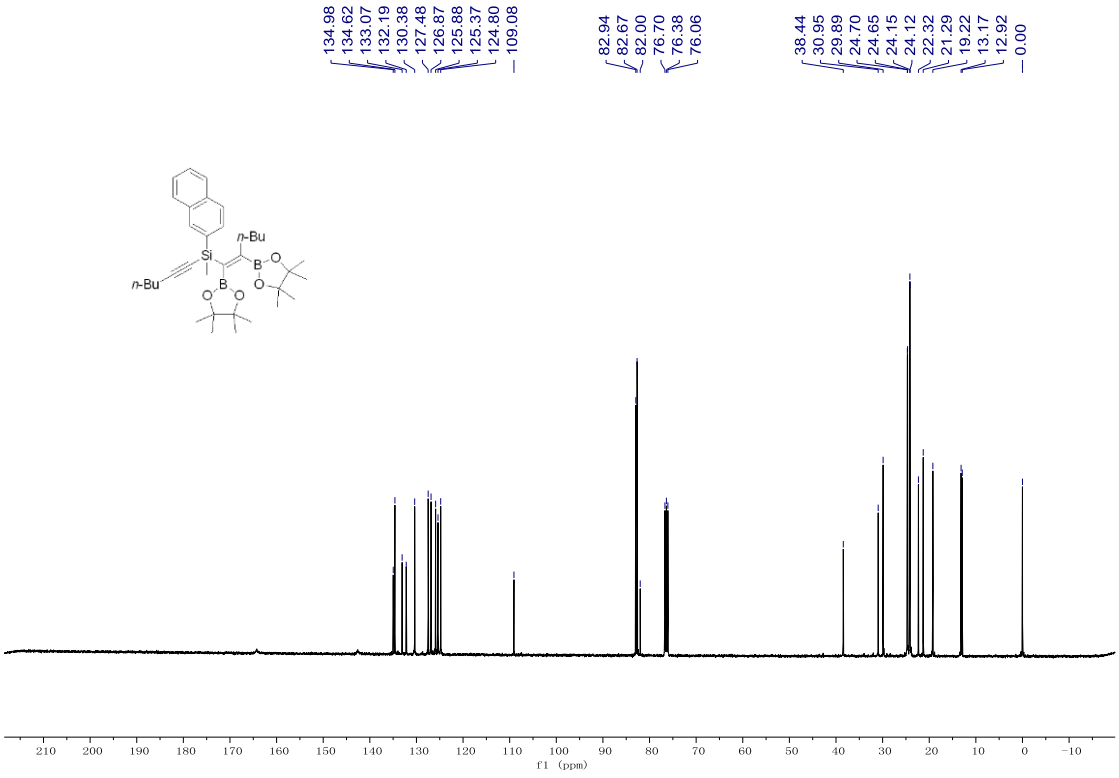
^{13}C NMR of **3e**



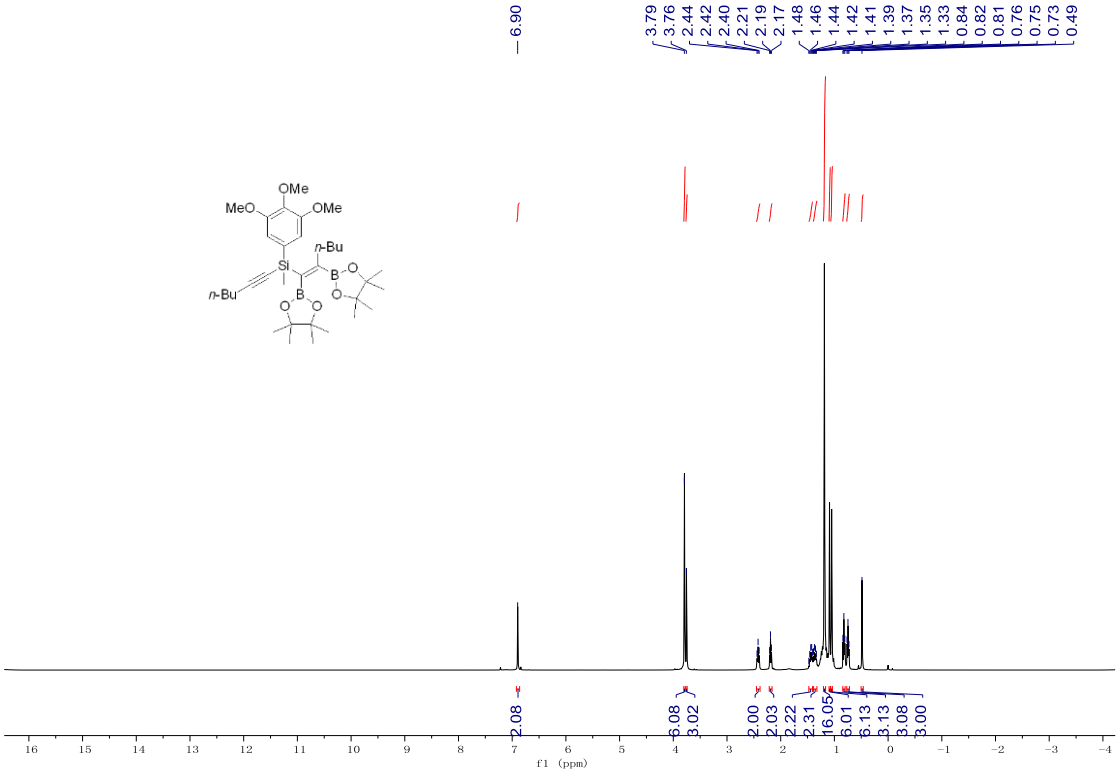
^{1}H NMR of **3f**



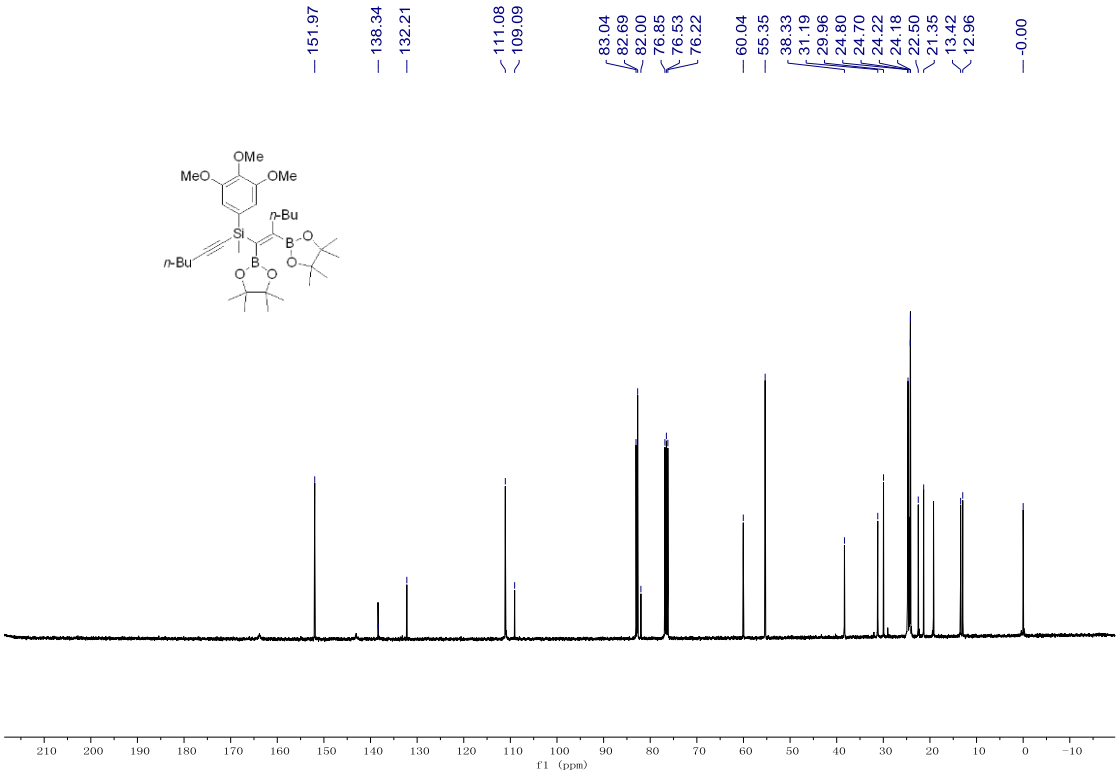
^{13}C NMR of **3f**



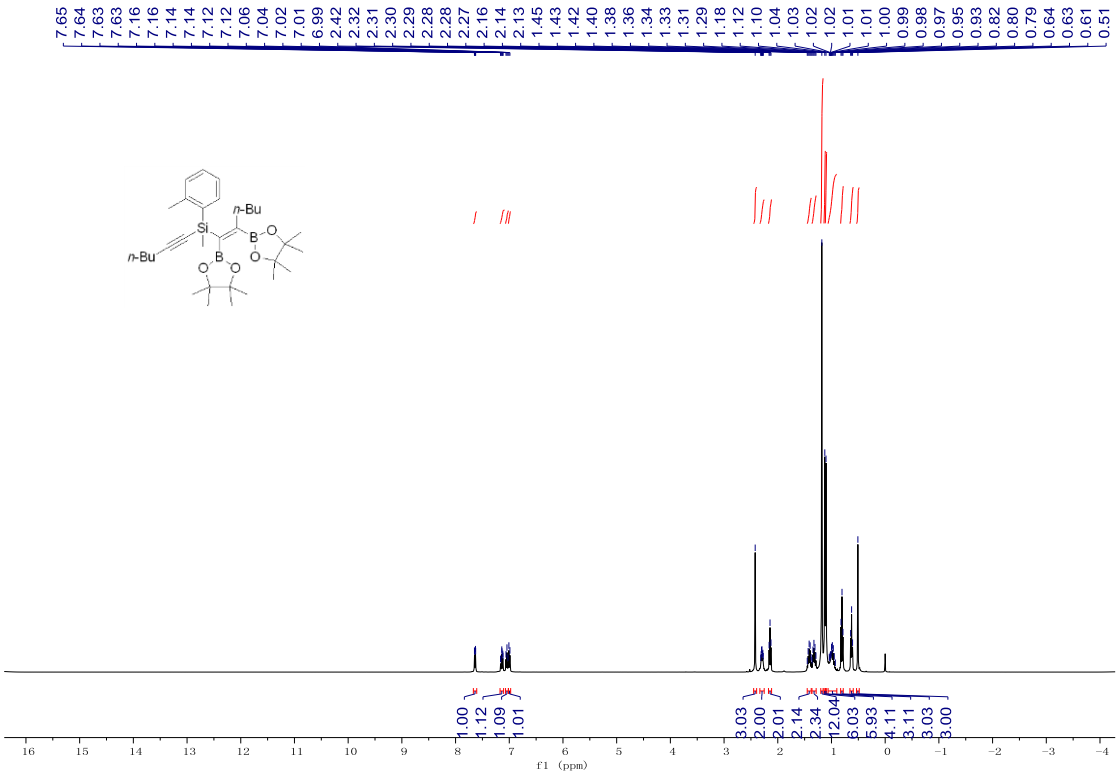
^{1}H NMR of **3g**



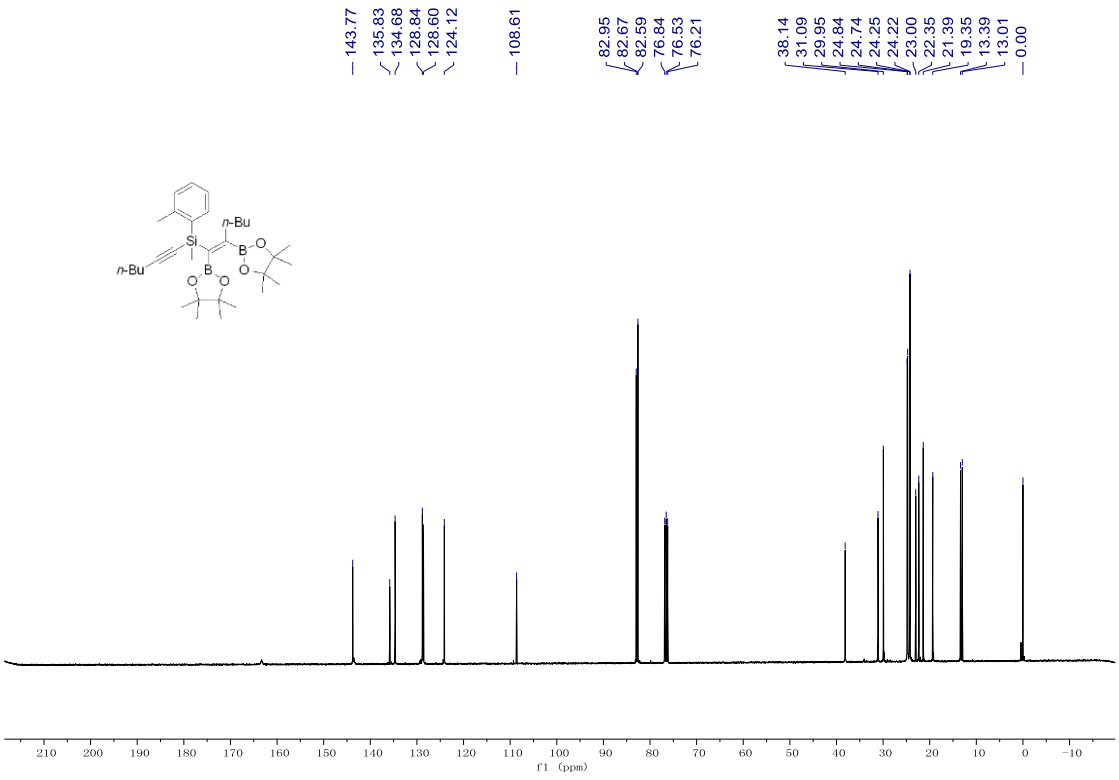
^{13}C NMR of **3g**



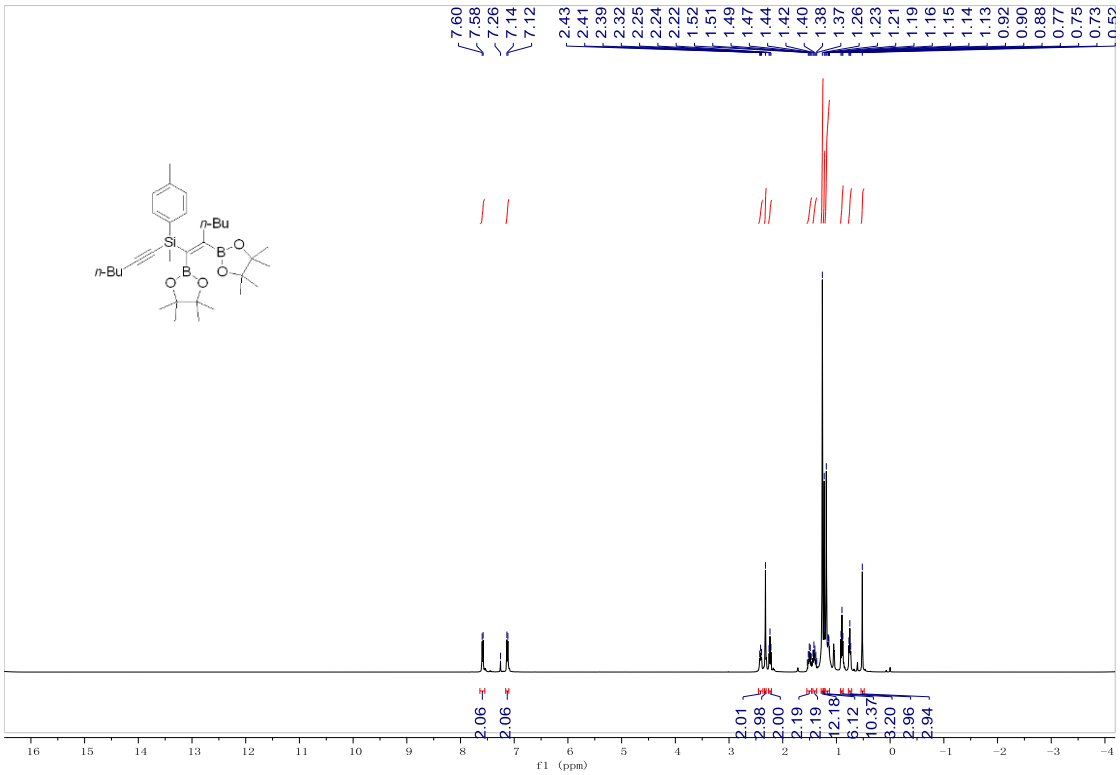
^{1}H NMR of **3h**



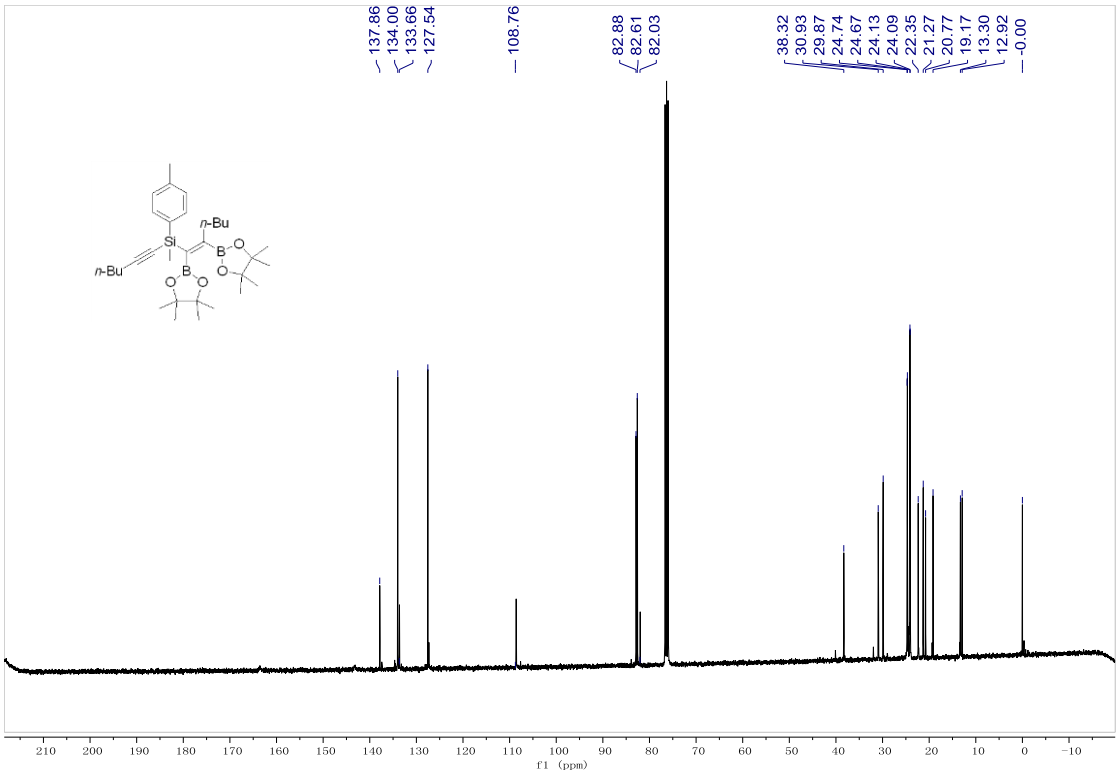
^{13}C NMR of **3h**



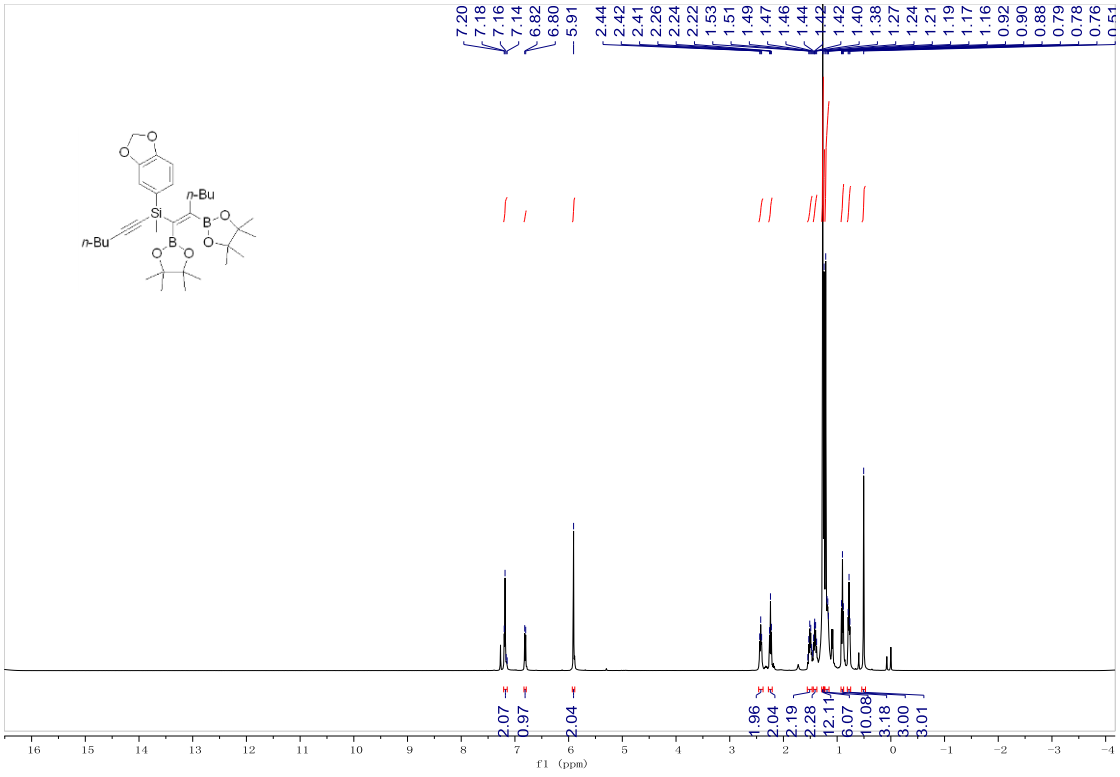
^{1}H NMR of **3i**



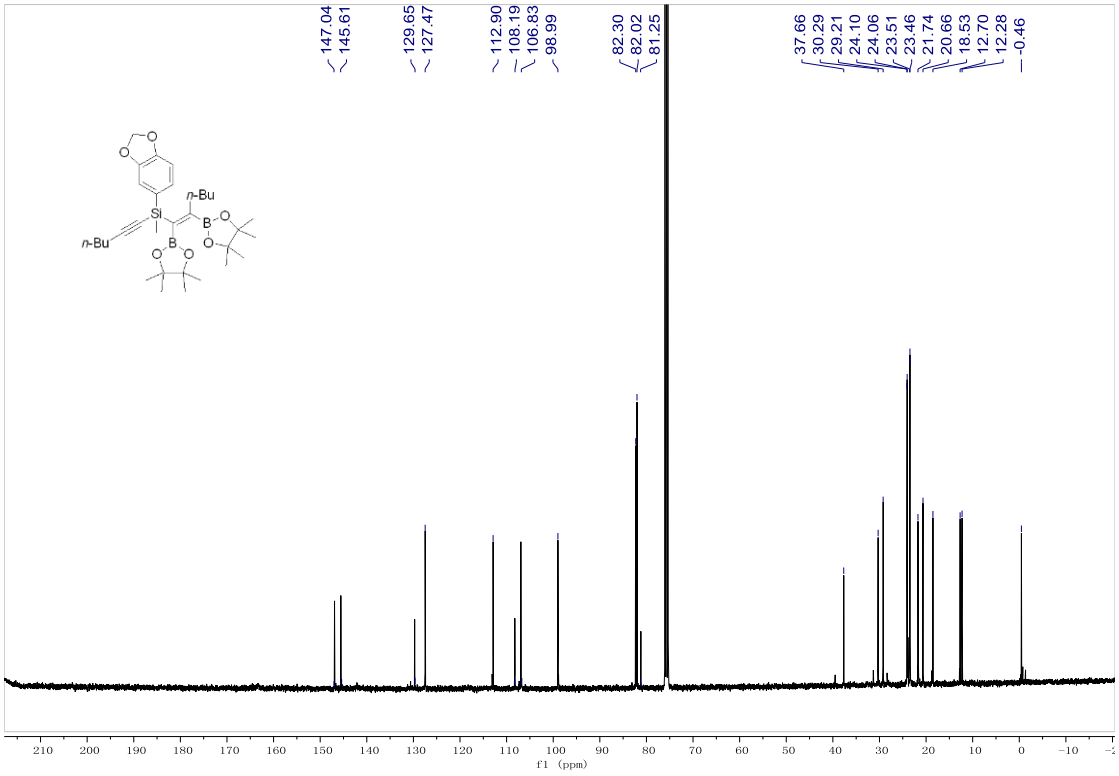
^{13}C NMR of **3i**



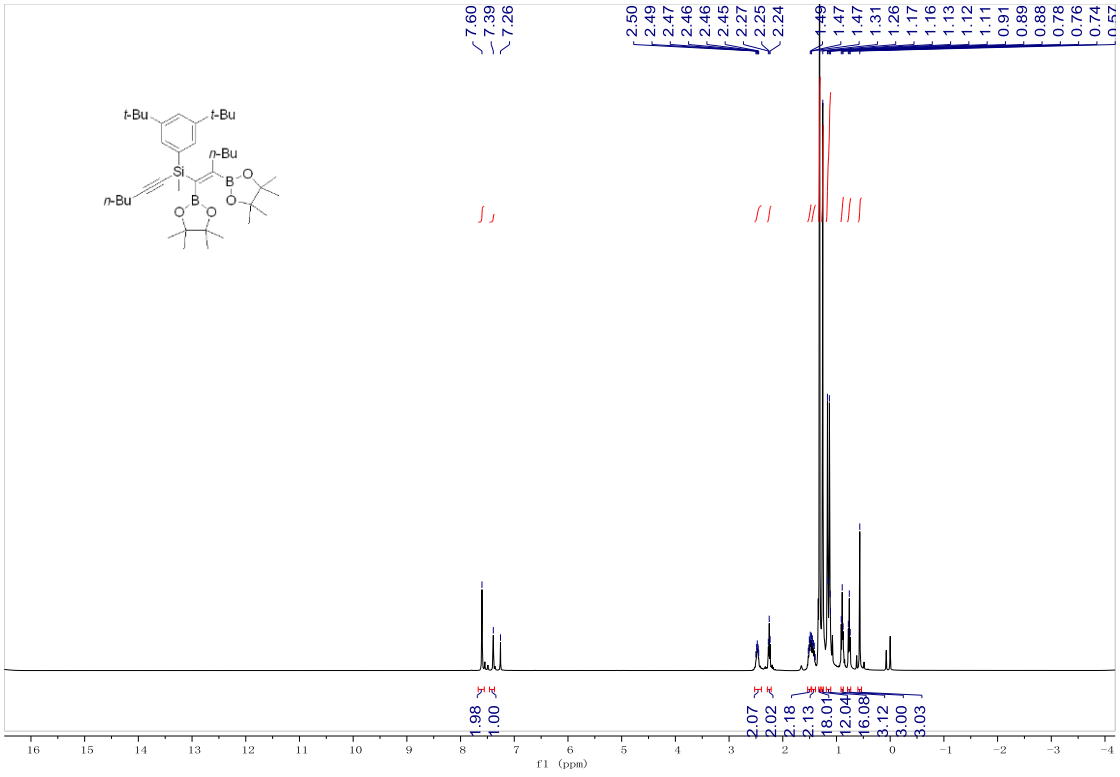
^{1}H NMR of **3j**



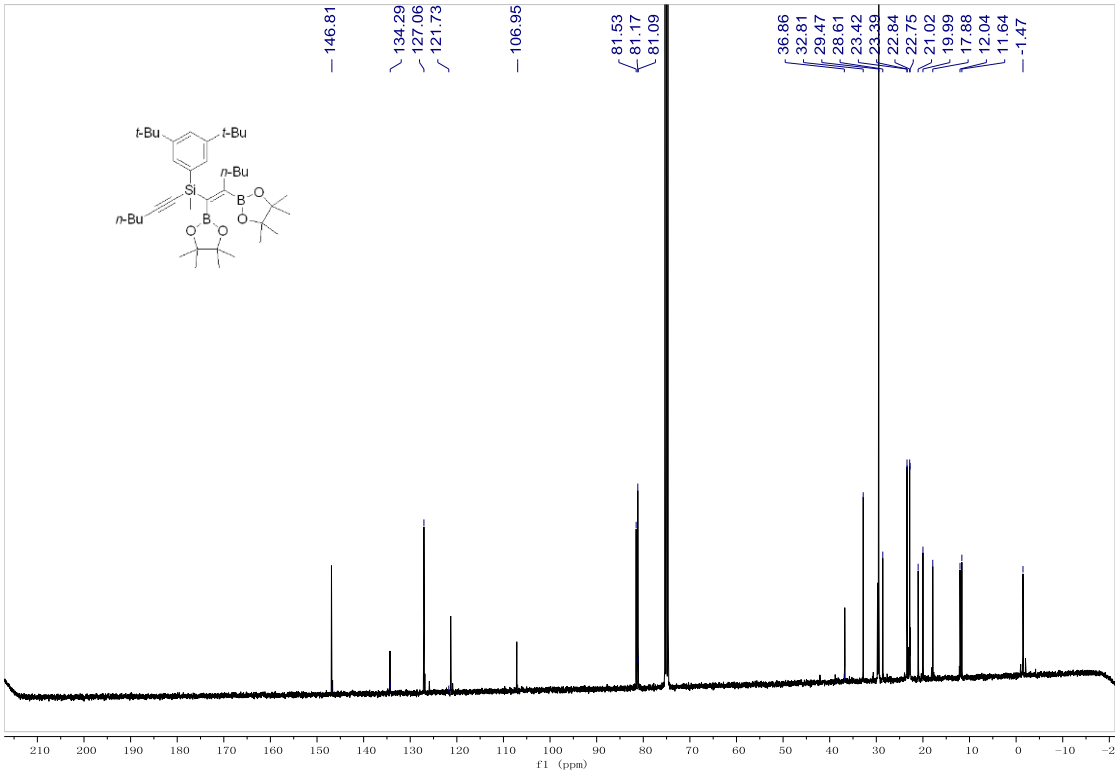
^{13}C NMR of **3j**



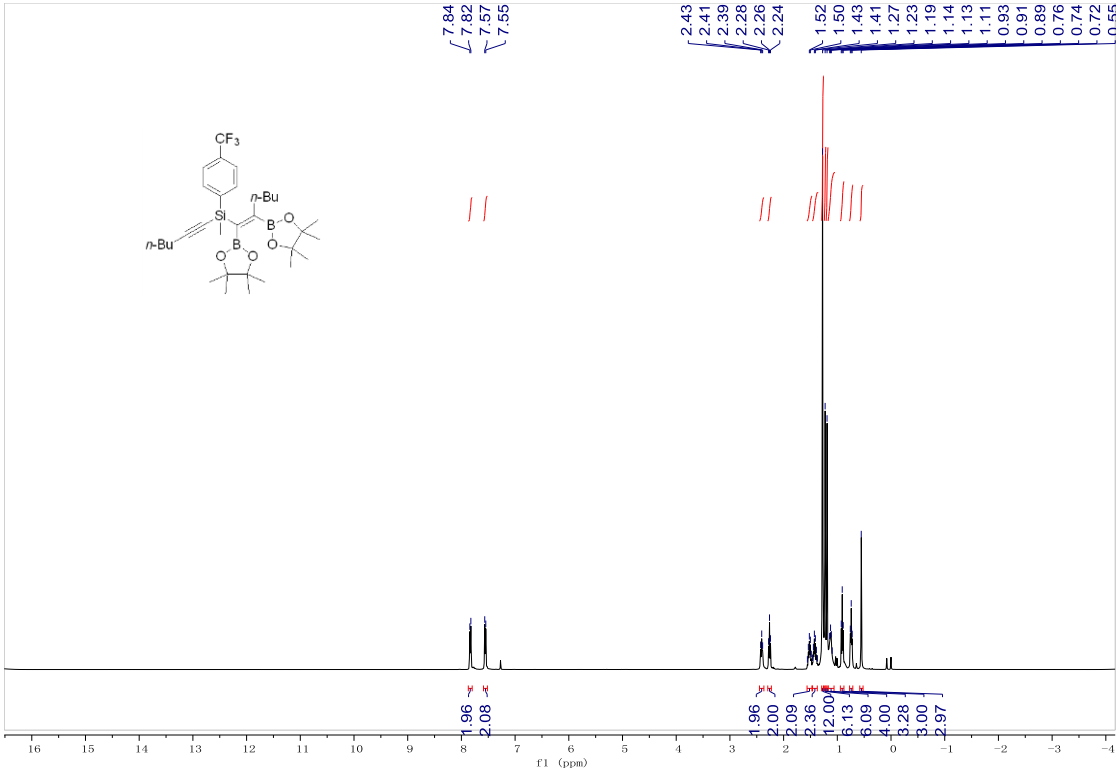
^{1}H NMR of **3k**



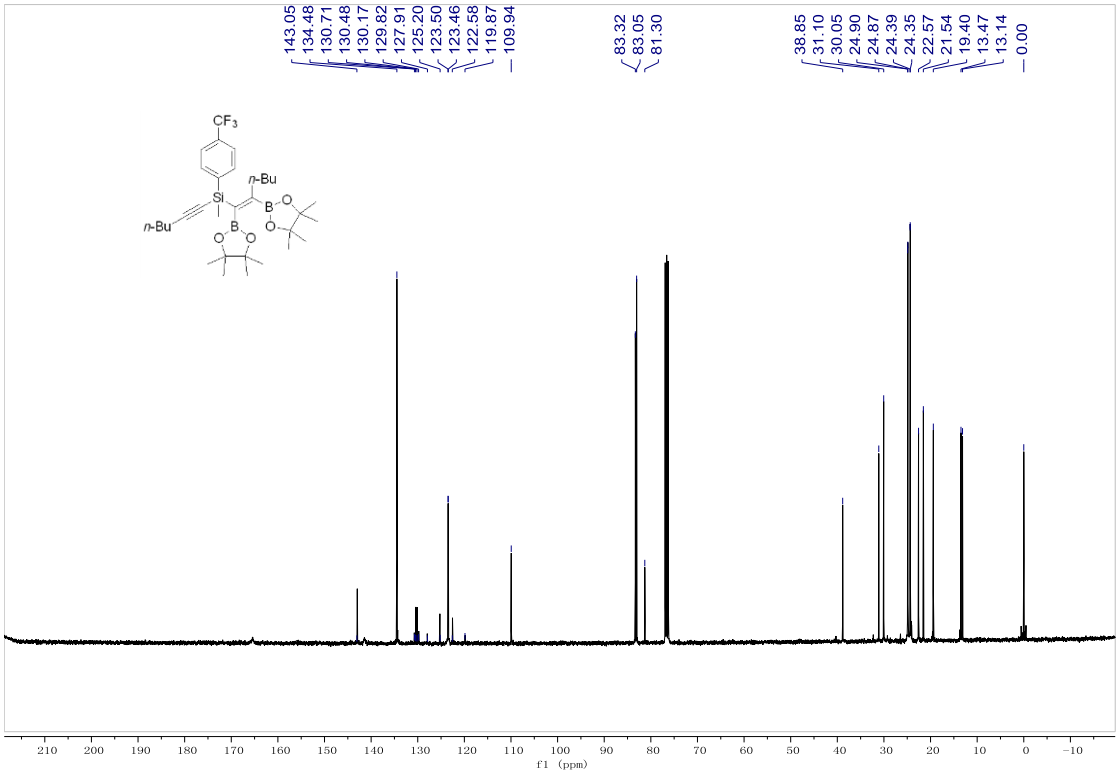
^{13}C NMR of **3k**



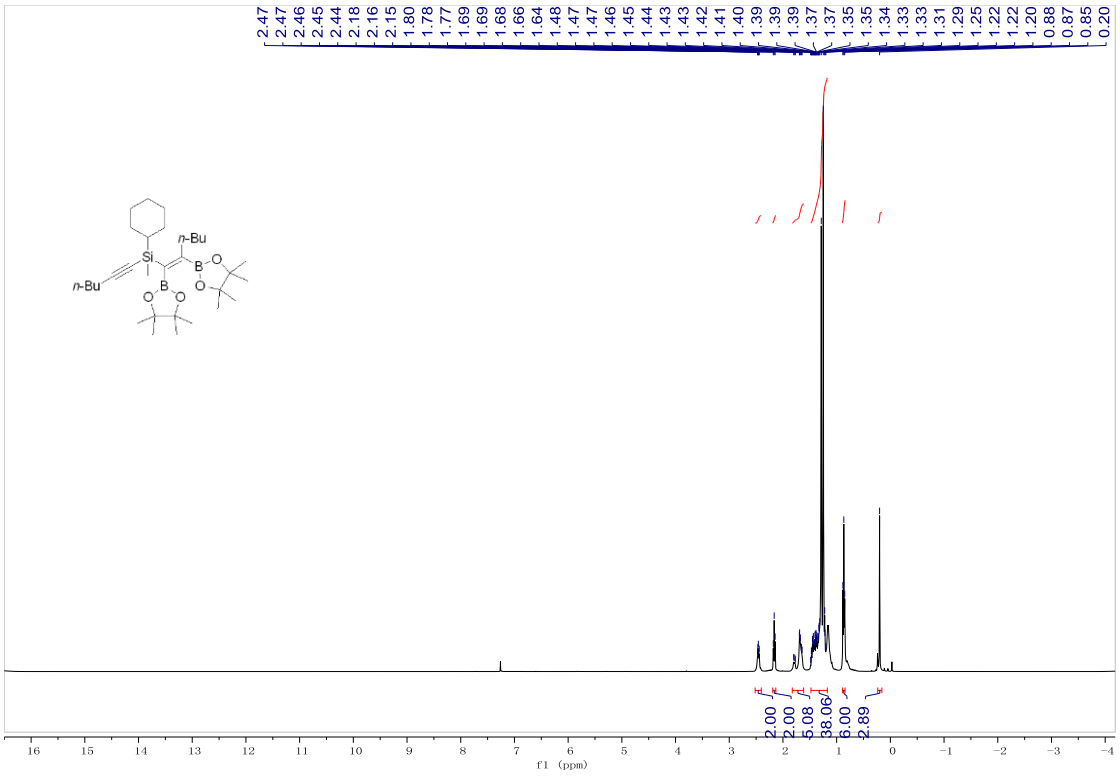
^{1}H NMR of **3l**



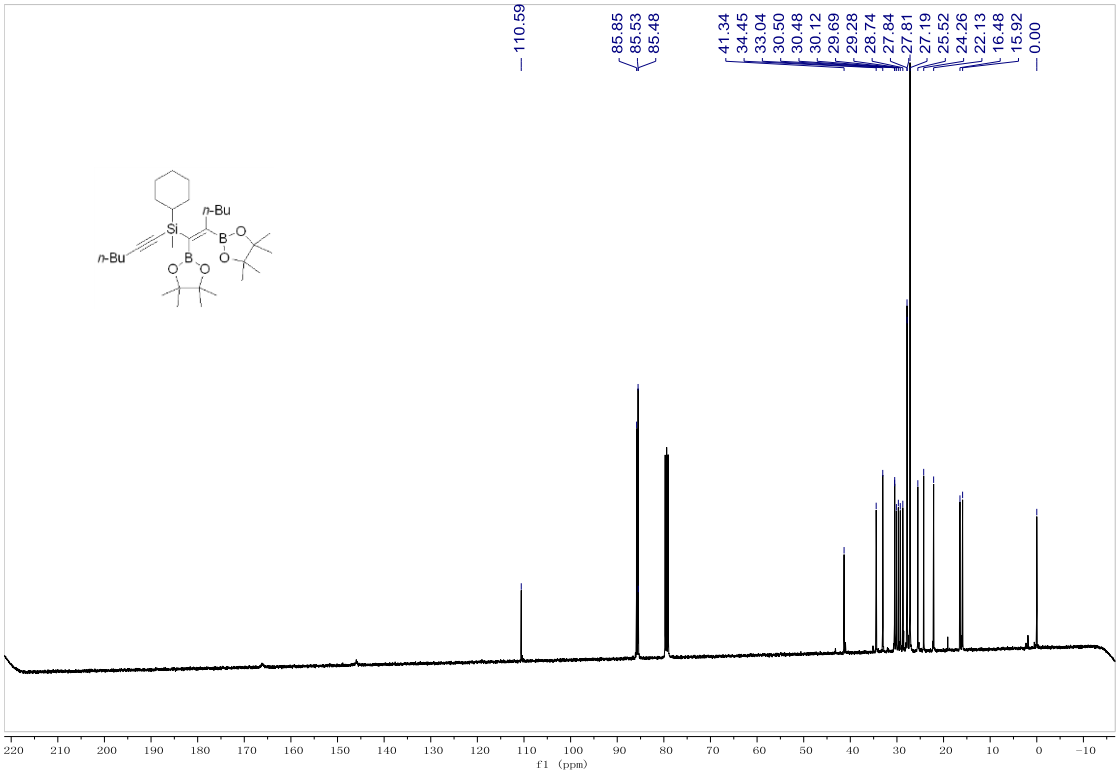
^{13}C NMR of **3l**



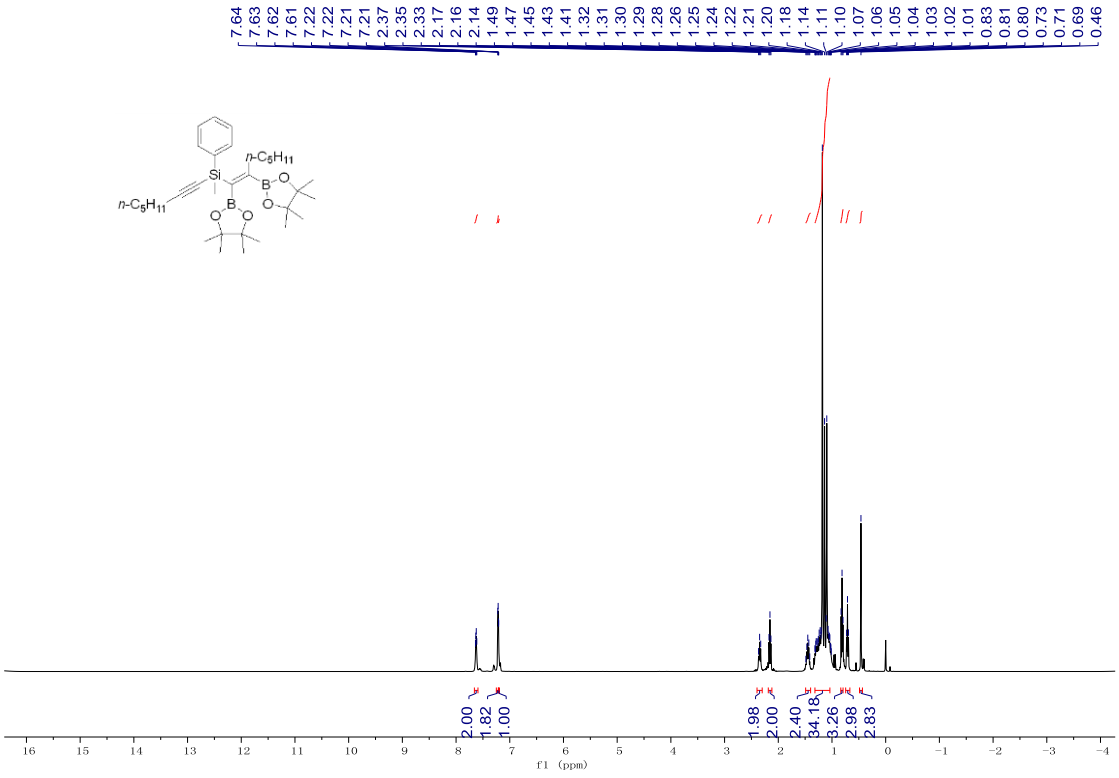
^{1}H NMR of **3m**



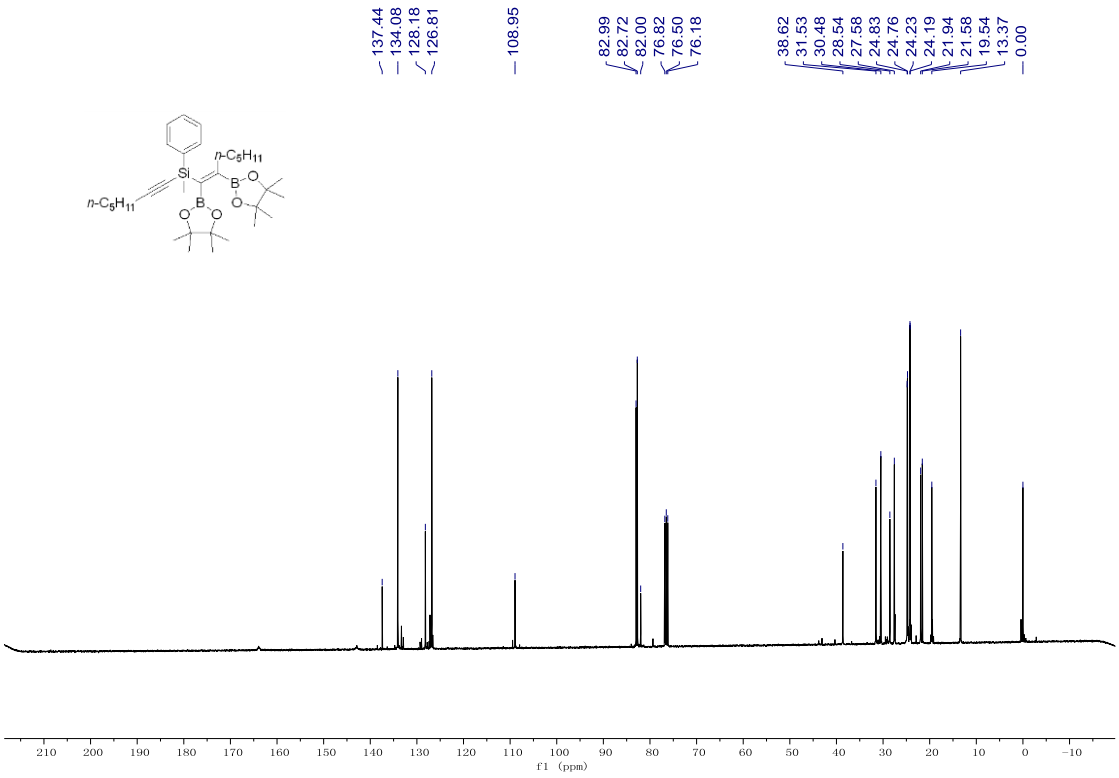
^{13}C NMR of **3m**



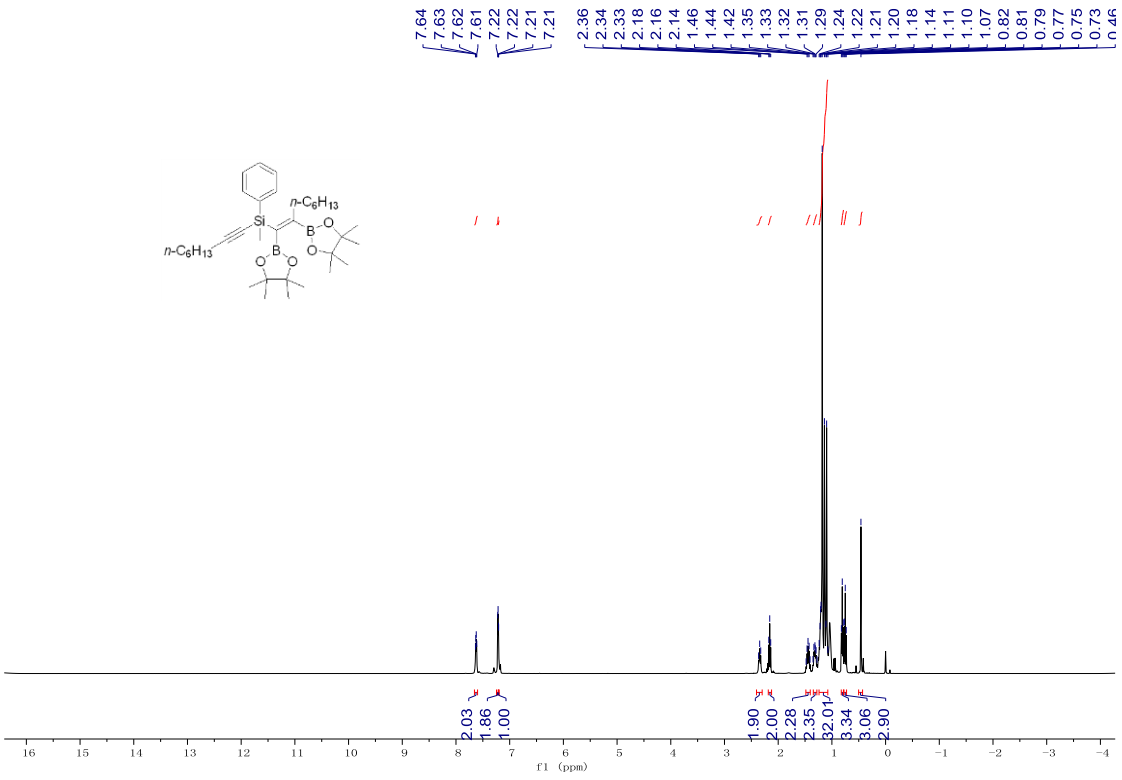
^{1}H NMR of **3n**



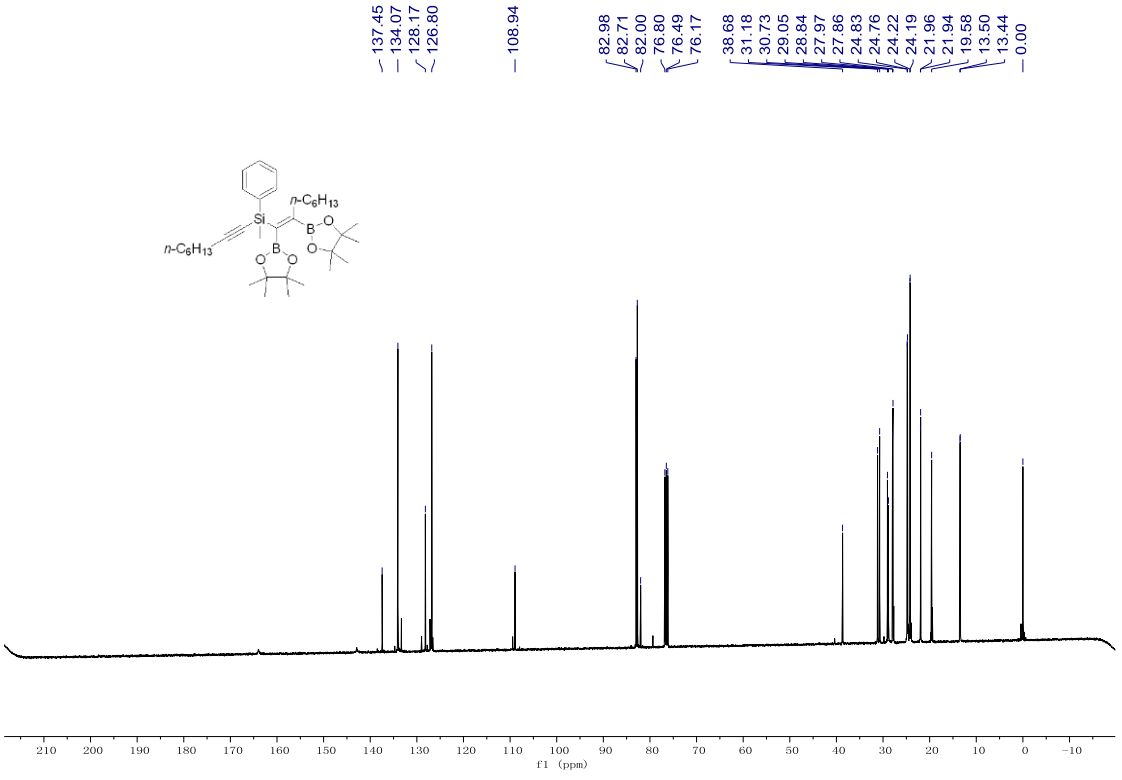
^{13}C NMR of **3n**



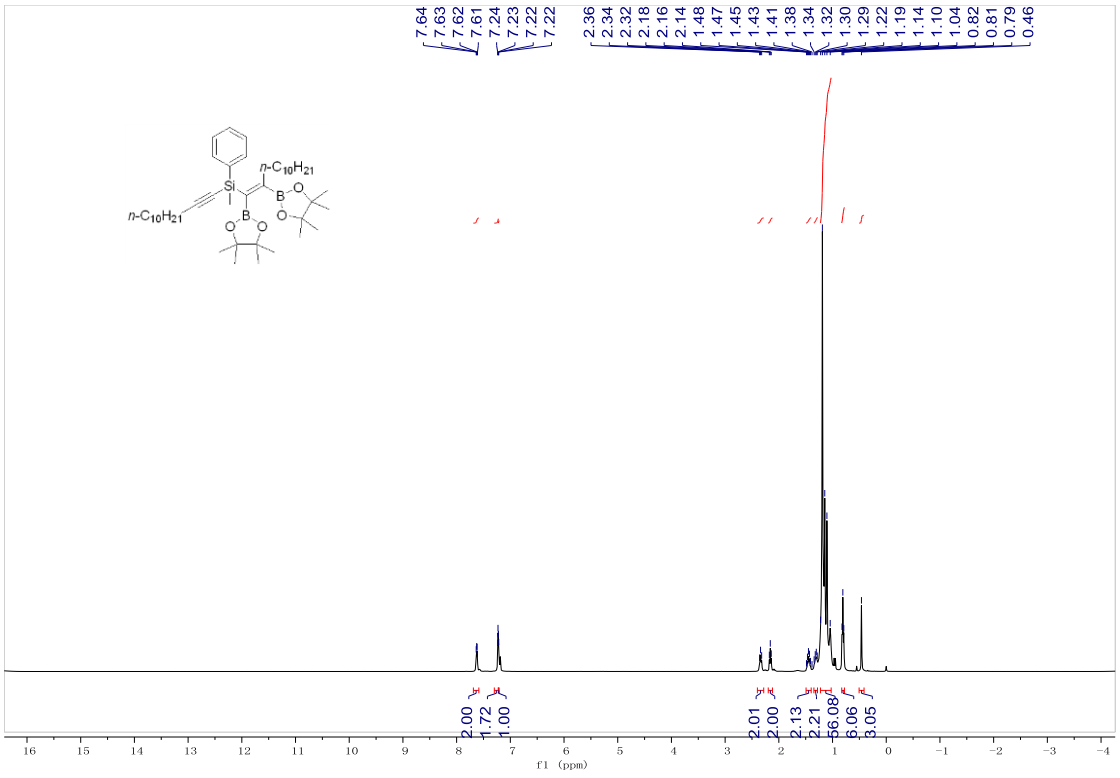
^{1}H NMR of **3o**



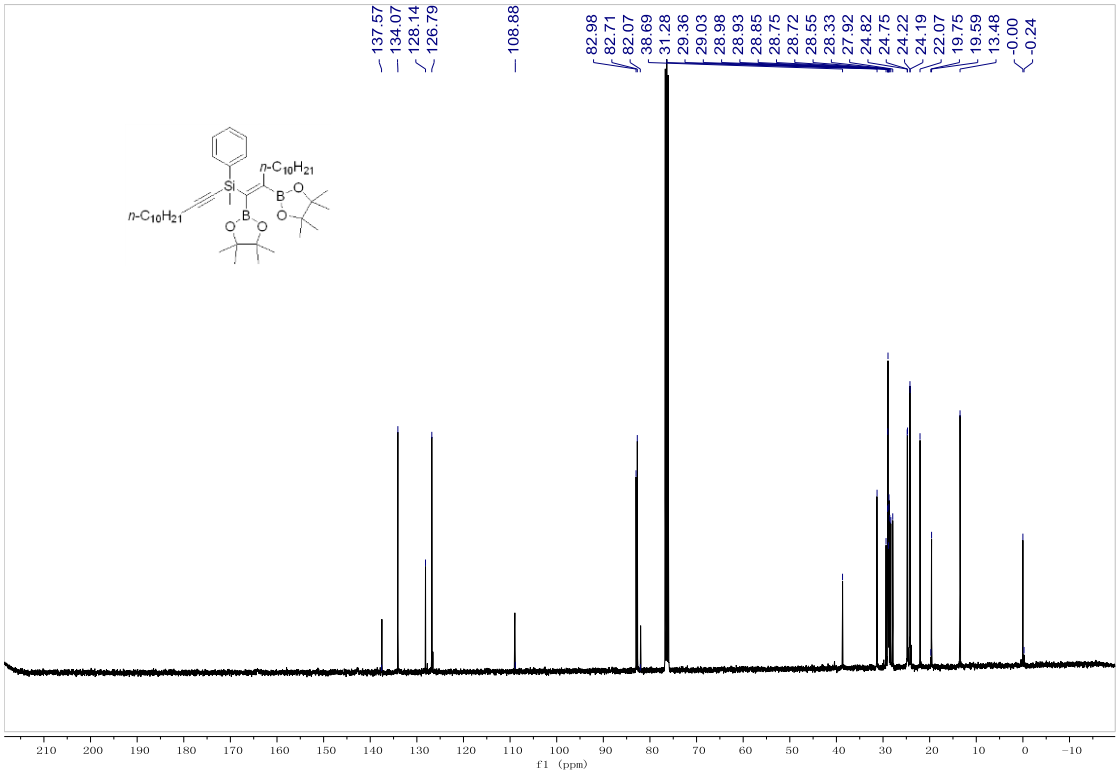
^{13}C NMR of **3o**



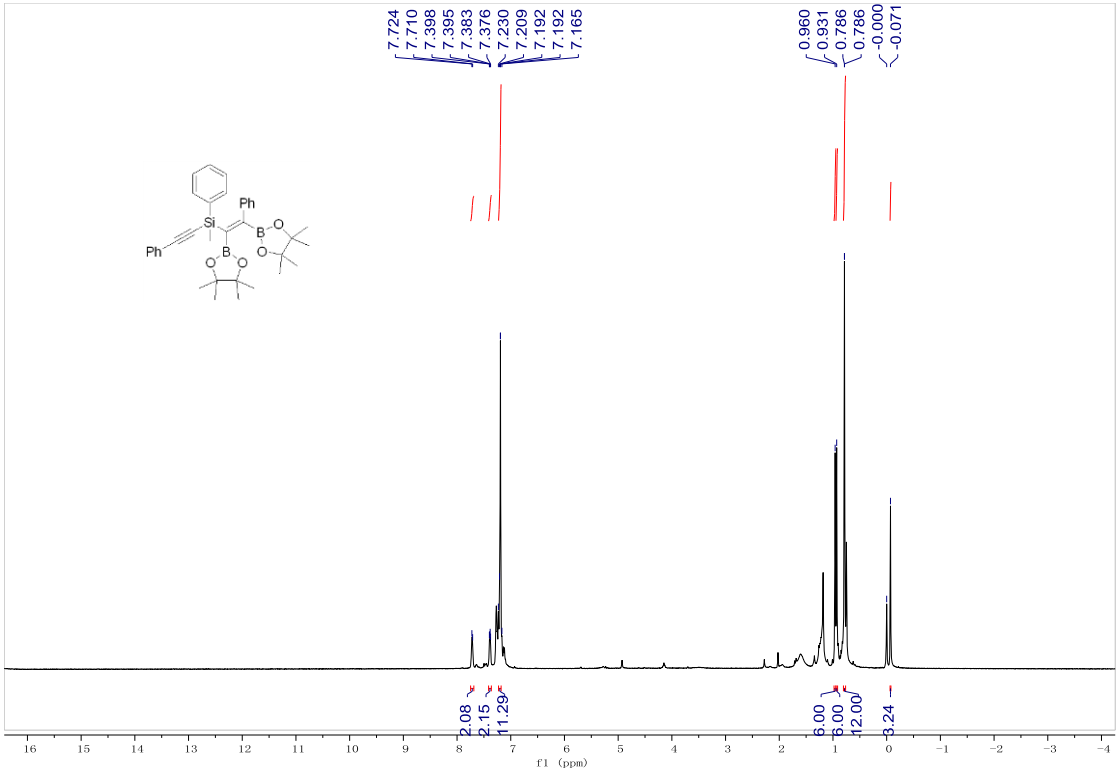
^{1}H NMR of **3p**



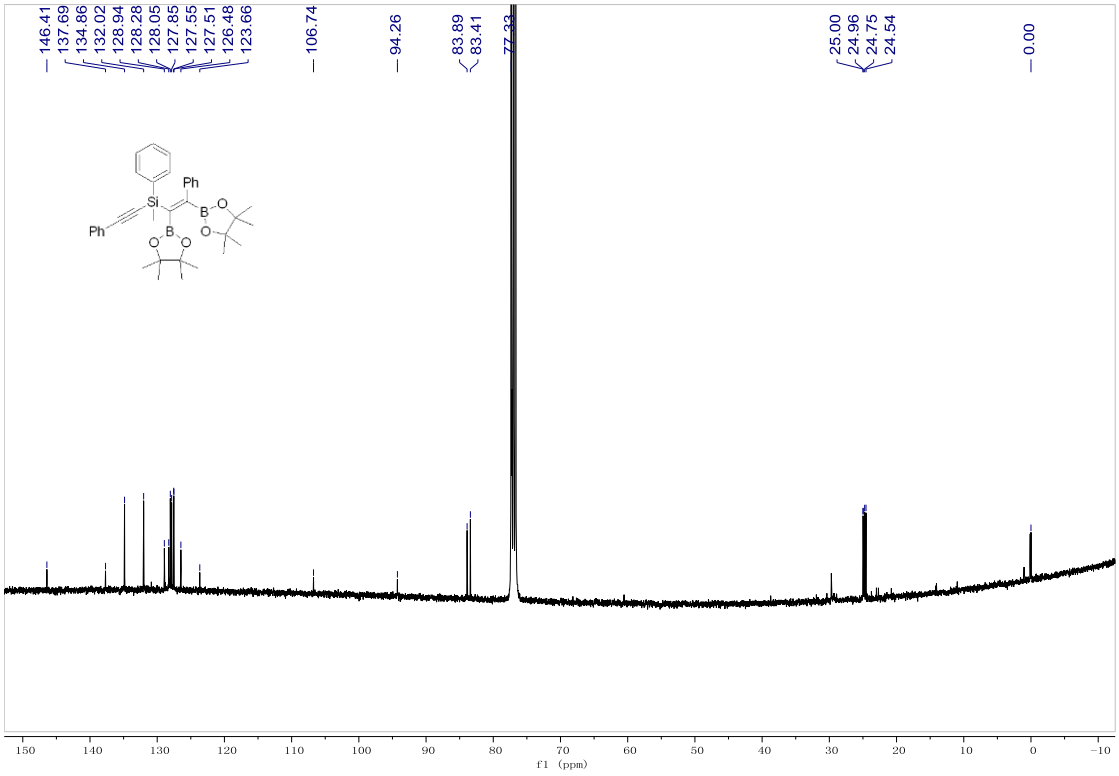
^{13}C NMR of **3p**



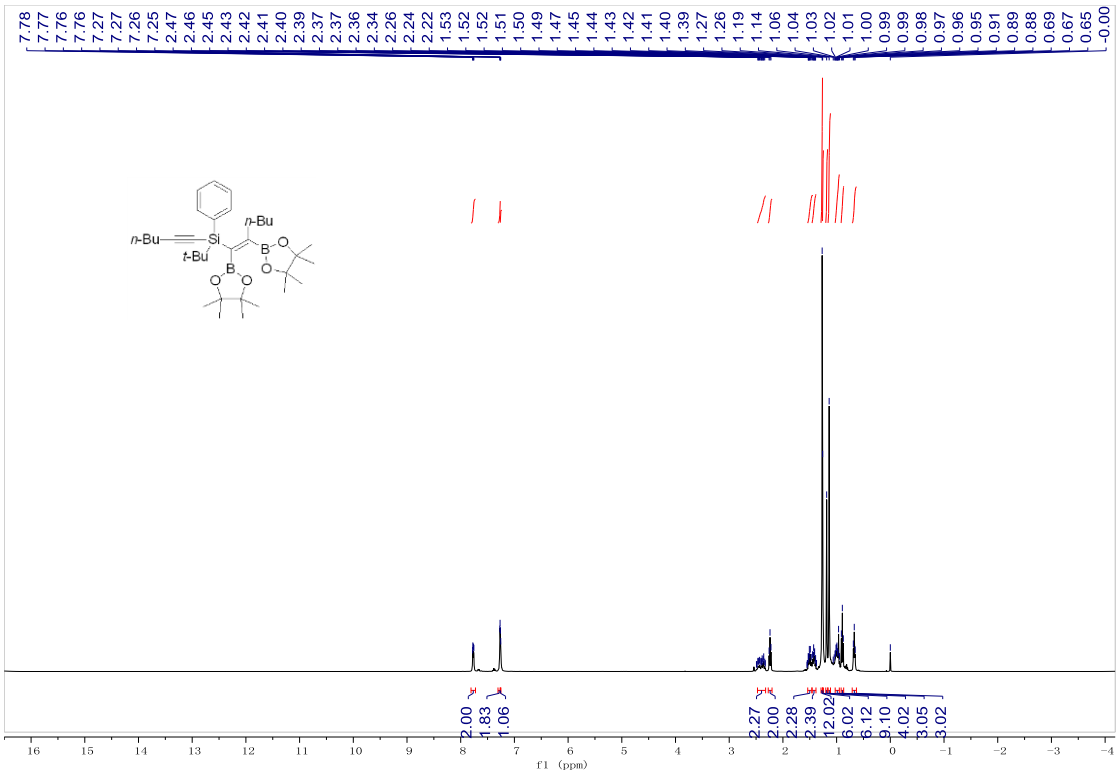
^{1}H NMR of **3q**



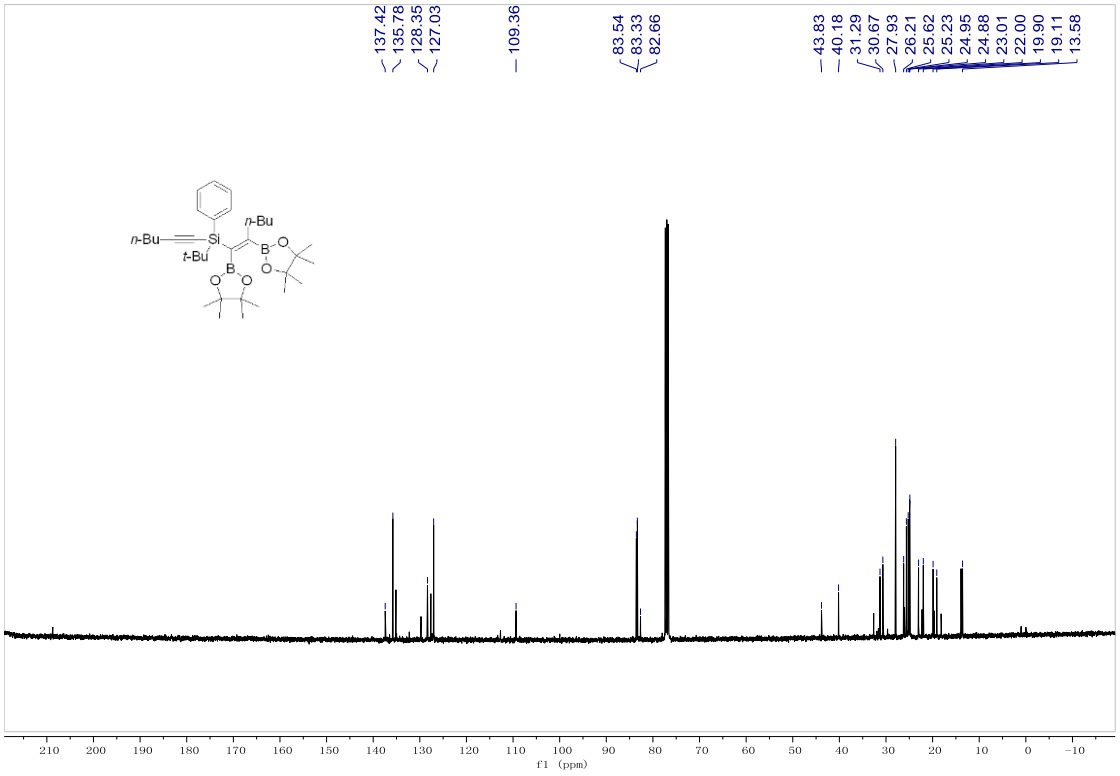
^{13}C NMR of **3q**



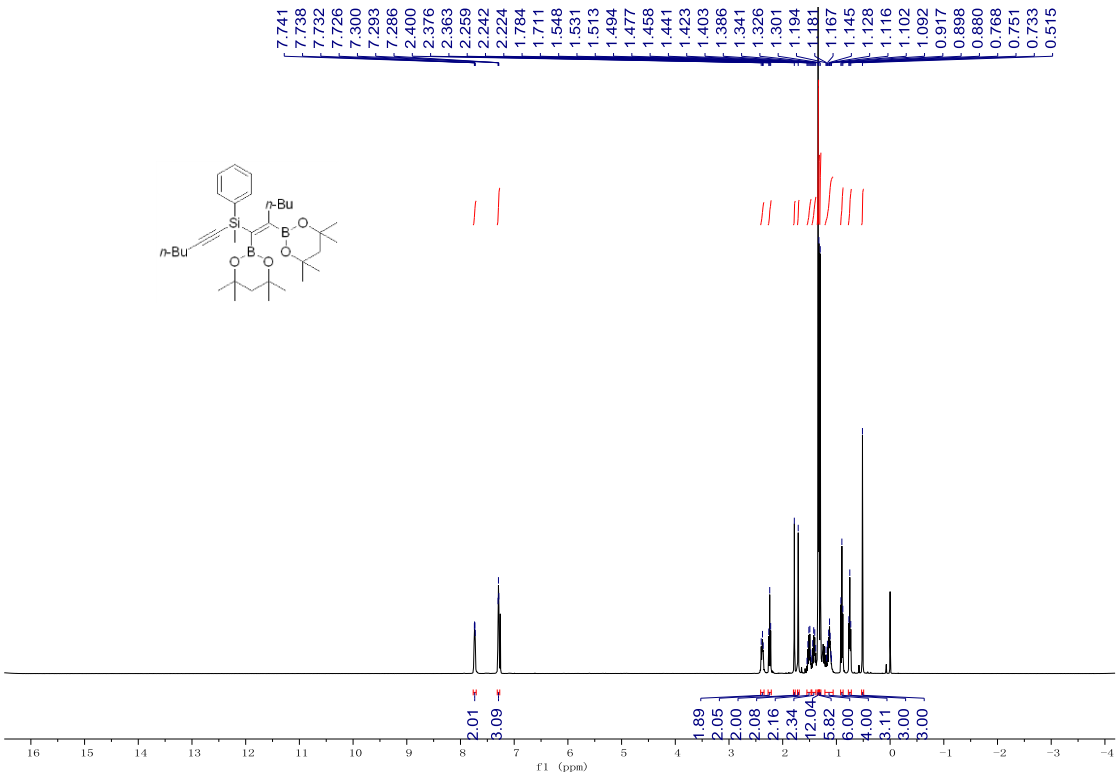
^{1}H NMR of **3r**



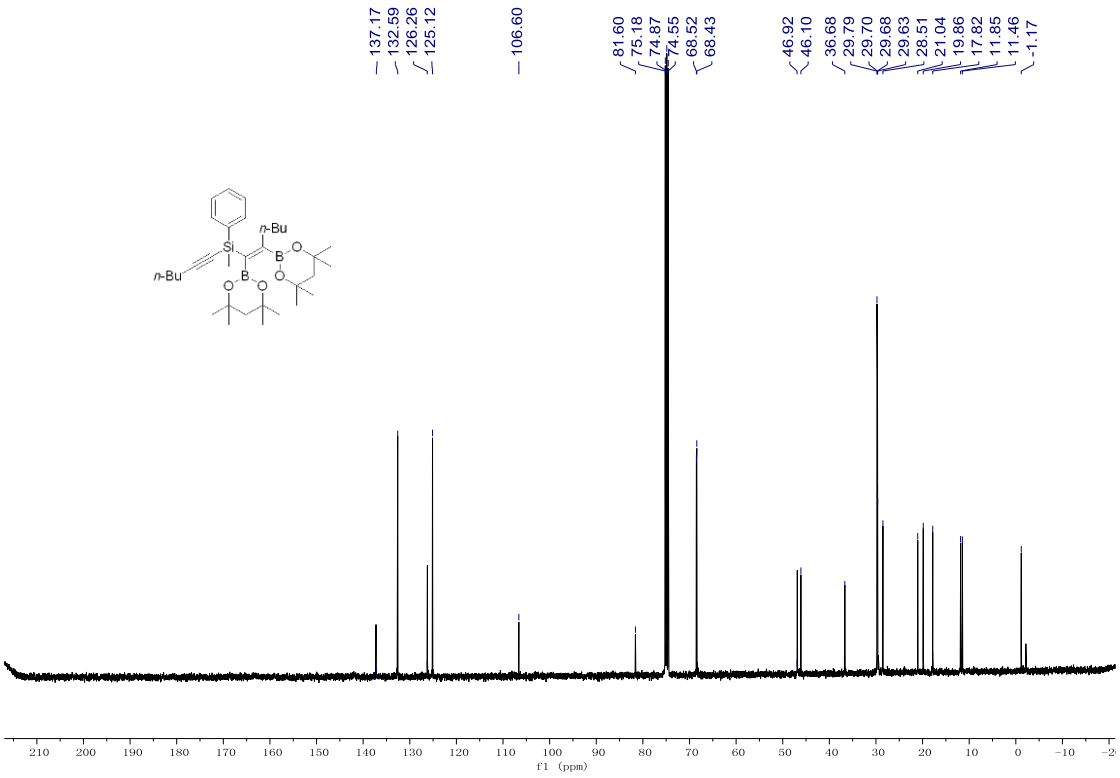
^{13}C NMR of **3r**



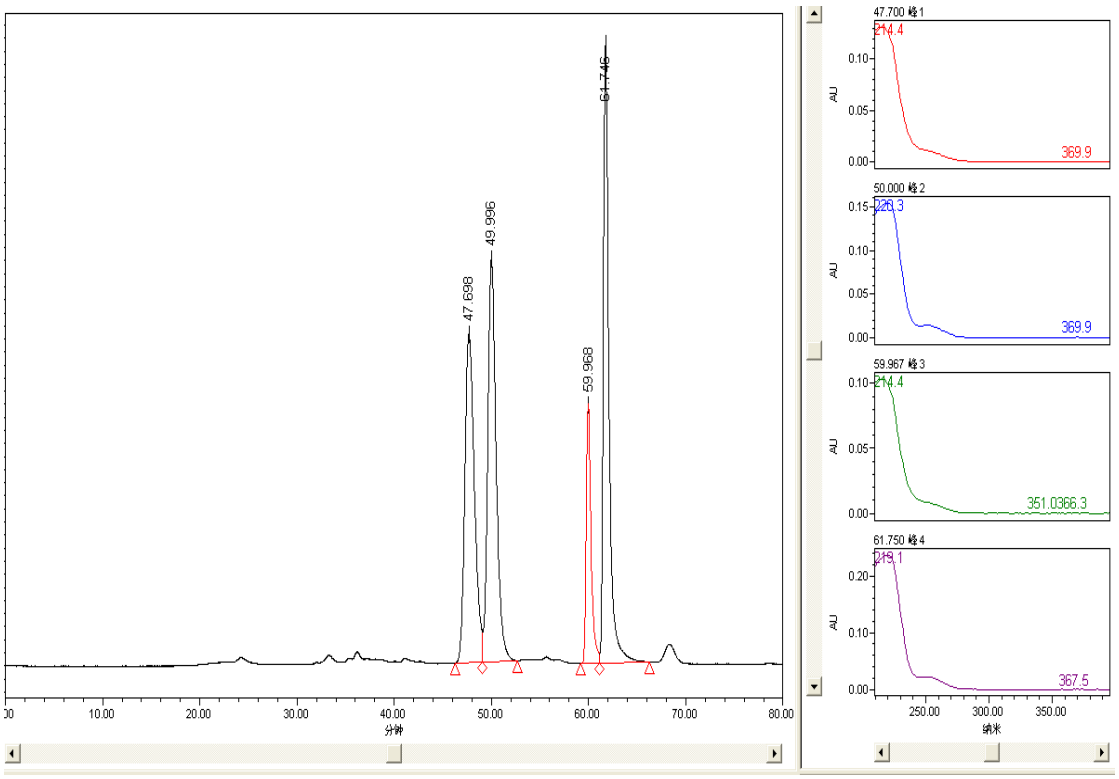
^{1}H NMR of **3s**



^{13}C NMR of **3s**



HPLC Spectra

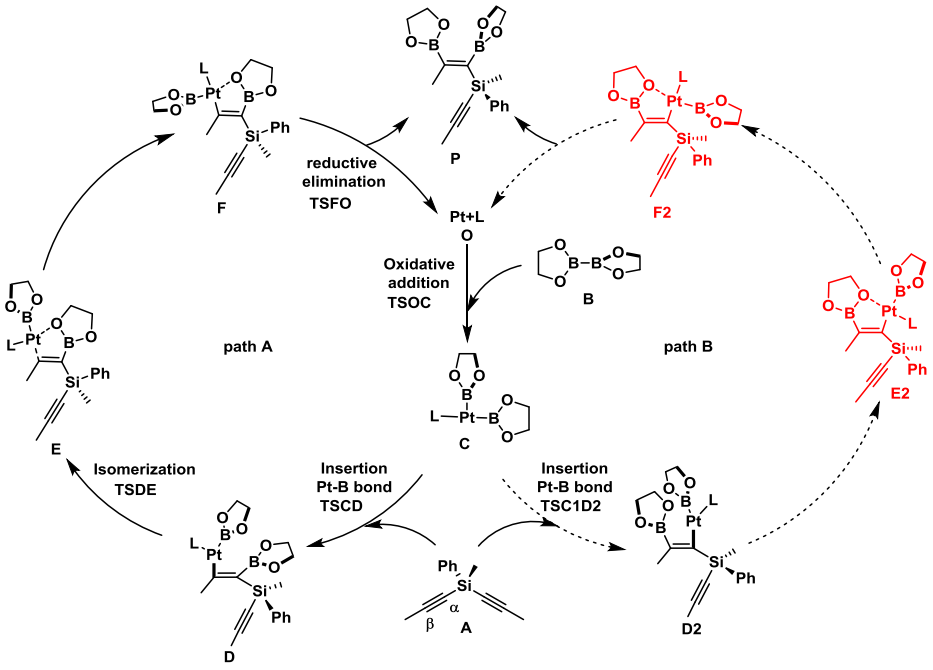


Peak	RetTime/min	Area%
1	47.698	72
2	59.968	28

Peak	RetTime/min	Area%
3	49.996	50
4	61.746	50

Computational studies by DFT

Ⅰ. A proposed catalytic cycles for the model reaction system



Ⅱ. Calculated Potential Energy Surface

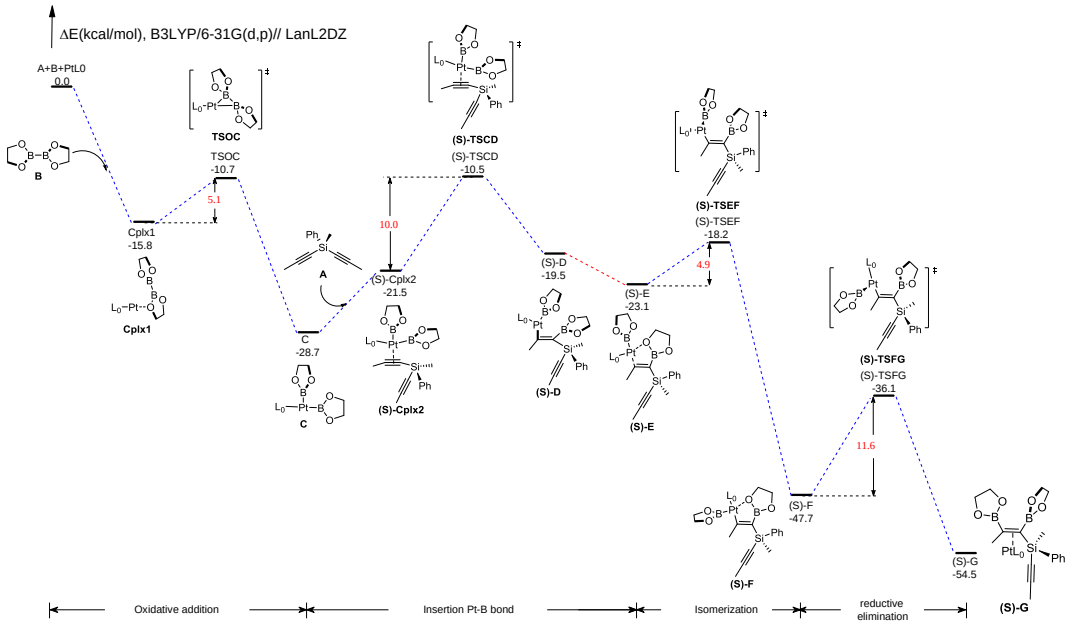


Figure S1. The energy profile [kcal/mol] for P-ligated Pt Catalyst **[PtL0]** of reaction. The energy of **A, B** and P-ligated Pt complex **[PtL0]** is set to be relative zero reference.

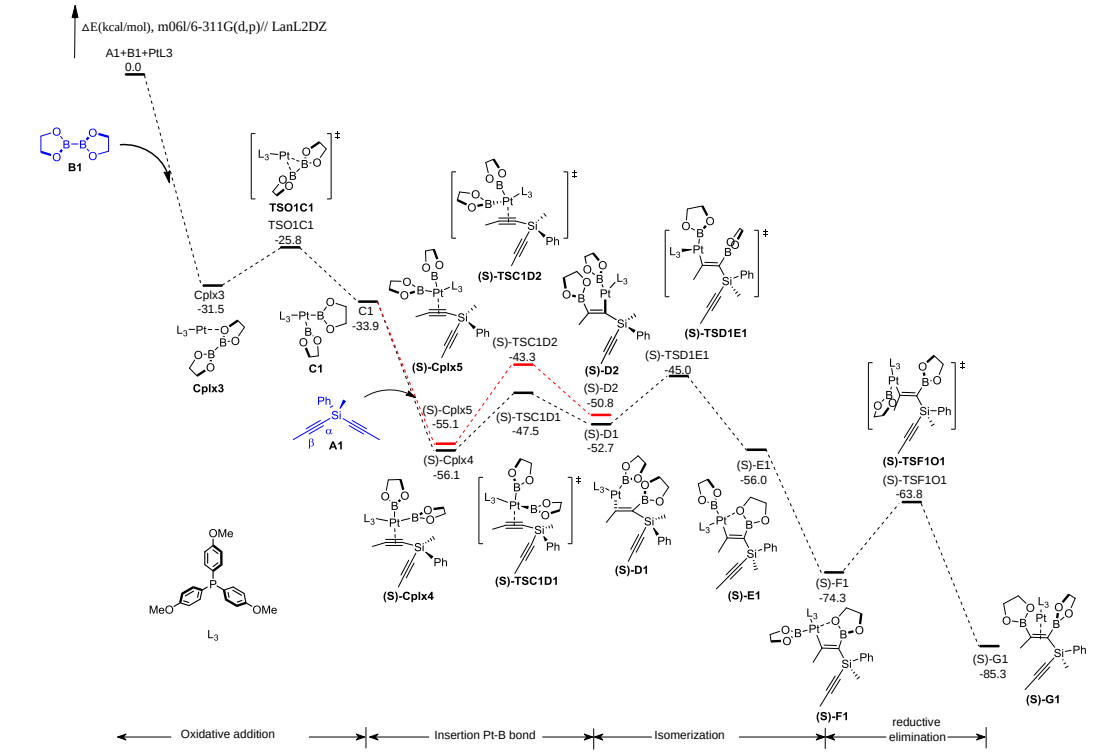


Figure S2. The energy profile [kcal/mol] for P-ligated Pt Catalyst **[PtL3]** of reaction. The energy of **A1, B1** and P-ligated Pt complex **[PtL3]** is set to be relative zero reference.

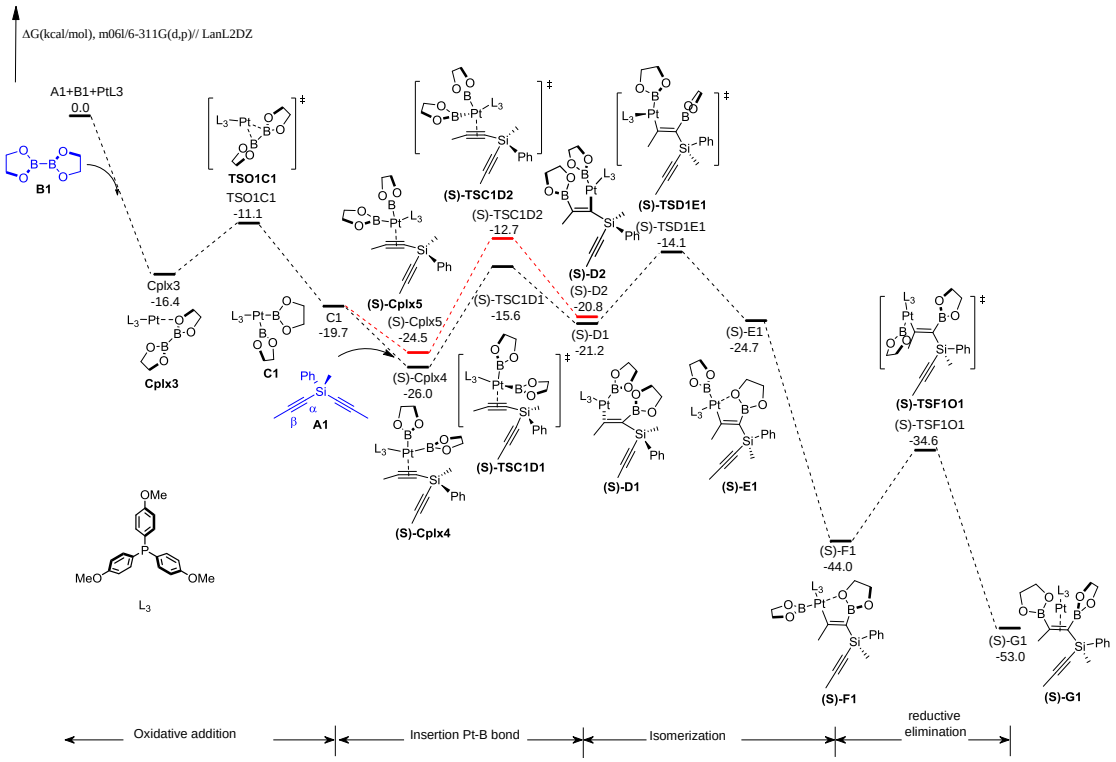


Figure S3. The free-energy profile [kcal/mol] for P-ligated Pt Catalyst **[PtL3]** of reaction. The free-energy of **A1, B1** and P-ligated Pt complex **[PtL3]** is set to be relative zero reference.

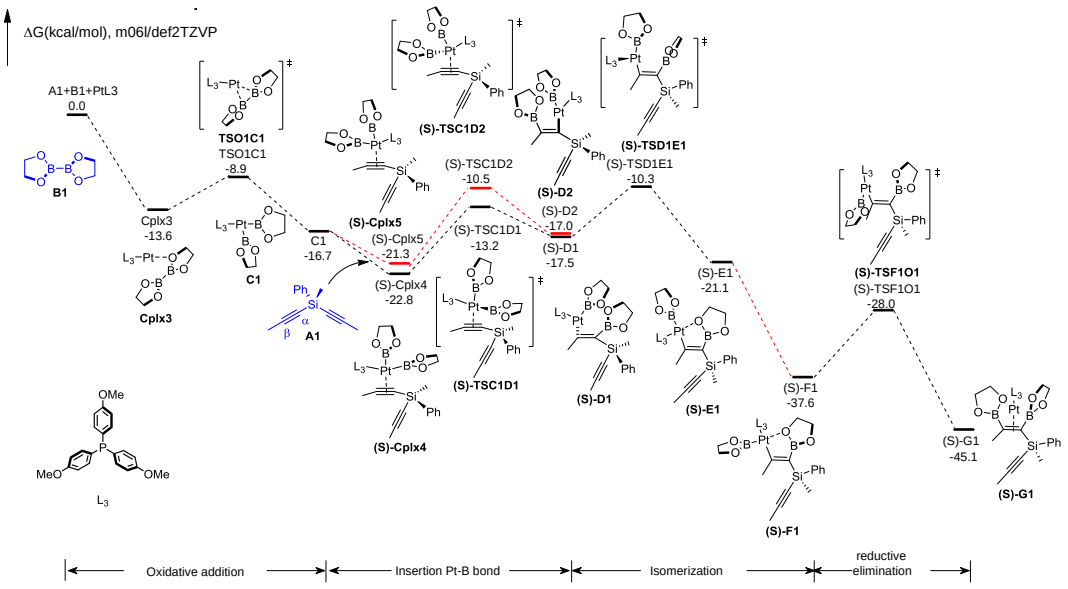


Figure S4. The **s**ingle point energy profile [kcal/mol] for P-ligated Pt Catalyst **[PtL3]** of reaction. The **s**ingle point energy of **A1, B1** and P-ligated Pt complex **[PtL3]** is set to be relative zero reference.

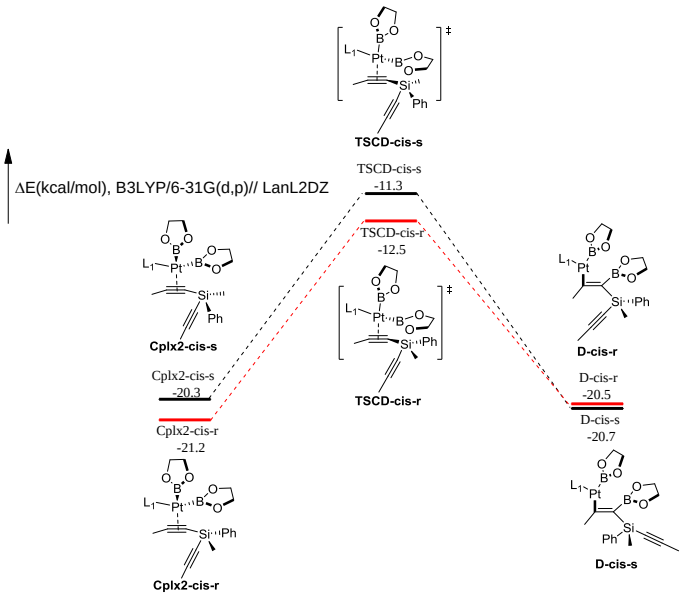


Figure S5. The energy profile [kcal/mol] for P-ligated Pt Catalyst **[PtL1]** of reaction. The energy of **A, B** and P-ligated Pt complex **[PtL1]** is set to be relative zero reference.

Ⅲ. Calculated energy parameters

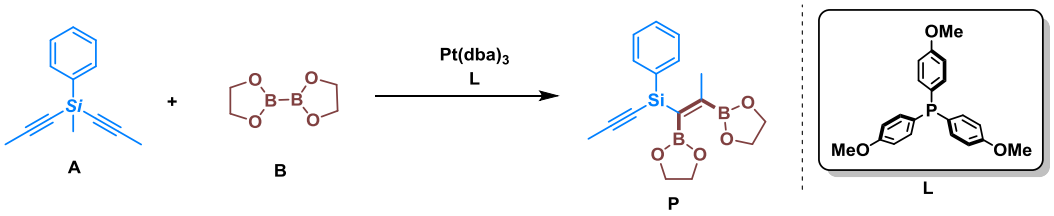


Table S9. Reaction parameters for Mono-Lateral diboration of methyl(phenyl)di(prop-1-yn-1-yl)silane **A** with 2,2'-bi(1,3,2-dioxaborolane) **B** Catalyzed by P-ligated Pt Catalyst [**PtL0**] Calculated at B3LYP/LANL2DZ(Pt), 6-31G(d,p) (C, H, P, O, B, Si) level of theory at 298.15 K in gas phase. [a,b]

System[c]	ΔE[d]	ΔH[d]	ΔS[e]	ΔG[d]
Cplx1	-15.8	-15.5	-45.5	-2.0
TSOC	-10.7	-10.7	-49.6	4.0
C	-28.7	-28.1	-41.0	-15.9
(*S*)-Cplx2	-21.5	-20.9	-97.9	8.3
(*S*)-TSCD	-10.5	-10.7	-103.4	20.1
(*S*)-D	-19.5	-19.4	-98.7	10.0
(*S*)-E	-23.1	-23.4	-103.9	7.5
(*S*)-TSEF	-18.2	-19.3	-107.2	12.7
(*S*)-F	-47.7	-48.0	-102.4	-17.5
(S)-TSFO	-36.1	-36.3	-97.2	-7.4
(*S*)-G	-54.5	-54.8	-105.2	-23.4

[a] Basis set (BS) refers to the standard 6-31G(d,p) basis for C, H, P, O, B and Si atoms and LANL2DZ valence basis set in combination with the corresponding effective core potential for Pt. [b] Relative activation energy and reaction parameters were calculated based on those of free **A+B** + **PdL0**. [c] Parameters for all the transition state (TSs) should read as those with double dagger like $\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$, and $\Delta G^{\neq}$. [d] In kcal/mol. [e] In kcal/(mol K).

Table S10. Reaction parameters for Mono-Lateral diboration of methyl(phenyl)di(prop-1-yn-1-yl)silane **A1** with 2,2'-bi(1,3,2-dioxaborolane) **B1** Catalyzed by P-ligated Pt Catalyst [**PtL3**] Calculated at M06L/LANL2DZ(Pt), 6-311G(d,p) (C, H, P, O, B, Si) level of theory at 298.15 K in gas phase. [a,b]

System[c]	ΔE[d]	ΔH[d]	ΔS[e]	ΔG[d]
Cplx3	-31.5	-31.4	-50.4	-16.4
TSO1C1	-25.8	-25.8	-49.4	-11.1
C1	-33.9	-33.5	-46.2	-19.7
(*S*)-Cplx4	-56.1	-55.8	-100.0	-26.0
(*S*)-TSC1D1	-47.5	-48.0	-108.6	-15.6
(*S*)-D1	-52.7	-53.3	-107.7	-21.2
(*S*)-Cplx5	-55.1	-55.1	-102.5	-24.5
(*S*)-TSC1D2	-43.3	-43.7	-103.8	-12.7
(*S*)-D2	-50.8	-50.9	-101.0	-20.8
(*S*)-TSD1E1	-45.0	-45.6	-105.3	-14.1
(*S*)-E1	-56.0	-56.6	-107.0	-24.7
(*S*)-F1	-74.3	-74.7	-103.0	-44.0
(*S*)-TSF1O1	-63.8	-64.1	-98.8	-34.6
(*S*)-G1	-85.3	-86.1	-111.0	-53.0
(*S*)-P1	-43.3	-44.2	-55.0	-27.8

[a] Basis set (BS) refers to the standard 6-311G(d,p) basis for C, H, P, O, B and Si atoms and LANL2DZ valence basis set in combination with the corresponding effective core potential for Pt. [b] Relative activation energy and reaction parameters were calculated based on those of free **A1+B1** + **PdL3**. [c] Parameters for all the transition state (TSs) should read as those with double dagger like $\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$, and $\Delta G^{\neq}$. [d] In kcal/mol. [e] In kcal/(mol K).

Table S11. Reaction parameters for Mono-Lateral diboration of methyl(phenyl)di(prop-1-yn-1-yl)silane **A1** with 2,2'-bi(1,3,2-dioxaborolane) **B1** Catalyzed by P-ligated Pt Catalyst [**PtL3**] Calculated at M06L/ def2TZVP (Pt, C, H, P, O, B, Si) level of theory at 298.15 K in gas phase. [a,b]

System[c]	ΔE[d]	ΔH[d]	ΔS[e]	ΔG[d]
Cplx3	-28.1	-28.6	-50.4	-13.6
TSO1C1	-23.0	-23.6	-49.4	-8.9
C1	-29.9	-30.5	-46.2	-16.7
(*S*)-Cplx4	-51.4	-52.6	-100.0	-22.8
(*S*)-TSC1D1	-44.5	-45.6	-108.6	-13.2
(*S*)-D1	-48.4	-49.6	-107.7	-17.5
(*S*)-Cplx5	-50.7	-51.9	-102.5	-21.3
(*S*)-TSC1D2	-40.2	-41.4	-103.8	-10.5
(*S*)-D2	-45.9	-47.1	-101.0	-17.0
(*S*)-TSD1E1	-40.5	-41.7	-105.3	-10.3
(*S*)-E1	-51.8	-53.0	-107.0	-21.1
(*S*)-F1	-67.1	-68.3	-103.0	-37.6
(*S*)-TSF1O1	-56.3	-57.5	-98.8	-28.0
(*S*)-G1	-77.0	-78.1	-111.0	-45.1
(*S*)-P1	-39.2	-39.8	-55.0	-23.4

[a] Basis set (BS) refers to def2TZVP basis for C, H, P, O, B, Si and Pt atoms [b] Relative activation energy and reaction parameters were calculated based on those of free **A1+B1** + **PdL3**. [c] Parameters for all the transition state (TSs) should read as those with double dagger like $\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$, and $\Delta G^{\neq}$. [d] In kcal/mol. [e] In kcal/(mol K).

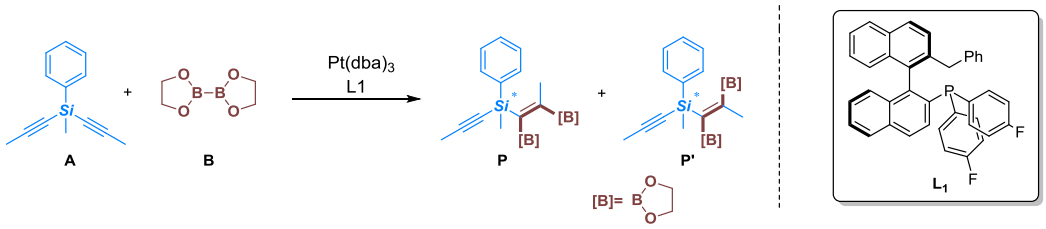


Table S12. Reaction parameters for Mono-Lateral diboration of methyl(phenyl)di(prop-1-yn-1-yl)silane **A** with 2,2'-bi(1,3,2-dioxaborolane) **B** Catalyzed by P-ligated Pt Catalyst [**PtL1**] Calculated at B3LYP/LANL2DZ(Pt), 6-31G(d,p) (C, H, P, O, B, F, Si) level of theory at 298.15 K in gas phase. [a,b]

System[c]	ΔE[d]	ΔH[d]	ΔS[e]	ΔG[d]
cplx2-cis-s	-20.3	-19.8	-102.0	10.6
TSCD-cis-s	-11.3	-11.4	-110.0	21.4
D-cis-s	-20.8	-20.6	-100.6	9.4
cplx2-cis-r	-21.2	-20.8	-103.0	9.9
TSCD-cis-r	-12.5	-12.7	-108.9	19.8
D-cis-r	-20.5	-20.5	-104.6	10.7
F-cis-s	-46.0	-46.4	-106.7	-14.6
F-cis-r	-42.8	-42.6	-97.0	-13.7
F-trans-s	-40.8	-40.8	-102.2	-10.3
F-trans-r	-39.2	-39.2	-102.1	-8.8

[a] Basis set (BS) refers to the standard 6-31G(d,p) basis for C, H, P, O, B, F and Si atoms and LANL2DZ valence basis set in combination with the corresponding effective core potential for Pt. [b] Relative activation energy and reaction parameters were calculated based on those of free **A+B** + **PdL1**. [c] Parameters for all the transition state (TSs) should read as those with double dagger like $\Delta E^{\neq}$, $\Delta H^{\neq}$, $\Delta S^{\neq}$, and $\Delta G^{\neq}$. [d] In kcal/mol. [e] In kcal/(mol K).

Ⅳ. Computational Details

All calculations were performed with the Gaussian09 suites of programs[1]. The geometries of all stationary points and transition states were optimized by using the M06L functional in conjunction with the standard 6-311G(d,p) basis for all atoms (C, H, O, N, P) except for palladium and iodide, which were described by the LANL2DZ valence basis set in combination with the corresponding effective core potential. We label this basis set combination as BS. Geometries were fully optimized, normally without symmetry constraints. Frequencies calculations were carried out at the same level of theory to verify the stationary points as minima or saddle points. The connectivity of the stationary points to transition state was verified by intrinsic reaction coordinate (IRC) runs or the vibrational mode of the imaginary frequencies. Solvent effects were included with fully optimization calculations at the same level of theory by using the integral equation formalism variant of the polarizable continuum model (IEFPCM) in toluene with those geometries optimized in gas phase as initial structures. The frequencies calculated at M06L/BS level were used to obtain the reported energies as zero-point energy-corrected energies, enthalpies, and free energies.

References:

[1] Frisch, M., Trucks, G., Schlegel, H., Scuseria, G., Robb, M., Cheeseman, J., Scalmani, G., Barone, V., Mennucci, B., Petersson, G., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H., Izmaylov, A., Bloino, J., Zheng, G., Sonnenberg, J., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, J., Peralta, J., Ogliaro, F., Bearpark, M., Heyd, J., Brothers, E., Kudin, K., Staroverov, V., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J., Iyengar, S., Tomasi, J., Cossi, M., Rega, N., Millam, J., Klene, M., Knox, J., Cross, J., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R., Yazyev, O., Austin, A., Cammi, R., Pomelli, C., Ochterski, J., Martin, R., Morokuma, K., Zakrzewski, V., Voth, G., Salvador, P., Dannenberg, J., Dapprich, S., Daniels, A., Farkas, Foresman, J., Ortiz, J., Cioslowski, J., Fox, D., 2009. Gaussian 09, Revision C.01, Gaussian Inc Wallingford CT.

Ⅴ. Cartesian coordinates of calculated intermediates and transition states

47

O

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-1498.687698

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-1498.661112

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-1498.748138

P	0.00094000	-0.00367100	0.36157500
Pt	-0.00486500	-0.01187800	2.50877500
C	-1.48185500	-0.79146200	-0.39130800
C	-2.05935900	-1.89725700	0.24610300
C	-2.05707600	-0.33842000	-1.59224700
C	-3.16793500	-2.54997500	-0.29337700
H	-1.64076800	-2.23926800	1.18859100
C	-3.16297300	-0.97763500	-2.13846500
H	-1.64260900	0.52548900	-2.10197500
C	-3.72583200	-2.08951900	-1.49357400
H	-3.58952200	-3.39974700	0.23030700
H	-3.61481600	-0.63070000	-3.06212700
C	0.05979300	1.67926700	-0.37963600
C	0.75011700	1.96236100	-1.57207800
C	-0.62392300	2.72404700	0.25574400
C	0.74423300	3.24218700	-2.11259400
H	1.30311100	1.17868900	-2.08004300
C	-0.64024700	4.01270600	-0.27808600
H	-1.13868100	2.52406800	1.19144400
C	0.04691200	4.27672400	-1.47062000
H	1.27797000	3.46832900	-3.03002500
H	-1.17768900	4.79591900	0.24324900
C	1.43033300	-0.88991900	-0.38443700
C	1.33031500	-1.62822800	-1.57740300
C	2.67819400	-0.81551000	0.24830600
C	2.44286700	-2.25842900	-2.12061200
H	0.37450900	-1.71739000	-2.08372400
C	3.80373200	-1.44078500	-0.28856200
H	2.76183900	-0.27052800	1.18452800
C	3.68842500	-2.16788600	-1.48107300
H	2.37231800	-2.83332800	-3.03832800
H	4.75169400	-1.36366800	0.23045800
O	0.10350600	5.49429400	-2.07847500
O	4.71472900	-2.82290600	-2.09168100
O	-4.80928100	-2.64254400	-2.10624300

C	5.99960800	-2.77650000	-1.48910400
H	6.65653100	-3.35861700	-2.13709600
H	6.37805400	-1.74863700	-1.42130800
H	5.99306800	-3.22337300	-0.48691500
C	-5.43074500	-3.76357400	-1.49512700
H	-6.26314800	-4.03721200	-2.14511700
H	-4.74186600	-4.61389900	-1.41372000
H	-5.81699200	-3.51797300	-0.49781400
C	-0.57617700	6.58324500	-1.47156400
H	-0.40076700	7.44467700	-2.11764300
H	-1.65557900	6.39802200	-1.40176600
H	-0.18331700	6.79735600	-0.46959600

28

A

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-793.041914

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-793.024016

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-793.090745

Si	-0.64935700	0.00009100	0.65785500
C	1.16147800	-0.00010700	0.13164000
C	1.86438600	1.20466100	-0.04518400
C	1.86392600	-1.20499800	-0.04609600
C	3.22015100	1.20704500	-0.37561900
H	1.34177500	2.15181900	0.06330600
C	3.21969900	-1.20764400	-0.37653100
H	1.34093500	-2.15202500	0.06167600
C	3.90109300	-0.00037000	-0.53973500
H	3.74371900	2.14969500	-0.51004800
H	3.74290700	-2.15039200	-0.51167200
H	4.95612900	-0.00046700	-0.79940100
C	-0.80634600	0.00024300	2.53664700
H	-0.32542500	0.88641500	2.96314400
H	-1.85767800	0.00041300	2.84034500
H	-0.32568600	-0.88602500	2.96324000
C	-1.46366100	1.49609300	-0.01289700
C	-1.99587500	2.50089000	-0.44858800
C	-1.46393900	-1.49586800	-0.01265300
C	-1.99634100	-2.50062000	-0.44822100
C	-2.63870900	3.69773300	-0.97774800
H	-3.65884200	3.47955600	-1.31266700
H	-2.69752300	4.48507400	-0.21805800
H	-2.08433400	4.09806400	-1.83379000
C	-2.63948100	-3.69736900	-0.97723000

H	-2.68184400	-4.49104900	-0.22306300
H	-3.66591000	-3.48315500	-1.29503100
H	-2.09552100	-4.08733000	-1.84466100

18

B

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-507.874068

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-507.863583

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-507.912102

B	-0.85167600	0.00000700	-0.00014800
B	0.85167700	0.00001500	-0.00017800
O	1.60892500	0.99548000	-0.56837000
O	1.60873700	-0.99547000	0.56826900
O	-1.60889200	-0.99543700	-0.56842200
O	-1.60876300	0.99546600	0.56830400
C	-2.99722700	0.64564700	0.42693200
C	-2.99732400	-0.64560100	-0.42675200
C	2.99720400	-0.64562500	0.42700300
C	2.99734100	0.64553200	-0.42681100
H	-3.52752300	-1.47338200	0.05422900
H	-3.52752500	1.47343000	-0.05393500
H	-3.42679900	0.49186600	1.42283500
H	-3.42710300	-0.49181900	-1.42256400
H	3.42666700	-0.49171200	1.42293500
H	3.52758600	-1.47343900	-0.05371600
H	3.42699300	0.49159800	-1.42265600
H	3.52767600	1.47331000	0.05402200

65

Cplx1

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.586983

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.549451

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.663151

P	0.70089400	0.12297700	0.07343800
C	0.59171500	-0.40725000	1.83366400
C	-0.66914100	-0.71292900	2.36554100
C	1.71443700	-0.51217700	2.67301900
C	-0.81647700	-1.10243100	3.69744900
H	-1.55173200	-0.65146900	1.73505100
C	1.57968200	-0.90428700	3.99962600
H	2.70491900	-0.29462200	2.28626300
C	0.31241300	-1.20203100	4.52149200

H	-1.80679100	-1.33299300	4.07191600
H	2.44308200	-0.99366200	4.65111500
C	2.49134900	-0.01989200	-0.33918600
C	3.41849500	1.01895800	-0.14198500
C	2.95762200	-1.22780800	-0.87476100
C	4.76026400	0.84987300	-0.46033800
H	3.08917800	1.97349000	0.25569800
C	4.30330800	-1.41379600	-1.19423000
H	2.24976600	-2.03265000	-1.05425600
C	5.21321000	-0.36883000	-0.98761400
H	5.47850900	1.65047300	-0.31561900
H	4.62474800	-2.36226000	-1.60816600
C	0.38886100	1.93878800	0.13743000
C	0.64338600	2.72048700	1.27904100
C	-0.11920100	2.57647400	-1.00160000
C	0.41099000	4.09015200	1.27424500
H	1.01788100	2.25202800	2.18404700
C	-0.35440300	3.95326300	-1.02197000
H	-0.34736600	1.98013900	-1.88105300
C	-0.08677400	4.71746900	0.12158300
H	0.60257700	4.69777400	2.15283800
H	-0.74517800	4.41127000	-1.92302700
O	6.54469900	-0.43311300	-1.27029800
O	-0.28226700	6.06249200	0.21872800
O	0.28583000	-1.58065700	5.83100500
C	-0.77774200	6.75584500	-0.91673900
H	-0.84878200	7.80384100	-0.62184100
H	-0.09822700	6.66708000	-1.77378800
H	-1.77221200	6.39539900	-1.20951600
C	-0.96730200	-1.90738900	6.41200100
H	-0.75670100	-2.18116600	7.44704700
H	-1.65597900	-1.05293300	6.39814100
H	-1.44097100	-2.75645300	5.90312700
C	7.05902800	-1.63668300	-1.81974700
H	8.12636200	-1.46720400	-1.96949800
H	6.92079100	-2.48506000	-1.13732300
H	6.59206800	-1.87299300	-2.78432900
Pt	-0.63022900	-0.95298700	-1.29845900
C	-4.12152500	1.85016300	-0.77809200
C	-4.21480300	1.30746300	0.66900300
H	-3.33049900	2.60034700	-0.88694300
H	-5.06412100	2.28078200	-1.13208000
H	-3.58204000	1.86383700	1.36773800
H	-5.24142800	1.30812600	1.05396000

C	-2.44276900	-4.08318100	-1.34232700
C	-2.08633100	-3.45338900	-2.69788900
H	-1.54660100	-4.29608400	-0.74757400
H	-3.03614300	-4.99673100	-1.44007100
H	-1.07491100	-3.67626000	-3.04017800
H	-2.80535400	-3.71292300	-3.48245000
B	-3.50797500	-0.34668700	-0.74167500
B	-2.94859100	-1.85832300	-1.25011600
O	-3.79130700	0.70793600	-1.58231100
O	-3.75032600	-0.04875900	0.58622100
O	-2.20729800	-2.02586300	-2.46272600
O	-3.21774400	-3.07790300	-0.67159200

65

TSOC

imaginary frequencies -104.46

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.578869

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.541818

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.653788

P	0.72922100	0.03439000	0.06694500
C	0.72989600	-0.20498300	1.89159100
C	-0.47981500	-0.09788800	2.59300700
C	1.90225700	-0.48326400	2.61745800
C	-0.52404100	-0.25017900	3.97970300
H	-1.40303100	0.09689800	2.05439000
C	1.86752000	-0.63966500	3.99750100
H	2.85066600	-0.58902000	2.10039100
C	0.65262700	-0.52337500	4.68914700
H	-1.47713100	-0.16506900	4.48810300
H	2.76767000	-0.85989200	4.56231800
C	2.30595400	-0.73798200	-0.49577700
C	3.52127800	-0.03688800	-0.59185000
C	2.29488600	-2.09285500	-0.85158900
C	4.68122200	-0.67303800	-1.01635800
H	3.56111500	1.01829300	-0.34130600
C	3.45317400	-2.74637900	-1.27360000
H	1.35919500	-2.64429600	-0.80794600
C	4.65640900	-2.03352200	-1.35813500
H	5.62053900	-0.13560500	-1.09761500
H	3.40398000	-3.79495100	-1.54213600
C	0.99069200	1.84091700	-0.16962300
C	1.62305400	2.65374000	0.78850000
C	0.54608100	2.43747800	-1.35662400
C	1.81632400	4.00999900	0.55800600

H	1.95845600	2.22521100	1.72786300
C	0.73670400	3.79864800	-1.60229500
H	0.02815800	1.82789600	-2.09222500
C	1.37757600	4.59196900	-0.64141300
H	2.30043500	4.64331000	1.29442300
H	0.37970100	4.22431700	-2.53257900
O	5.84402400	-2.56290900	-1.76490600
O	1.61251900	5.92751600	-0.77112300
O	0.72160300	-0.69756600	6.03909400
C	1.19267100	6.57314000	-1.96410000
H	1.48086100	7.61989400	-1.85689400
H	1.68711100	6.15090500	-2.84808000
H	0.10521600	6.50986400	-2.09724700
C	-0.47837000	-0.60417700	6.79206900
H	-0.19531200	-0.77677900	7.83158600
H	-0.93621000	0.38920000	6.70272800
H	-1.20867200	-1.36356600	6.48536300
C	5.87937000	-3.93209000	-2.13845500
H	6.91088200	-4.13832000	-2.42785800
H	5.60131000	-4.58735800	-1.30307500
H	5.21785600	-4.13630800	-2.98990300
Pt	-1.09527000	-0.70847200	-0.93703100
C	-3.48877700	2.50267600	-0.86055200
C	-3.77813800	2.09960000	0.60068300
H	-2.56351200	3.08644200	-0.94687700
H	-4.30436400	3.07230800	-1.31810900
H	-3.23074600	2.71302900	1.32414100
H	-4.84825500	2.15417600	0.84129000
C	-4.30259400	-3.51150100	-0.80133900
C	-3.41741300	-3.44498800	-2.06405300
H	-4.03062300	-4.33582000	-0.13590900
H	-5.36861200	-3.59527400	-1.04335800
H	-2.50474100	-4.04251400	-1.97210300
H	-3.94188100	-3.73716900	-2.97765100
B	-3.08966100	0.26685000	-0.59586700
B	-3.37132600	-1.43565400	-0.96347800
O	-3.32985200	1.25874600	-1.55295800
O	-3.34781700	0.73795700	0.69725400
O	-3.04553900	-2.05202900	-2.16601700
O	-4.07664800	-2.26335700	-0.12286800

65

C

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.607528
H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.569476
G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2006.685562

P	-0.85219900	-0.03934000	-0.03959800
C	-1.52475500	-0.69500500	1.53942100
C	-0.64733200	-1.33684000	2.42493200
C	-2.87936800	-0.58161800	1.90310000
C	-1.10377500	-1.87156500	3.63135900
H	0.40872800	-1.41657200	2.18098500
C	-3.34259300	-1.10697600	3.10197800
H	-3.57558600	-0.06702700	1.24758400
C	-2.45700900	-1.75910300	3.97435000
H	-0.39695900	-2.35767300	4.29328100
H	-4.38508400	-1.02020100	3.39092600
C	-2.02500000	1.29702400	-0.51401300
C	-3.04425900	1.14883100	-1.47036700
C	-1.86418000	2.55206800	0.09137900
C	-3.87488100	2.21311300	-1.79885200
H	-3.18584900	0.19429700	-1.96677000
C	-2.69378800	3.62809800	-0.22524200
H	-1.07921700	2.69923200	0.83040000
C	-3.70701500	3.46033700	-1.17859700
H	-4.66182600	2.10498800	-2.53829300
H	-2.53692900	4.58155100	0.26475600
C	-1.11416500	-1.38016700	-1.26656800
C	-2.17252500	-2.30486100	-1.18772900
C	-0.20618900	-1.49721900	-2.32738000
C	-2.32600000	-3.29597500	-2.14716000
H	-2.87527400	-2.25607100	-0.36152400
C	-0.35136900	-2.48835000	-3.30029900
H	0.63847400	-0.81670000	-2.38545600
C	-1.41682600	-3.39257400	-3.21370500
H	-3.13748100	-4.01441800	-2.09160800
H	0.37288500	-2.54934900	-4.10373200
O	-4.56974500	4.43787200	-1.57170800
O	-1.65194900	-4.40008900	-4.09918700
O	-3.00759600	-2.23735900	5.12517100
C	-0.76211800	-4.55553800	-5.19512000
H	-1.13489500	-5.40706600	-5.76622100
H	-0.75211200	-3.66606000	-5.83758900
H	0.26084300	-4.76602200	-4.85850000
C	-2.15982000	-2.89487600	6.05508200
H	-2.79935000	-3.19051800	6.88812200
H	-1.69800900	-3.78984800	5.61908100

H	-1.37045200	-2.22811700	6.42448300
C	-4.43774000	5.72774300	-0.99247500
H	-5.21317600	6.34340900	-1.45052400
H	-4.59281600	5.70154900	0.09364800
H	-3.45509400	6.16753800	-1.20464000
Pt	1.46512300	0.80866000	0.05111800
C	3.67213600	-2.71140200	-0.46635000
C	3.65172400	-2.61760400	1.07477200
H	3.03794200	-3.52533800	-0.84021200
H	4.68054300	-2.84296800	-0.87091600
H	3.27589900	-3.52725900	1.55395500
H	4.64162200	-2.38836200	1.48691000
C	5.51083900	2.30671300	0.24804900
C	4.66379500	3.58702200	0.08882300
H	6.17843200	2.34184900	1.11521700
H	6.11491600	2.09578000	-0.64361800
H	4.66504900	4.20127800	0.99838200
H	4.98878500	4.21279400	-0.74878100
B	2.57503900	-0.82120400	0.17830900
B	3.28835200	1.74594600	0.11321800
O	3.13634600	-1.45791600	-0.91315000
O	2.76615800	-1.52364400	1.35815100
O	3.33228100	3.11062800	-0.15588900
O	4.55021800	1.25658200	0.42329700

93

(*S*)-Cplx2

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.637863

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.581996

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.737739

P	1.61960000	0.44244800	0.13955200
Pt	-0.53571200	-0.52651200	-0.43520200
C	3.02105700	-0.70966800	0.49075300
C	3.76457700	-0.68336900	1.68236300
C	3.37485800	-1.64769600	-0.48920400
C	4.82556900	-1.56013600	1.88380300
C	4.44290600	-2.52622400	-0.30389000
C	5.17568400	-2.48523600	0.89037500
C	2.34590600	1.48938300	-1.18918000
C	1.61028000	1.74450200	-2.36056000
C	3.65128000	1.99518400	-1.10627800
C	2.14765400	2.50364200	-3.39247700
C	4.20149800	2.76518700	-2.13183800

C	3.44456500	3.02655800	-3.28267200
O	6.23341100	-3.29599100	1.17958400
C	1.52319600	1.47173000	1.66173300
C	0.83707100	0.91894400	2.76464400
C	2.03367600	2.76782500	1.77931600
C	0.69170800	1.63676500	3.94214400
C	1.88042900	3.50549000	2.95850700
C	1.21066500	2.93819900	4.04789700
O	3.88038200	3.75991800	-4.34362300
O	1.00580500	3.56047700	5.24251400
C	5.19110300	4.30352300	-4.29751600
C	6.63717900	-4.24901600	0.20853500
C	1.48890700	4.88483200	5.40418700
B	0.19037800	-2.30861900	0.32723600
O	0.74581200	-3.42356900	-0.28650200
C	1.09903500	-4.38448500	0.71662000
C	0.91976400	-3.64016800	2.05815100
B	-1.46618000	-2.14366700	-1.34066600
O	-2.36485700	-3.06156300	-0.79707300
C	-2.61851300	-4.08266200	-1.77399000
O	0.22785300	-2.43218200	1.71314300
O	-1.25054900	-2.39076700	-2.68576300
C	-2.04372600	-3.51398800	-3.08930300
H	3.51385900	0.02685400	2.46296400
H	2.80546300	-1.70750200	-1.41140000
H	5.40165500	-1.54278500	2.80344000
H	4.68734700	-3.23329100	-1.08767600
H	0.61307800	1.32651700	-2.46265700
H	4.26254800	1.77713700	-0.23532300
H	1.58442500	2.69774300	-4.29938600
H	5.21306000	3.14023100	-2.03028600
H	0.41666300	-0.08077200	2.69033600
H	2.55038800	3.22810600	0.94378600
H	0.16631500	1.21731400	4.79390600
H	2.28266900	4.51044300	3.00988700
H	5.95306000	3.51711100	-4.22467700
H	5.31148400	4.99887400	-3.45701700
H	5.32441500	4.84649100	-5.23428100
H	6.94669700	-3.76763100	-0.72792000
H	5.83924800	-4.97106000	-0.00786100
H	7.48966400	-4.77589000	0.63997100
H	1.02758300	5.57451100	4.68574100
H	2.58033900	4.93421300	5.29787000
H	1.21364700	5.18444200	6.41649300

Si	-4.21266900	0.38789900	-1.01243400
C	-4.58939200	-0.81215100	-2.41231600
H	-4.34375600	-1.83196800	-2.10747600
H	-5.65456900	-0.77446300	-2.66184200
H	-4.01160500	-0.56653500	-3.30848000
C	-2.39418000	0.64224900	-0.77804100
C	-1.47622200	1.48627300	-0.54867600
C	-4.89618900	2.03867700	-1.45169700
C	-5.34099100	3.13137400	-1.75611200
C	-5.00661600	-0.17689300	0.60171900
C	-5.99710400	0.59254800	1.23709800
C	-4.62644200	-1.39471300	1.20042800
C	-6.59141800	0.16510800	2.42646200
H	-6.30477600	1.53718200	0.79653400
C	-5.21899400	-1.82117500	2.39013900
H	-3.86165100	-2.01388100	0.73853600
C	-6.20240800	-1.04331700	3.00569200
H	-7.35549200	0.77600700	2.90049900
H	-4.91019500	-2.76207600	2.83821700
H	-6.66205300	-1.37721200	3.93242900
H	2.12923200	-4.71658500	0.55237400
H	0.43494500	-5.25332200	0.63012100
H	0.32610200	-4.20648500	2.78300100
H	1.88063100	-3.38188400	2.51866900
H	-1.41233200	-4.23349700	-3.62052900
H	-2.11043900	-5.00395000	-1.46434800
H	-2.83074300	-3.17313700	-3.77290000
C	-5.87723600	4.43682300	-2.12583800
H	-5.87597800	5.12300600	-1.27127200
H	-5.28324400	4.89650400	-2.92397100
H	-6.90934500	4.35348000	-2.48493400
C	-1.09349000	2.90267400	-0.35820300
H	-0.72390600	3.07155800	0.65788400
H	-0.29629600	3.20202400	-1.04509500
H	-1.96295200	3.54758300	-0.52860500
H	-3.69404300	-4.28149200	-1.82587800

93

(*S*)-TSCD

imaginary frequencies -207.89

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.620377

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.565745

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.718876

P	1.67133700	0.40400200	0.14156500

Pt	-0.41774000	-0.44561400	-0.46583100
C	3.03034800	-0.79992600	0.45589400
C	3.93019500	-0.68063500	1.52813700
C	3.21343300	-1.85069500	-0.45202400
C	4.97919300	-1.57965400	1.68324200
C	4.26640900	-2.75595100	-0.31145900
C	5.15789400	-2.62129500	0.76116500
C	2.44948100	1.53359200	-1.08631900
C	1.80099900	1.80401700	-2.30347400
C	3.71732700	2.09371400	-0.87456500
C	2.38517700	2.62577900	-3.25932000
C	4.31235800	2.92861800	-1.82096200
C	3.64197100	3.20107800	-3.02187500
O	6.21657600	-3.44770400	0.99692100
C	1.51403000	1.34373400	1.71170200
C	0.96921700	0.66497800	2.82382200
C	1.81711300	2.70194400	1.84208400
C	0.76664200	1.32709000	4.02464000
C	1.60648200	3.37988200	3.04795000
C	1.08393100	2.69046500	4.14683500
O	4.12835600	3.99632400	-4.01451400
O	0.84363800	3.24534800	5.36848900
C	5.40350100	4.59474600	-3.83795400
C	6.44940800	-4.51723300	0.09334400
C	1.12207300	4.62459700	5.54793800
B	0.07562700	-2.32142500	0.29683400
O	0.30109900	-3.51798400	-0.38537300
C	0.52424300	-4.56983100	0.56256600
C	0.69782600	-3.84929400	1.91469900
B	-1.81381700	-1.59453300	-1.60404900
O	-2.66881300	-2.59666000	-1.14249600
C	-2.68896200	-3.63408400	-2.13158200
O	0.23443400	-2.51513100	1.67147800
O	-1.49686200	-1.77306500	-2.94288700
C	-2.15031700	-2.95914700	-3.40948600
H	3.80554600	0.11590500	2.25484900
H	2.51358600	-1.98120900	-1.27167500
H	5.67355700	-1.49660600	2.51319900
H	4.37552800	-3.55572400	-1.03422000
H	0.83461800	1.34905500	-2.49843500
H	4.26231800	1.87409900	0.03884000
H	1.88968800	2.83176800	-4.20250000
H	5.29155600	3.34671600	-1.61914300
H	0.69422900	-0.38304800	2.73467000

H	2.22049900	3.25365500	0.99961400
H	0.34891200	0.81353900	4.88448000
H	1.85185800	4.43343800	3.11226800
H	6.19290400	3.84040100	-3.72785600
H	5.42068500	5.26202000	-2.96672900
H	5.58899900	5.17891300	-4.74047500
H	6.64260400	-4.15361300	-0.92397100
H	5.60494800	-5.21789300	0.06796100
H	7.33485300	-5.03649500	0.46323700
H	0.52404000	5.24985700	4.87257600
H	2.18593900	4.84712100	5.39347400
H	0.85442800	4.85444400	6.58041700
C	-5.16116100	-1.00338200	-2.19895500
H	-5.05430100	-2.04500400	-1.89158400
H	-6.22765400	-0.75632800	-2.22144400
H	-4.76678000	-0.88965300	-3.21394100
C	-2.41107300	0.22897100	-1.19716900
C	-1.58861500	1.23818500	-1.07426300
C	-4.76014100	-0.20450200	0.79129100
C	-5.52061200	0.71404700	1.53732900
C	-4.37397300	-1.40605100	1.41814600
C	-5.88773300	0.44493400	2.85755100
H	-5.82746400	1.65095200	1.08059800
C	-4.73864300	-1.67431700	2.73815400
H	-3.77821200	-2.13094200	0.87175600
C	-5.49664000	-0.75063100	3.46116200
H	-6.47605100	1.16998000	3.41415700
H	-4.42707100	-2.60553800	3.20405100
H	-5.77871200	-0.96105600	4.48954600
H	1.41021500	-5.14465000	0.27153900
H	-0.33996100	-5.24682000	0.56243100
H	0.10933100	-4.30348300	2.71874700
H	1.74759100	-3.81258100	2.23182100
H	-1.43164200	-3.58567100	-3.94663100
H	-2.03442300	-4.44647400	-1.79660600
H	-2.95379000	-2.67867700	-4.10268000
C	-1.56303200	2.71910700	-1.11978300
H	-1.23262300	3.11106200	-0.15108800
H	-0.82886700	3.06314700	-1.85710900
H	-2.54024500	3.14555800	-1.36832400
H	-3.70822300	-4.01785000	-2.24470300
Si	-4.28895300	0.16216900	-0.99925900
C	-4.89108000	1.85257000	-1.41294800
C	-5.35897100	2.93659200	-1.71416600

C	-5.91402500	4.23643700	-2.07644300
H	-5.52850000	5.02901100	-1.42516800
H	-5.66037400	4.49953500	-3.10961200
H	-7.00661500	4.23668600	-1.99162600

93

(*S*)-D

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.634825

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.579602

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.734971

P	-1.70468800	-0.15824700	0.12128300
Pt	0.47818800	-0.08776000	-0.49349900
C	-2.49635200	1.37855600	0.75634900
C	-3.39736300	1.37875600	1.83487100
C	-2.22080000	2.59548300	0.12056600
C	-4.00822300	2.55458100	2.25481000
C	-2.83130000	3.78212700	0.52830900
C	-3.73263800	3.76442700	1.60112100
C	-2.85220500	-0.67249900	-1.22995600
C	-2.35139000	-1.32988100	-2.36736500
C	-4.23046200	-0.42598700	-1.16048400
C	-3.19996600	-1.73885700	-3.38716200
C	-5.09493900	-0.83357900	-2.17827500
C	-4.57885100	-1.49574500	-3.30010400
O	-4.38134000	4.86063200	2.08701000
C	-1.94328400	-1.38679600	1.46822800
C	-1.11919100	-1.30928100	2.61132900
C	-2.88373200	-2.41869500	1.39119700
C	-1.25288900	-2.23033300	3.63919000
C	-3.01919600	-3.35601700	2.42063100
C	-2.20237900	-3.26219700	3.55201800
O	-5.32623200	-1.93097000	-4.35278400
O	-2.24672600	-4.11546900	4.61416500
C	-6.72621400	-1.69974200	-4.32829500
C	-4.13808700	6.11623300	1.47161100
C	-3.17747100	-5.18578200	4.57981200
B	0.82987100	1.47578100	0.83564400
O	1.12381000	2.77697800	0.43779200
C	1.55775200	3.52899200	1.58258100
C	1.24781300	2.62169100	2.79251700
B	2.18934600	0.75048500	-2.33729200
O	3.09492200	1.79008800	-2.18094800
C	2.56240800	2.92776500	-2.86996100

O	0.91836800	1.34818600	2.21766300
O	1.24662200	1.02806300	-3.31680200
C	1.53838500	2.32406000	-3.85282400
H	-3.61698400	0.45275700	2.35661700
H	-1.50034800	2.62385800	-0.69071500
H	-4.69951800	2.56270000	3.09135200
H	-2.59038800	4.70521000	0.01459700
H	-1.28140700	-1.49888800	-2.44665000
H	-4.64719600	0.09838900	-0.30635900
H	-2.81671600	-2.23965600	-4.27039400
H	-6.15427700	-0.62316400	-2.08995100
H	-0.37148300	-0.52484000	2.68739600
H	-3.52440500	-2.50653900	0.52015000
H	-0.62482700	-2.17855000	4.52275900
H	-3.75560400	-4.14509400	2.32455000
H	-6.95912600	-0.62789500	-4.29093600
H	-7.20478200	-2.20016800	-3.47666300
H	-7.11704000	-2.11959400	-5.25638100
H	-4.43106800	6.11323100	0.41392700
H	-3.08310000	6.40843500	1.54983500
H	-4.75121900	6.83961800	2.01130000
H	-2.98845300	-5.86017800	3.73472000
H	-4.21166800	-4.82218400	4.52285500
H	-3.04137700	-5.73384300	5.51341100
Si	4.20005100	-0.91973600	-1.04503500
C	5.41356700	-0.62182900	-2.46306200
H	5.30483500	0.39220600	-2.85791800
H	6.44746100	-0.75909700	-2.13047400
H	5.22478100	-1.32591900	-3.28032100
C	2.40434900	-0.64210900	-1.64784300
C	1.36022700	-1.56137700	-1.58991000
C	4.45140800	-2.64287800	-0.44832900
C	4.69990100	-3.75978000	-0.02949400
C	4.60771700	0.19966600	0.42677300
C	5.15295300	1.48499500	0.25208400
C	4.39580800	-0.24623100	1.74390100
C	5.47853700	2.28841300	1.34661400
H	5.31091900	1.87044400	-0.74981000
C	4.71396500	0.55460600	2.84243300
H	3.98661900	-1.23821700	1.91393400
C	5.26010700	1.82459800	2.64626800
H	5.90785500	3.27414900	1.18531300
H	4.54161100	0.18437800	3.84963000
H	5.51998600	2.44607800	3.49955300

H	1.01884500	4.48231400	1.61801300
H	2.63008100	3.73476900	1.48776500
H	2.10648500	2.50577300	3.46095800
H	0.39298200	2.98236000	3.37810100
H	0.61716300	2.91081300	-3.92088300
H	2.08539800	3.58470400	-2.13405800
H	1.95172000	2.20755000	-4.86336900
C	4.98154300	-5.10238700	0.46622200
H	5.27343400	-5.08100100	1.52229800
H	4.10177000	-5.75006300	0.37644800
H	5.79856900	-5.56881400	-0.09597300
C	1.39957900	-3.04448300	-1.69439800
H	0.79402300	-3.50652700	-0.90742900
H	0.90750000	-3.30342400	-2.64396400
H	2.40245000	-3.48307600	-1.70209000
H	3.37147100	3.47003200	-3.36935300

93

(*S*)-E

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.640561

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.586044

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.738962

P	1.58682000	0.38203100	0.18728800
Pt	0.06893300	-1.12000300	-0.45824300
C	1.04005000	2.14229900	0.29588100
C	1.03213400	2.87387000	1.49389600
C	0.63007400	2.78800400	-0.87821800
C	0.62701700	4.20397100	1.51583300
C	0.22599200	4.12200800	-0.87219800
C	0.22071600	4.83798400	0.33391900
C	2.22696900	0.01228300	1.86892600
C	1.30031700	-0.39745100	2.84738200
C	3.57196900	0.11201500	2.23264800
C	1.70538300	-0.67092000	4.14502500
C	3.99532900	-0.17085900	3.53434500
C	3.05945700	-0.55971300	4.49901300
O	-0.15435900	6.14148700	0.45799000
C	3.03933100	0.59031100	-0.93497700
C	3.25336900	-0.24734500	-2.04267300
C	3.93818900	1.64911000	-0.73042900
C	4.33759500	-0.05360900	-2.88935000
C	5.03846900	1.84788000	-1.56511200
C	5.24476600	0.98868300	-2.65304100

O	3.35797600	-0.85552800	5.79493600
O	6.27638900	1.09000300	-3.53543600
C	4.71328100	-0.78063900	6.20851500
C	-0.60232200	6.82843000	-0.70075900
C	7.21864600	2.13717600	-3.35796500
B	1.65285600	-2.50654300	-0.52768900
B	-2.58716400	-2.09011300	-1.54186800
H	1.34320700	2.40348500	2.42043400
H	0.61541400	2.24224700	-1.81766500
H	0.61525800	4.77241100	2.44007200
H	-0.08543500	4.58666800	-1.80013800
H	0.25475800	-0.51718100	2.57883700
H	4.31700200	0.39715300	1.49840200
H	0.99465700	-0.98665800	4.90163000
H	5.04852400	-0.09149800	3.77661600
H	2.55596900	-1.05130600	-2.24872500
H	3.77685300	2.34706300	0.08526100
H	4.49811600	-0.69610000	-3.74901600
H	5.71089900	2.67450100	-1.36826500
H	5.11552100	0.23457300	6.09731200
H	5.34659500	-1.48044500	5.64838200
H	4.72159900	-1.05554700	7.26430500
H	-1.49027500	6.35205000	-1.13509700
H	0.18289300	6.88833700	-1.46530100
H	-0.85983400	7.83631600	-0.37193200
H	7.73689500	2.05639300	-2.39397100
H	6.74458500	3.12427100	-3.42934100
H	7.94431100	2.02866900	-4.16528000
O	-1.31557500	-2.66037500	-1.26190300
O	-3.27549800	-2.89607100	-2.41680600
O	2.54497500	-2.81035700	0.49130300
O	1.84851800	-3.37010300	-1.61225200
Si	-4.74690500	-0.18963400	-0.80233600
C	-5.87382000	-1.28906800	-1.85356100
H	-5.86922800	-2.32099200	-1.48977000
H	-6.90242400	-0.91552400	-1.81429300
H	-5.55024600	-1.30682900	-2.89820800
C	-2.95907700	-0.78319500	-0.85507100
C	-1.88068100	-0.13630000	-0.27952800
C	-4.93370900	1.52219000	-1.46670900
C	-5.07893200	2.64108900	-1.92638400
C	-5.43466500	-0.18276800	0.96961000
C	-6.47074800	0.68730400	1.35484100
C	-4.96687100	-1.10130500	1.92692600

C	-7.02200300	0.63863400	2.63669300
H	-6.84290000	1.42183200	0.64444600
C	-5.51465900	-1.15701100	3.21022100
H	-4.15229200	-1.77411900	1.66845700
C	-6.54597400	-0.28658200	3.56797600
H	-7.81987100	1.32456100	2.91049500
H	-5.13380000	-1.87542200	3.93191000
H	-6.97249700	-0.32556300	4.56698400
C	-5.24704500	3.98208100	-2.47640600
H	-5.04087400	4.75029700	-1.72176400
H	-4.56769600	4.15254200	-3.31992000
H	-6.26959300	4.13961100	-2.83884300
C	-2.10352100	1.13909200	0.49214500
H	-1.83555000	2.00156000	-0.12920000
H	-3.13887700	1.28365200	0.82143000
H	-1.45746800	1.19094400	1.37436900
C	-1.08777300	-3.75486600	-2.17807500
C	-2.51088000	-4.08391300	-2.66199800
C	2.84195800	-4.34933000	-1.26834200
C	3.43890700	-3.84495200	0.06160300
H	-0.60123900	-4.57322100	-1.64660200
H	-0.42674100	-3.41592400	-2.97866400
H	-2.95392000	-4.91596800	-2.10060400
H	-2.54478100	-4.32679900	-3.72804200
H	2.36087900	-5.33028500	-1.16281200
H	3.58270400	-4.41694700	-2.07186300
H	3.49304100	-4.62467300	0.82815900
H	4.44214600	-3.42022100	-0.06829700

93

(*S*)-TSEF

imaginary frequencies -90.11

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.632624

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.579433

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.730773

P	1.81868600	0.33697900	0.16485900
Pt	-0.06767000	-0.78138300	-0.20564400
C	1.38653300	2.06170200	0.65570600
C	1.80140000	2.64572900	1.86403700
C	0.60896400	2.83091100	-0.22153400
C	1.45365700	3.95415200	2.17938800
C	0.25895800	4.14632800	0.07974400
C	0.68093500	4.71481400	1.29033700
C	2.91703800	-0.24477300	1.51578900

C	2.33409200	-0.75023900	2.69508600
C	4.31233800	-0.19744000	1.43092300
C	3.12317800	-1.16956600	3.75469000
C	5.11858300	-0.62933100	2.48809400
C	4.52384700	-1.11287900	3.65912100
O	0.39561600	5.98435500	1.68961200
C	2.89801700	0.62387700	-1.30012400
C	2.93454500	-0.28929400	-2.36985500
C	3.70392900	1.76958600	-1.37860700
C	3.75482600	-0.06500800	-3.46734600
C	4.53659000	2.00166800	-2.47445600
C	4.56327000	1.07989500	-3.52935000
O	5.20823400	-1.55456300	4.75009000
O	5.32710600	1.20708400	-4.64833900
C	6.62715900	-1.52339600	4.71502000
C	-0.42403000	6.78805600	0.85298700
C	6.15400100	2.35447600	-4.77706400
B	1.17036800	-2.40117400	-0.16946600
B	-2.68371500	-1.82472700	-1.71708900
H	2.40189900	2.07739200	2.56598200
H	0.25944100	2.39510200	-1.15357300
H	1.76829500	4.40938100	3.11281500
H	-0.34521800	4.70797800	-0.62254800
H	1.25377500	-0.82599800	2.76939000
H	4.79009700	0.17563400	0.53128400
H	2.68059400	-1.55955900	4.66528800
H	6.19618900	-0.58309000	2.38484500
H	2.32002600	-1.18102600	-2.33798100
H	3.68284700	2.50420200	-0.57996400
H	3.78221800	-0.76328400	-4.29759900
H	5.14331100	2.89902400	-2.49828800
H	7.00603000	-0.50153400	4.58609300
H	7.02602600	-2.15753900	3.91298300
H	6.96053900	-1.91117500	5.67862200
H	-1.41334000	6.33764400	0.70519800
H	0.04251100	6.96143600	-0.12514100
H	-0.53645000	7.74194300	1.37026500
H	6.90157700	2.40661200	-3.97532400
H	5.56415500	3.27975600	-4.77886400
H	6.66335700	2.25158800	-5.73623500
O	-1.51398100	-2.55940200	-1.47713400
O	-3.29288900	-2.23996500	-2.88564800
O	1.31116300	-3.16145800	0.97607600
O	1.70815000	-3.04520600	-1.27920400

Si	-4.95553400	-0.24094500	-0.63376700
C	-6.04337500	-1.43647500	-1.61973800
H	-5.93955500	-2.45891600	-1.23981700
H	-7.09598100	-1.14930700	-1.52735400
H	-5.76904000	-1.44488700	-2.67733100
C	-3.12733600	-0.69796000	-0.77172900
C	-2.10849100	-0.07539700	-0.08675600
C	-5.30260500	1.45167000	-1.28249800
C	-5.54171500	2.55949800	-1.73000500
C	-5.56049500	-0.28589800	1.16690600
C	-6.59228900	0.55594200	1.61931200
C	-5.03247100	-1.21678900	2.08008200
C	-7.08114700	0.46989700	2.92453800
H	-7.01036300	1.29807300	0.94324600
C	-5.51760300	-1.30949300	3.38617400
H	-4.21876200	-1.86880300	1.77018000
C	-6.54549200	-0.46562100	3.81177600
H	-7.87722000	1.13491200	3.25049900
H	-5.08998400	-2.03572300	4.07301700
H	-6.92285500	-0.53338700	4.82890200
C	-5.82224300	3.88623900	-2.26862600
H	-5.78058900	4.65121400	-1.48433400
H	-5.09492400	4.16221000	-3.04117500
H	-6.81941600	3.93026600	-2.72196800
C	-2.38399800	1.06755600	0.86307700
H	-1.74316400	1.92484200	0.63322100
H	-3.42403600	1.41419800	0.87665500
H	-2.11824400	0.76195400	1.88394400
C	-1.22278700	-3.33540000	-2.65108400
C	-2.56097500	-3.34932200	-3.41680400
C	2.13098200	-4.35998800	-0.88081800
C	2.07503900	-4.33351300	0.66209900
H	-0.88602900	-4.33284800	-2.35535200
H	-0.41934300	-2.84811400	-3.21273900
H	-3.12775700	-4.27271800	-3.24048400
H	-2.43336300	-3.22290900	-4.49642900
H	1.44353400	-5.10080900	-1.30767800
H	3.13446900	-4.55441300	-1.27189400
H	1.58399700	-5.21511200	1.08515800
H	3.07072500	-4.24034000	1.11275000

93

(*S*)-F

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.679753
H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.625265
G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.778862

P	-2.03455400	0.11005200	-0.02516000
Pt	0.32921900	-0.23502300	-0.33778100
C	-2.75711100	1.53911800	-0.93239800
C	-4.14532200	1.77757100	-0.97686900
C	-1.91643800	2.39989400	-1.64855100
C	-4.66492200	2.85174800	-1.68339900
C	-2.42696200	3.48404600	-2.36885200
C	-3.80695000	3.71670900	-2.38414100
C	-3.18073500	-1.26033800	-0.47981600
C	-3.04563000	-1.85193500	-1.75146200
C	-4.19059600	-1.72990100	0.36533500
C	-3.89810100	-2.86765900	-2.15908000
C	-5.05210400	-2.75813300	-0.03102100
C	-4.90945100	-3.32963700	-1.30032600
O	-4.41502300	4.73721700	-3.04747400
C	-2.37171000	0.40712300	1.75882600
C	-1.83032500	-0.51349500	2.68310900
C	-3.07779400	1.50731700	2.25487200
C	-2.01577800	-0.34177200	4.04635800
C	-3.25939900	1.69618500	3.62961500
C	-2.73195200	0.76582400	4.53141600
O	-5.68924900	-4.33305300	-1.79199800
O	-2.85245200	0.84321300	5.88607100
C	-6.72840300	-4.84296000	-0.97051500
C	-3.60593000	5.63444200	-3.79516700
C	-3.56388100	1.93993800	6.43853800
B	0.02068200	-2.19018300	-0.51256400
B	2.38307400	1.94317800	0.21754000
H	-4.82619000	1.10611200	-0.46220700
H	-0.84611900	2.21863100	-1.65440000
H	-5.73308400	3.03958000	-1.72150300
H	-1.74539400	4.12338600	-2.91735000
H	-2.25394100	-1.52592400	-2.41867200
H	-4.31262900	-1.29966500	1.35399300
H	-3.80004500	-3.32488700	-3.13835800
H	-5.82019400	-3.09840400	0.65350700
H	-1.26103100	-1.36676400	2.32362500
H	-3.49655700	2.23849700	1.57112300
H	-1.60638400	-1.04742400	4.76194900
H	-3.80989400	2.56275800	3.97673300
H	-7.46290700	-4.06730100	-0.71890600

H	-6.33487000	-5.27820200	-0.04297900
H	-7.21756200	-5.62425700	-1.55407400
H	-3.06189200	5.11676000	-4.59491100
H	-2.88754100	6.16057000	-3.15394300
H	-4.29101700	6.35927800	-4.23698200
H	-4.60788600	1.95709000	6.10020500
H	-3.09019600	2.89768700	6.18763200
H	-3.53951200	1.80052500	7.52026300
O	2.86387400	3.02026400	0.93140400
O	0.98678800	2.05981500	0.03636500
O	0.03208100	-2.90953900	-1.69807200
O	-0.27323200	-3.00567000	0.57581900
Si	5.02150200	0.76428000	-0.46104200
C	5.70267700	2.50969300	-0.19361900
H	5.46383800	2.88455500	0.80472900
H	6.79107900	2.50203600	-0.31442500
H	5.28607500	3.21193900	-0.92312700
C	3.14230700	0.71463500	-0.28982900
C	2.37111200	-0.39898000	-0.55084000
C	5.56726900	0.27093700	-2.15267900
C	5.93928300	-0.02582500	-3.27435300
C	5.86489900	-0.40511600	0.77322400
C	7.16838500	-0.88514400	0.54967800
C	5.22969400	-0.77682200	1.97133100
C	7.81420700	-1.69518100	1.48518200
H	7.68054200	-0.63211400	-0.37591500
C	5.87014100	-1.58643000	2.91215200
H	4.21522600	-0.43708600	2.16555400
C	7.16578600	-2.04657800	2.67128700
H	8.82065100	-2.05591800	1.28793000
H	5.35645300	-1.86146700	3.82991800
H	7.66580500	-2.67884900	3.40045900
C	6.37339800	-0.38793100	-4.61937000
H	6.85812500	-1.37105700	-4.62865600
H	5.52353000	-0.43057900	-5.31031400
H	7.08989000	0.34011300	-5.01726300
C	2.98382800	-1.70988200	-0.97650700
H	2.47205000	-2.09477900	-1.86412800
H	4.05646800	-1.65878800	-1.18450900
H	2.82793300	-2.45394000	-0.18375700
C	1.78798400	3.93334100	1.17451100
C	0.51560600	3.11325900	0.90060700
C	-0.58896600	-4.31899500	0.08876500
C	-0.15063100	-4.29879800	-1.39139600

H	1.88065000	4.78912200	0.49364800
H	1.84265600	4.29960000	2.20381500
H	-0.26886700	3.67820800	0.39164500
H	0.10113300	2.66869700	1.81209600
H	-0.05449800	-5.06743800	0.68231000
H	-1.66657700	-4.49112400	0.19788200
H	0.79761600	-4.82724600	-1.55081300
H	-0.90270600	-4.72539000	-2.06243600

93

(*S*)-TSFO

imaginary frequencies -113.10

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.661244

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.606629

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.762723

P	2.22153200	0.17571600	0.19218000
Pt	-0.05124800	0.17791400	0.36040500
C	2.95080100	1.84182800	-0.10302500
C	4.13536500	2.29771600	0.50097600
C	2.27281400	2.71018000	-0.97051200
C	4.62815200	3.56991700	0.23606300
C	2.75908600	3.98800300	-1.24897400
C	3.94479700	4.42368700	-0.64243000
C	3.08897400	-0.46279000	1.68226600
C	2.47415400	-0.29178400	2.93736600
C	4.32850700	-1.11080400	1.63424100
C	3.08941400	-0.73264100	4.09962400
C	4.95673100	-1.56571600	2.79711600
C	4.33744000	-1.37289900	4.03811800
O	4.50826100	5.64971600	-0.83387300
C	2.85483000	-0.84400200	-1.20438100
C	2.09467400	-1.94647000	-1.64034400
C	4.06146800	-0.56886900	-1.85812100
C	2.54452900	-2.75357000	-2.67634200
C	4.52231200	-1.37174100	-2.90555300
C	3.76300000	-2.47404100	-3.31547300
O	4.85446500	-1.77537800	5.23273300
O	4.11125000	-3.32314500	-4.32356700
C	6.10636600	-2.44320400	5.23607400
C	3.85223800	6.56550900	-1.69772000
C	5.32641100	-3.08380700	-5.01627400
B	-1.26990300	-1.44984200	0.74107800
B	-2.61494500	-0.52916100	-1.84528300
H	4.67353900	1.65599000	1.19148600

H	1.34555900	2.38507400	-1.43655500
H	5.53950400	3.92925400	0.70314300
H	2.20619800	4.63049000	-1.92387300
H	1.49430300	0.17486700	2.98546200
H	4.81620600	-1.28034700	0.67933000
H	2.61811600	-0.60740000	5.06898600
H	5.91311500	-2.06963600	2.72093300
H	1.13452500	-2.14998900	-1.17485300
H	4.65449400	0.29161700	-1.56231100
H	1.96548500	-3.60565700	-3.01816100
H	5.45882700	-1.12414900	-3.39138400
H	6.90572600	-1.80831000	4.83267200
H	6.06810900	-3.37851200	4.66302400
H	6.32312000	-2.67145500	6.28073300
H	2.84625600	6.81310000	-1.33590100
H	3.77906300	6.17582300	-2.72112000
H	4.46503600	7.46819000	-1.70059400
H	6.19333400	-3.13906400	-4.34531600
H	5.32218400	-2.10657000	-5.51583300
H	5.40470800	-3.87056800	-5.76816200
O	-3.44676100	-1.48607300	-2.39990900
O	-1.53673500	-0.23583000	-2.64416800
O	-1.41484100	-2.03203700	1.99978500
O	-1.39874000	-2.41291300	-0.27637600
Si	-4.69251300	1.07710100	-0.55050800
C	-5.22494700	1.32430000	-2.34786700
H	-5.34600500	0.36142800	-2.85210700
H	-6.17799600	1.86079900	-2.38976400
H	-4.48332500	1.91073500	-2.90132000
C	-2.99548300	0.20449000	-0.51535200
C	-2.20820000	0.13532200	0.60039500
C	-4.61891100	2.74016600	0.22538300
C	-4.58719100	3.86052800	0.70264800
C	-5.98147700	0.03062800	0.35623400
C	-6.78229300	0.55231800	1.38677800
C	-6.17591900	-1.31475700	-0.01451500
C	-7.74494900	-0.23499800	2.02312500
H	-6.64890100	1.58608200	1.69510400
C	-7.13788500	-2.10295300	0.61831400
H	-5.56626700	-1.75088000	-0.80289500
C	-7.92504500	-1.56444300	1.63925800
H	-8.35236500	0.18936100	2.81840500
H	-7.27333000	-3.13848300	0.31655500
H	-8.67325200	-2.17886100	2.13311700

C	-4.53950800	5.19928900	1.27991300
H	-5.53366500	5.66033000	1.29598400
H	-4.16580300	5.17336700	2.30984800
H	-3.87790900	5.85426400	0.70170100
C	-2.61979200	0.73765100	1.93547600
H	-2.06029100	0.28739900	2.75618900
H	-2.42928600	1.81624700	1.93863400
H	-3.68820500	0.59248300	2.13682500
C	-2.77897500	-2.03436400	-3.54378600
C	-1.60096700	-1.06621800	-3.81134800
C	-1.53681200	-3.69825400	0.33710700
C	-1.81165700	-3.39411400	1.82570700
H	-3.48025400	-2.09727200	-4.38201400
H	-2.43161100	-3.04475200	-3.29979900
H	-1.77214400	-0.43161900	-4.68924000
H	-0.64589400	-1.58480700	-3.93738700
H	-2.35358300	-4.24923600	-0.14131200
H	-0.60761700	-4.26721800	0.20016900
H	-2.87623100	-3.49418300	2.07457000
H	-1.23717600	-4.03468000	2.50290100

93

(*S*)-G

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.690516

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.636033

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2799.78833

P	-1.86085900	0.24499200	-0.02928300
Pt	0.39458900	-0.13538600	-0.10720900
C	-2.45234600	1.79905800	-0.81694600
C	-3.76034100	1.96730000	-1.30727600
C	-1.55555300	2.86819200	-0.93712900
C	-4.16041100	3.16819800	-1.87852000
C	-1.94600300	4.08174000	-1.50738600
C	-3.25535800	4.23629600	-1.97991800
C	-2.89932300	-1.06004700	-0.81278300
C	-2.49090500	-1.59225700	-2.05165000
C	-4.08577700	-1.53605800	-0.24591800
C	-3.25756500	-2.54820000	-2.70254000
C	-4.86056600	-2.50941900	-0.88617700
C	-4.44902300	-3.01601100	-2.12337900
O	-3.74272300	5.36936300	-2.55942100
C	-2.45099900	0.33209900	1.71285400
C	-1.80056900	-0.46491800	2.67737200

C	-3.50070200	1.15677300	2.13229000
C	-2.20631400	-0.44739400	4.00401800
C	-3.91367700	1.18686400	3.46764500
C	-3.26702000	0.37833700	4.40968400
O	-5.12195000	-3.96161100	-2.83863800
O	-3.58319900	0.32742000	5.73452100
C	-6.33467700	-4.47105300	-2.30623800
C	-2.87070400	6.47912100	-2.70964900
C	-4.62999900	1.15899300	6.21019000
B	1.54706300	-2.18323200	-1.58839800
B	2.63954100	-1.76121000	1.18924200
H	-4.46922600	1.14644300	-1.25342400
H	-0.53243800	2.73948000	-0.59249400
H	-5.16599400	3.30316700	-2.26376200
H	-1.22374500	4.88506900	-1.59115400
H	-1.55616400	-1.26305300	-2.49669700
H	-4.41837600	-1.15384000	0.71418800
H	-2.95573200	-2.95409200	-3.66297100
H	-5.77040000	-2.85874800	-0.41218100
H	-0.95786000	-1.08514700	2.38104500
H	-4.00621200	1.79891600	1.41785400
H	-1.70683200	-1.05420700	4.75229100
H	-4.72631400	1.84310300	3.75628800
H	-7.08491600	-3.68000200	-2.17946500
H	-6.17565200	-4.97126000	-1.34227300
H	-6.70033600	-5.19904200	-3.03199600
H	-2.00989400	6.23462600	-3.34495000
H	-2.50855600	6.84423400	-1.73998800
H	-3.45985600	7.26185500	-3.18988400
H	-5.58794200	0.91963000	5.73065900
H	-4.40638900	2.22180200	6.05219400
H	-4.70683800	0.96395000	7.28093600
O	3.75000200	-2.58625400	1.21812800
O	1.78068400	-2.00752200	2.24117600
O	0.97155900	-2.42695000	-2.82262500
O	1.54768000	-3.30417800	-0.77614100
Si	3.55440700	0.93259600	0.72581400
C	3.68240000	0.87783600	2.61280200
H	4.26808900	0.01209000	2.94069600
H	4.17654200	1.77861100	2.98954400
H	2.68831700	0.81114600	3.06605100
C	2.54424800	-0.57544000	0.16264900
C	2.18230600	-0.81217500	-1.19357400
C	2.80264700	2.55443500	0.28152000

C	2.38569800	3.67435500	0.04221700
C	5.28935600	0.89750400	-0.04039800
C	5.92563300	2.07366900	-0.47581500
C	5.99579700	-0.31524600	-0.16431100
C	7.21680300	2.04625900	-1.00694200
H	5.39889800	3.02192100	-0.40711200
C	7.28654400	-0.34602600	-0.69577000
H	5.53312600	-1.24647400	0.15306900
C	7.90092700	0.83477700	-1.11797300
H	7.68623200	2.96915500	-1.33821500
H	7.81174200	-1.29375100	-0.78378900
H	8.90471400	0.81013500	-1.53417900
C	1.87332900	5.00918700	-0.24846600
H	0.86782300	5.14524400	0.16663700
H	2.51708500	5.78446800	0.18276000
H	1.81923300	5.18569800	-1.32914000
C	2.56617200	0.11613200	-2.33109800
H	1.82318700	0.07466800	-3.13198700
H	2.67817000	1.15457100	-2.01122000
H	3.52612000	-0.21024600	-2.75541700
C	3.53337100	-3.58506900	2.22090700
C	2.35298100	-3.03995500	3.05536900
C	0.72811100	-4.29646200	-1.40600400
C	0.58955100	-3.80821000	-2.86527600
H	4.44656200	-3.72325900	2.80812900
H	3.28532900	-4.53251000	1.72785000
H	2.68238100	-2.60196100	4.00595100
H	1.59603700	-3.80101400	3.26848800
H	1.21037200	-5.27566500	-1.32612500
H	-0.24203000	-4.33721100	-0.89622900
H	1.26117900	-4.34282700	-3.54864700
H	-0.43389900	-3.89581000	-3.24170900

46

(*S*)-P

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-1300.973729

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-1300.94607

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-1301.037201

Si	1.34898000	0.03997900	0.88871500
C	2.02662700	1.67343800	1.38519100
C	2.47920000	2.74737800	1.74019700
C	-0.45142100	0.17211100	0.28901100
C	-0.88288700	1.01809900	-0.68455000

C	-4.30498900	1.64004400	-2.17219800
C	-4.57497500	0.40848700	-1.27364700
B	-2.38170000	1.00878200	-1.12865700
O	-2.94458200	2.00232600	-1.89596500
O	-3.27821400	0.01324300	-0.80318800
C	-2.25765800	-2.86595200	1.61816500
C	-2.97626100	-1.72503800	2.37771000
B	-1.41454700	-0.84701800	0.98354300
O	-2.24507700	-0.53975600	2.03680900
O	-1.39074300	-2.19544200	0.69188400
C	2.44173200	-0.68831000	-0.47153900
C	3.69319400	-0.14076000	-0.80038600
C	2.02131500	-1.83808100	-1.16739700
C	4.49941300	-0.71978500	-1.78248600
H	4.03708600	0.75211300	-0.28481600
C	2.82477700	-2.42023800	-2.14803600
H	1.05307700	-2.28154600	-0.94504800
C	4.06686300	-1.86178500	-2.45737600
H	5.46335400	-0.27853500	-2.02175200
H	2.48104400	-3.30721900	-2.67348000
H	4.69245800	-2.31337600	-3.22253200
C	1.39662300	-1.08406800	2.40838100
H	0.73069800	-0.71254800	3.19434700
H	1.08634500	-2.10110300	2.14805100
H	2.41093800	-1.13195700	2.81581500
C	0.00103800	2.00467300	-1.41856200
H	-0.45810800	2.99978600	-1.42251500
H	1.00130300	2.09045400	-0.99117600
H	0.10283500	1.71361500	-2.47207600
C	3.01159400	4.03759100	2.16292800
H	2.33372100	4.52986800	2.86912200
H	3.98294300	3.92345700	2.65695500
H	3.14771400	4.70896000	1.30772300
H	-4.40117600	1.40689900	-3.23891000
H	-4.96081600	2.48509800	-1.94228700
H	-5.03366100	-0.42307000	-1.81705100
H	-5.20676100	0.65319700	-0.41203500
H	-2.94988500	-3.51100300	1.06837700
H	-4.01619800	-1.60599500	2.05172500
H	-1.65242400	-3.49374600	2.28288000
H	-2.96515400	-1.86167900	3.46347900

70

PtL1

imaginary frequencies no
E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2162.103513
H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2162.067015
G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-2162.175879

C	2.23187000	0.48012300	-0.43217400
C	1.36226300	1.09485500	0.46578600
C	1.15128200	2.51402500	0.41360600
C	1.79223700	3.28336300	-0.61060700
C	2.63901700	2.61810000	-1.53446300
C	2.85639500	1.26643800	-1.43901500
H	-0.15175500	2.63477700	2.14134100
C	0.32931100	3.20062700	1.35060600
C	1.57438800	4.68569900	-0.66961200
H	3.12560600	3.19930700	-2.31375200
H	3.52905000	0.77642700	-2.13571700
C	0.76909100	5.31718200	0.25125400
C	0.14635400	4.56424400	1.27438500
H	2.06223500	5.25407800	-1.45751600
H	0.61356900	6.39082000	0.19797000
H	-0.48061400	5.06675300	2.00573100
C	0.71177800	0.28944400	1.55340200
C	1.39251100	0.22842100	2.82531300
C	-0.46865600	-0.43207900	1.37632000
C	2.59287300	0.95348100	3.07557200
C	0.87239100	-0.58899000	3.87963400
C	-0.94924600	-1.26623800	2.43408700
C	3.22996900	0.87866300	4.29540400
H	3.00420900	1.57813000	2.29164100
C	1.55124600	-0.64562600	5.12493100
C	-0.30778500	-1.33959700	3.64132000
H	-1.83938500	-1.86352000	2.27047400
C	2.70676900	0.07280900	5.33295700
H	4.14152900	1.44528200	4.46185900
H	1.14058400	-1.27264800	5.91207800
H	-0.69450000	-1.98197700	4.42808200
H	3.21888100	0.02160600	6.28936400
C	2.50994500	-1.01868600	-0.37815400
H	2.30485400	-1.38238600	0.63276400
H	1.78138300	-1.53534000	-1.02072600
C	3.91788800	-1.42250400	-0.77052600
C	5.00287000	-1.12192100	0.06741200
C	4.16952400	-2.11120700	-1.96341100
C	6.29985900	-1.49788300	-0.27855600
H	4.82285300	-0.59256300	1.00008900

C	5.46817300	-2.49005800	-2.31425400
H	3.33900900	-2.35730000	-2.62094600
C	6.53759300	-2.18364100	-1.47294700
H	7.12643700	-1.25961100	0.38539700
H	5.64130400	-3.02646800	-3.24321500
H	7.54780700	-2.47878400	-1.74212000
Pt	-1.00632900	-2.43830600	-1.19868900
C	-1.34374200	0.89864500	-1.25549000
C	-1.98553300	2.10421500	-0.92839700
C	-0.67454000	0.80020800	-2.48528600
C	-1.94440400	3.19358200	-1.79524800
H	-2.53163900	2.20215200	0.00257200
C	-0.62632700	1.88138000	-3.36265400
H	-0.20353600	-0.14085800	-2.75184300
C	-1.26129900	3.06288200	-2.99903200
H	-2.42975500	4.13201900	-1.55185100
H	-0.11285600	1.81746700	-4.31571300
C	-3.20881100	-0.50092300	0.42337600
C	-3.58921100	0.29044100	1.52020400
C	-4.20198100	-1.19754800	-0.28326100
C	-4.92716500	0.39261300	1.90029200
H	-2.83892700	0.82075500	2.09809600
C	-5.54350900	-1.10234200	0.08321700
H	-3.90818200	-1.82531000	-1.11937100
C	-5.88335800	-0.30566900	1.17081600
H	-5.23346500	0.99560200	2.74831500
H	-6.31891200	-1.63833100	-0.45329900
P	-1.46408800	-0.59804000	-0.18584300
F	-1.22323200	4.11240300	-3.84403400
F	-7.17687800	-0.21248900	1.53568400

116

cplx2-cis-s

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.051817

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3462.98615

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.161776

B	-1.08692100	2.06611200	-1.52085100
O	-0.46740600	3.25697500	-1.87081100
C	-0.39179700	3.33608400	-3.30346500
C	-1.27956700	2.17597400	-3.80461400
B	-2.47393500	2.74835500	0.07742200
O	-3.59563600	2.90635200	-0.72702600
C	-4.13974300	4.21759800	-0.50471100

O	-1.52564600	1.37447500	-2.63973100
O	-2.30509200	3.83519600	0.92436900
C	-3.41695000	4.72848800	0.75852700
C	-5.60497900	1.24511800	1.48772000
H	-5.44121900	1.97524600	0.69204500
H	-6.67270500	1.00651500	1.52796600
H	-5.31597900	1.69119500	2.44492500
C	-2.78084000	-0.01399300	1.27954900
C	-1.69399600	-0.39378000	1.83556000
C	-5.01282900	-1.03330700	-0.55509000
C	-5.94868200	-2.07530100	-0.68484000
C	-4.41122700	-0.53287300	-1.72582300
C	-6.28255500	-2.59603100	-1.93666600
H	-6.41240000	-2.49331000	0.20506900
C	-4.73979400	-1.05681900	-2.97815300
H	-3.67687900	0.26470200	-1.66901200
C	-5.67755300	-2.08675900	-3.08770500
H	-7.00919900	-3.40085500	-2.01288500
H	-4.25888100	-0.65889200	-3.86774100
H	-5.93440600	-2.49077900	-4.06369000
H	0.65439600	3.22237200	-3.60845000
H	-0.74565100	4.31834800	-3.63206900
H	-2.23900100	2.52638800	-4.20339400
H	-0.78499200	1.56692800	-4.56752400
H	-3.04799500	5.75340700	0.65341300
H	-3.93487200	4.84004900	-1.38372100
H	-4.05277700	4.67791400	1.65025300
C	-1.12060100	-1.25690900	2.89492400
H	-0.25728800	-1.82652400	2.54527400
H	-0.77523800	-0.64811100	3.73663900
H	-1.88352600	-1.95362400	3.26001500
H	-5.22410900	4.14485400	-0.37685800
Si	-4.60373000	-0.31231600	1.13959700
C	-5.01925500	-1.56832100	2.41663500
C	-5.29187400	-2.39607900	3.26818500
C	-5.61956000	-3.38920400	4.28528000
H	-5.22811700	-4.37632500	4.01453600
H	-5.19364700	-3.11550200	5.25727400
H	-6.70410100	-3.48303400	4.41202200
C	2.01668700	-2.67867200	-0.66523800
C	2.95622200	-1.83025600	-0.07962900
C	4.20953900	-1.58056900	-0.73108700
C	4.46774000	-2.17151900	-2.01126300
C	3.47922300	-3.00721600	-2.58734100

C	2.29711700	-3.25480400	-1.93162900
H	5.06015000	-0.33742800	0.82817500
C	5.22883200	-0.77319200	-0.15076900
C	5.70540800	-1.91691800	-2.66173200
H	3.67251000	-3.45881300	-3.55723600
H	1.55725100	-3.90628800	-2.38294000
C	6.66434200	-1.12434000	-2.07437400
C	6.42231800	-0.55306000	-0.80206600
H	5.88194000	-2.36676100	-3.63556700
H	7.60783300	-0.93977900	-2.57984500
H	7.18639000	0.06262100	-0.33567600
C	2.72565500	-1.27499100	1.29904600
C	3.21393200	-2.07907000	2.39907000
C	2.08634600	-0.06467600	1.57137800
C	3.88379000	-3.31873600	2.18981500
C	3.03812200	-1.63860500	3.74976400
C	1.90060800	0.33516700	2.93331900
C	4.34731000	-4.06890100	3.24910400
H	4.03155200	-3.67333300	1.17686800
C	3.52754600	-2.43161700	4.82032900
C	2.36493500	-0.41201600	3.98140800
H	1.37533400	1.26149900	3.14073800
C	4.17041000	-3.62459600	4.57938400
H	4.85529000	-5.01003700	3.05928600
H	3.38261900	-2.07663300	5.83746500
H	2.21554600	-0.07372700	5.00356400
H	4.54105700	-4.22462400	5.40534400
C	0.70696500	-2.98776500	0.06153000
H	0.95965900	-3.40787300	1.04387100
H	0.19164900	-2.04310700	0.26836200
C	-0.26138800	-3.92047800	-0.63622400
C	-0.05768300	-5.30858900	-0.62840800
C	-1.39532200	-3.41526400	-1.28603700
C	-0.95702500	-6.16701600	-1.26136500
H	0.81240400	-5.71777200	-0.11969100
C	-2.30152200	-4.27140600	-1.91631100
H	-1.58594900	-2.34510500	-1.28215600
C	-2.08205500	-5.64956600	-1.90831000
H	-0.78364600	-7.23970300	-1.24303000
H	-3.18094100	-3.85636900	-2.39987600
H	-2.78679100	-6.31812100	-2.39500600
C	2.03807900	0.99523600	-1.28828400
C	3.15918400	1.74170600	-1.68220800
C	1.40736900	0.17911300	-2.24216600

C	3.65308500	1.66550900	-2.98451500
H	3.65188800	2.40170000	-0.97900500
C	1.89351000	0.08593600	-3.54462000
H	0.51865900	-0.38037300	-1.97418800
C	3.01381600	0.83180900	-3.89323100
H	4.52034000	2.23728200	-3.29599900
H	1.41883600	-0.55313800	-4.28073300
C	1.93594600	2.73747000	1.03183400
C	3.26243800	2.86105100	1.48453300
C	1.10404600	3.86638700	1.06177000
C	3.75481600	4.08128600	1.94215900
H	3.91844300	1.99650200	1.49276400
C	1.58528400	5.09380800	1.52018900
H	0.07378900	3.78902600	0.73792600
C	2.90258800	5.18155500	1.94963100
H	4.77496900	4.18808800	2.29496000
H	0.94827000	5.97093400	1.55327100
P	1.27146000	1.13529100	0.38842200
F	3.48656500	0.75137200	-5.15406300
F	3.37201400	6.36388200	2.39635400
Pt	-1.20373500	1.12965800	0.35062900

116

TSCD-cis-s

imaginary frequencies -211.55

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.037456

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3462.972851

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.144702

B	-1.07315900	-2.44449200	1.44808900
O	-0.91392300	-3.82762400	1.49724800
C	-0.92430700	-4.25923700	2.86663600
C	-1.36588400	-3.01437200	3.66535700
B	-2.92988600	-2.25130600	-0.44920600
O	-3.89266500	-2.48205200	0.53169600
C	-4.49766400	-3.75429500	0.26114100
O	-1.29261100	-1.93355900	2.72521300
O	-2.99156000	-3.19870500	-1.46142200
C	-4.09044700	-4.07752500	-1.19120900
C	-6.07070900	-0.74235200	-0.97047200
H	-6.14920300	-1.47138500	-0.16238900
H	-6.98267000	-0.13615500	-0.97826600
H	-6.01220300	-1.27184800	-1.92715900
C	-2.92193400	-0.40050000	-1.15456000
C	-1.88032000	0.06325600	-1.78878600

C	-4.52782500	1.12674400	1.00676800
C	-5.27029200	2.28738300	1.29356300
C	-3.77822200	0.54697500	2.04767700
C	-5.27653400	2.84450500	2.57394100
H	-5.83937800	2.77173600	0.50394600
C	-3.77676100	1.10814600	3.32693400
H	-3.18367700	-0.34218100	1.86875600
C	-4.52737500	2.25510200	3.59479800
H	-5.86130700	3.73905900	2.77258200
H	-3.18450700	0.64414700	4.11090400
H	-4.52709100	2.68885200	4.59145300
H	0.08185700	-4.59650500	3.14322600
H	-1.61216600	-5.10374200	2.97993500
H	-2.39516300	-3.09912500	4.03443200
H	-0.70954600	-2.80408200	4.51642800
H	-3.77015000	-5.11568500	-1.32162000
H	-4.10213000	-4.49079700	0.97062700
H	-4.89901200	-3.87175200	-1.90414100
C	-1.52777700	1.00013400	-2.87781700
H	-0.62726000	1.57277200	-2.64518900
H	-1.30242900	0.42174400	-3.78248900
H	-2.35387100	1.68317800	-3.10375500
H	-5.58146200	-3.68405700	0.39739100
Si	-4.57999200	0.38942200	-0.73017500
C	-4.79347800	1.77192300	-1.92411100
C	-4.99677600	2.69408900	-2.69433700
C	-5.23195200	3.80195000	-3.61389900
H	-4.58746500	4.65575300	-3.37669000
H	-5.02944500	3.50564000	-4.64935300
H	-6.27213500	4.14302400	-3.56321200
C	1.68899800	2.38765700	0.91563600
C	2.71423900	1.75090900	0.22136500
C	4.01340200	1.61133100	0.82222000
C	4.22959400	2.09179200	2.15415000
C	3.15214000	2.70965500	2.84130000
C	1.92928800	2.85501300	2.23772900
H	4.97068200	0.66041100	-0.87364000
C	5.11244300	1.01907300	0.14010000
C	5.51128500	1.94943000	2.74895800
H	3.31423800	3.07619500	3.85188700
H	1.11960200	3.35054500	2.76474800
C	6.55169200	1.36728400	2.06042700
C	6.34743000	0.90254200	0.74052500
H	5.65625500	2.31364800	3.76295400

H	7.52807700	1.26653500	2.52549400
H	7.17167300	0.45019600	0.19606000
C	2.52106400	1.30783100	-1.20263900
C	2.91215900	2.24801300	-2.22907200
C	1.98169200	0.07531600	-1.57458600
C	3.47772200	3.51798100	-1.91672000
C	2.73558200	1.92065200	-3.61145100
C	1.78323900	-0.20890700	-2.96246800
C	3.84713100	4.39981500	-2.90972600
H	3.62293000	3.78981700	-0.87824400
C	3.12630300	2.84887200	-4.61198900
C	2.15440900	0.67051300	-3.94393400
H	1.32305400	-1.14871300	-3.24668800
C	3.67211500	4.06582000	-4.27242600
H	4.27917200	5.35978200	-2.64217400
H	2.98273500	2.57851400	-5.65501600
H	1.99884400	0.41985100	-4.99016600
H	3.96733300	4.76949000	-5.04526800
C	0.30069000	2.58422000	0.31956800
H	0.35035500	2.42225700	-0.76019900
H	-0.36686900	1.80239300	0.70445500
C	-0.32460600	3.94125600	0.59067900
C	0.23964400	5.10802200	0.05189200
C	-1.48641500	4.05504200	1.36397100
C	-0.34143700	6.35396900	0.28273400
H	1.13722200	5.03484100	-0.55764700
C	-2.07134100	5.30308300	1.59554600
H	-1.94502100	3.16209400	1.78061600
C	-1.50031300	6.45613200	1.05775900
H	0.10783800	7.24656300	-0.14465600
H	-2.97661800	5.36458700	2.19268800
H	-1.95410300	7.42711200	1.23632900
C	2.21630800	-1.26757300	1.14245100
C	3.48796500	-1.85083900	1.26394900
C	1.59823800	-0.75434300	2.29375700
C	4.13477100	-1.91286700	2.49661400
H	3.98228100	-2.27639500	0.39894400
C	2.23469000	-0.80686800	3.53241500
H	0.60203700	-0.33430500	2.23165100
C	3.49588400	-1.38426900	3.61171100
H	5.11742800	-2.35939700	2.60018300
H	1.76500300	-0.41061500	4.42582100
C	1.85471300	-2.79730400	-1.28043900
C	3.09865300	-2.88762100	-1.93057600

C	1.03858900	-3.93844700	-1.22424600
C	3.52480100	-4.08356800	-2.50539400
H	3.73899800	-2.01488500	-2.00956200
C	1.45514400	-5.14166200	-1.79487800
H	0.07763400	-3.88738600	-0.72581100
C	2.69148400	-5.19465000	-2.42529200
H	4.47997300	-4.16251000	-3.01331300
H	0.83119800	-6.02805600	-1.75817700
P	1.28425500	-1.24595000	-0.45103300
F	4.11395900	-1.44507600	4.80907000
F	3.09682600	-6.35328200	-2.98264500
Pt	-1.06651300	-1.23614700	-0.26538900

116

D-cis-s

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.052565

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3462.987429

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.163753

B	1.63530100	-1.68833200	-1.87827300
O	1.73505700	-3.03945900	-2.19729600
C	1.97178300	-3.18425100	-3.60783700
C	2.26223300	-1.75199000	-4.10252200
B	3.67169000	-1.57470200	1.19488300
O	4.61223300	-2.38676100	0.58291800
C	4.79113900	-3.55283700	1.39590000
O	1.89121700	-0.90403800	-3.00285600
O	3.14742500	-2.15710700	2.33937300
C	3.61365000	-3.51049900	2.39349500
C	5.43822300	-0.26253300	-1.56307800
H	4.62949700	-0.53986400	-2.24706600
H	6.19984000	0.28150700	-2.13111800
H	5.87014100	-1.17880900	-1.15735400
C	3.38654600	-0.09418300	0.76747400
C	2.23320200	0.52252800	1.25589200
C	4.10036700	2.42179400	-0.98883200
C	4.59350100	3.68995000	-0.63420900
C	3.14459800	2.35298600	-2.02254800
C	4.15234600	4.84765500	-1.27942000
H	5.33857900	3.77010300	0.15318100
C	2.70405800	3.50877600	-2.67186900
H	2.74411800	1.39128900	-2.33543000
C	3.20665100	4.75932100	-2.30193100
H	4.55036100	5.81608800	-0.98763700

H	1.97627800	3.43162600	-3.47602100
H	2.86925100	5.65707100	-2.81363300
H	1.07844000	-3.61369200	-4.07695700
H	2.81055600	-3.86863400	-3.76831900
H	3.32381600	-1.59823300	-4.33008200
H	1.67648700	-1.48047800	-4.98660400
H	2.79873600	-4.18247400	2.09704900
H	4.78227300	-4.44520800	0.76298600
H	3.91130000	-3.75431100	3.41804700
C	2.07044000	1.89870400	1.78597700
H	1.16202200	2.37487200	1.40760900
H	1.92913600	1.79215100	2.87210900
H	2.93174800	2.55802000	1.62616000
H	5.76425100	-3.49169700	1.89933200
Si	4.75262900	0.83204200	-0.19197900
C	6.09305100	1.29386000	0.97786300
C	6.97484500	1.58888200	1.76557100
C	8.03467800	1.93787100	2.70512800
H	7.63930200	2.50219900	3.55739000
H	8.52447200	1.03986900	3.09850700
H	8.80377900	2.55329700	2.22457500
C	-2.73461500	2.09055600	-0.43853500
C	-3.30870800	0.99343700	0.19743000
C	-4.53740000	0.43732600	-0.29636100
C	-5.13682600	0.98723100	-1.47560300
C	-4.50937100	2.09019000	-2.11142200
C	-3.35320500	2.62430400	-1.60287700
H	-4.76778600	-1.06196000	1.25084600
C	-5.19701400	-0.64782800	0.34464100
C	-6.34152600	0.42381600	-1.97333200
H	-4.96429100	2.51104800	-3.00454100
H	-2.89387100	3.48189000	-2.08530900
C	-6.94743700	-0.63400100	-1.33333700
C	-6.36949200	-1.16925100	-0.15849900
H	-6.78008100	0.84786100	-2.87312500
H	-7.86984700	-1.05469800	-1.72312300
H	-6.85580800	-1.99599400	0.35175800
C	-2.70657400	0.45951600	1.46678100
C	-3.19251000	1.03192100	2.70418000
C	-1.68829000	-0.49012100	1.51236300
C	-4.25214000	1.98284400	2.73295800
C	-2.60719400	0.64807700	3.95256600
C	-1.09354600	-0.82627600	2.77057300
C	-4.70408400	2.51417300	3.92265300

H	-4.71632500	2.28430500	1.80161800
C	-3.09044700	1.21503100	5.16025200
C	-1.53769200	-0.28567500	3.94570000
H	-0.25364300	-1.51335200	2.78648000
C	-4.11896500	2.13037500	5.15045600
H	-5.51901100	3.23224900	3.91558200
H	-2.62891900	0.91200300	6.09656100
H	-1.06830900	-0.56119300	4.88645800
H	-4.48144300	2.55771000	6.08084100
C	-1.44124800	2.73028400	0.05066000
H	-1.21984100	2.36698200	1.05788800
H	-0.61298100	2.37964200	-0.57968600
C	-1.44274200	4.24959700	0.05609900
C	-2.35197100	4.96218800	0.85317400
C	-0.52067500	4.97036300	-0.71216900
C	-2.34100700	6.35588900	0.87585900
H	-3.06696100	4.41803900	1.46484800
C	-0.50720200	6.36763900	-0.69039100
H	0.20443100	4.43579200	-1.32039100
C	-1.41884200	7.06523300	0.10115800
H	-3.05077100	6.89043000	1.50152600
H	0.22072600	6.90691100	-1.29031500
H	-1.41000200	8.15143200	0.11978500
C	-1.80253800	-1.30464600	-1.45361000
C	-2.87170200	-2.17296000	-1.72471400
C	-1.38208900	-0.41338500	-2.45368400
C	-3.51955100	-2.14592000	-2.95839700
H	-3.20221700	-2.88428500	-0.97686800
C	-2.02569800	-0.37058800	-3.68847900
H	-0.52672300	0.22941100	-2.27586900
C	-3.08596400	-1.23981500	-3.91853200
H	-4.34816700	-2.80942900	-3.17900100
H	-1.71111400	0.31367100	-4.46875900
C	-1.07210100	-3.15722200	0.63787500
C	-2.14234800	-3.55709100	1.45513500
C	-0.17463800	-4.13342600	0.17223700
C	-2.31718900	-4.89520800	1.80810200
H	-2.84482000	-2.82200700	1.83194800
C	-0.34069400	-5.47443500	0.51837100
H	0.64560000	-3.85057500	-0.47857400
C	-1.40787200	-5.83313800	1.33366800
H	-3.13752900	-5.21322300	2.44250100
H	0.34398700	-6.23749600	0.16359800
P	-0.84216000	-1.39559700	0.11376100

F	-3.70577600	-1.21036700	-5.11590400
F	-1.56683500	-7.12760800	1.67511200
Pt	1.35972800	-0.80331900	-0.00465600

116

cplx2-cis-r

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.053258

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3462.987784

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.162965

B	1.06747100	-1.50982000	-1.93132100
O	0.80276600	-2.85816600	-2.12750500
C	0.43594300	-3.06068300	-3.50177700
C	0.77858500	-1.72491200	-4.19612100
B	2.91579300	-1.60488400	-0.70403400
O	3.85589000	-1.39861300	-1.69969200
C	4.92028200	-2.35389100	-1.54542900
O	0.99730800	-0.80066500	-3.12040500
O	3.25875500	-2.66931300	0.11258600
C	4.48196300	-3.25273300	-0.36440800
C	2.65406000	1.10452600	0.45537900
C	1.62405600	1.25121900	1.19780000
H	-0.63402100	-3.29177200	-3.55072400
H	0.99559100	-3.90989400	-3.90627600
H	1.69209800	-1.78961700	-4.79929700
H	-0.03369200	-1.35996200	-4.83253300
H	4.28558000	-4.28608200	-0.67246100
H	5.03690400	-2.91063100	-2.48115000
H	5.21551000	-3.25928900	0.44668500
C	1.05121600	2.03860000	2.31555300
H	1.07667800	1.45660800	3.24247100
H	1.63494900	2.95390900	2.46519900
H	0.00672800	2.30803700	2.14482500
H	5.84936200	-1.81578400	-1.33665800
Si	4.30125600	1.75352200	-0.08026700
C	4.49086900	3.38704100	0.74145700
C	4.61355300	4.47138500	1.28345000
C	4.76394500	5.77145800	1.92746000
H	3.91744800	6.42800700	1.69615100
H	4.82117100	5.66986500	3.01721500
H	5.67772400	6.27482100	1.59165500
C	-2.98002700	2.15729800	-0.57861300
C	-3.48782200	1.17819400	0.27443200
C	-4.74482200	0.54878600	-0.01625400

C	-5.45339200	0.90530300	-1.20993200
C	-4.89882300	1.89365300	-2.06055300
C	-3.70582300	2.49999400	-1.75023300
H	-4.82461500	-0.68515800	1.76435700
C	-5.33498900	-0.41898300	0.84521000
C	-6.69207800	0.27386300	-1.50364700
H	-5.43592900	2.17199100	-2.96391600
H	-3.30083600	3.25909500	-2.41035500
C	-7.22796600	-0.66427000	-0.65171000
C	-6.54172700	-1.00731000	0.53759600
H	-7.21164000	0.55120200	-2.41739300
H	-8.17709700	-1.13802400	-0.88505200
H	-6.97289000	-1.74004800	1.21405400
C	-2.81232600	0.86319600	1.58127100
C	-3.23888400	1.64511800	2.72172200
C	-1.84419900	-0.12694200	1.75636100
C	-4.22252300	2.66985500	2.61174400
C	-2.67746200	1.40006700	4.01577700
C	-1.28292500	-0.33051700	3.05716200
C	-4.61890500	3.40179900	3.71022300
H	-4.66580700	2.87347700	1.64437300
C	-3.10779700	2.16763900	5.12944300
C	-1.69006000	0.39074500	4.14656400
H	-0.51129400	-1.08178000	3.18506500
C	-4.05956600	3.15115000	4.98417500
H	-5.37045000	4.17766500	3.59597400
H	-2.66731500	1.96287800	6.10188800
H	-1.25164400	0.20116000	5.12307100
H	-4.38162900	3.73403900	5.84216000
C	-1.68005200	2.88693400	-0.23387900
H	-1.87788700	3.54153100	0.62600700
H	-0.94791900	2.15255100	0.11432500
C	-1.05273100	3.70693800	-1.34317600
C	-1.38888600	5.05670500	-1.51780100
C	-0.11636400	3.13359100	-2.21635800
C	-0.81635800	5.81318600	-2.54212100
H	-2.10452400	5.51933500	-0.84173400
C	0.45776300	3.88752200	-3.24169000
H	0.18338500	2.09673700	-2.08531800
C	0.10833600	5.22906700	-3.40952900
H	-1.08858100	6.85877700	-2.65818100
H	1.18332200	3.42448200	-3.90462900
H	0.55838200	5.81649600	-4.20489800
C	-2.14634000	-1.45912800	-0.96644000

C	-3.08033200	-2.50680900	-0.99023800
C	-2.02147500	-0.64900700	-2.10648500
C	-3.88055200	-2.73304000	-2.10980200
H	-3.18359300	-3.16891500	-0.13954500
C	-2.81850300	-0.85732700	-3.23060000
H	-1.28612000	0.14544800	-2.12769900
C	-3.73954100	-1.89828600	-3.21110100
H	-4.60533500	-3.53933900	-2.13466400
H	-2.73453300	-0.22561100	-4.10789100
C	-0.95441600	-2.81730200	1.29161600
C	-2.01790100	-3.27352300	2.09198900
C	0.15758900	-3.65271400	1.10530300
C	-1.98277600	-4.53436600	2.68383600
H	-2.87912300	-2.63710400	2.26862400
C	0.20394400	-4.91775100	1.69348800
H	0.99626500	-3.31680700	0.50748600
C	-0.86706400	-5.33829400	2.47043200
H	-2.79561500	-4.89530900	3.30484600
H	1.06123100	-5.56839000	1.55953300
P	-0.99560200	-1.16862300	0.45440200
F	-4.51046900	-2.11010100	-4.29743200
F	-0.82599800	-6.55787200	3.04404800
Pt	1.27850400	-0.44496100	-0.13870800
C	5.67924300	0.61836000	0.53910100
C	5.48710700	-0.22291900	1.64935500
C	6.94773800	0.62051600	-0.06967100
C	6.52056700	-1.02763400	2.13539600
H	4.51540300	-0.25362100	2.13496300
C	7.98467200	-0.18236400	0.41055700
H	7.13409400	1.25745000	-0.93108800
C	7.77224200	-1.00924500	1.51613900
H	6.34843800	-1.66741700	2.99702300
H	8.95650600	-0.16219000	-0.07572200
H	8.57785100	-1.63356900	1.89328900
C	4.36707900	1.98029300	-1.94364600
H	3.58494100	2.67831700	-2.25808800
H	5.33108200	2.38564100	-2.26884500
H	4.19662500	1.01878800	-2.43554100

116

TSCD-cis-r

imaginary frequencies -206.328

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.039484

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3462.974883

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.147238

B	0.98101500	-1.75179900	-1.87317500
O	1.15641700	-3.12881100	-1.98928200
C	1.20245800	-3.47984100	-3.38065500
C	0.72981500	-2.20984700	-4.11653700
B	3.04852200	-1.25370600	-0.28380800
O	3.88597400	-1.26189500	-1.39335700
C	4.87791500	-2.28549500	-1.21085400
O	0.79466600	-1.17354900	-3.12636800
O	3.42182700	-2.20486700	0.65321300
C	4.46777700	-3.01079900	0.09246200
C	2.79760900	0.55276000	0.51097900
C	1.77943600	0.84116100	1.27510100
H	0.55712000	-4.34504700	-3.56294600
H	2.23094300	-3.75364700	-3.64815000
H	1.36771500	-1.94603700	-4.96596600
H	-0.30436200	-2.30110700	-4.47246200
H	4.07725600	-4.01699000	-0.09827000
H	4.86766000	-2.94861400	-2.08182200
H	5.29149600	-3.08062900	0.80902000
C	1.41405000	1.75951400	2.37763400
H	1.36831600	1.19557200	3.31675800
H	2.14877000	2.56425100	2.49140400
H	0.41969300	2.18839500	2.22733700
H	5.86310100	-1.81608800	-1.13438900
Si	4.28145400	1.53911600	-0.09662000
C	4.24968700	3.12423900	0.83425400
C	4.28235700	4.19784300	1.40984800
C	4.32008500	5.48576900	2.09351900
H	3.36014700	6.00751500	2.00878900
H	4.54324900	5.36282900	3.15936700
H	5.09157100	6.13520100	1.66460200
C	-2.73273300	2.15182000	-0.76737200
C	-3.39667700	1.33735600	0.14882800
C	-4.72579000	0.87124600	-0.12681200
C	-5.35101500	1.21854200	-1.36861100
C	-4.63868300	2.03191300	-2.28445200
C	-3.37551500	2.48462900	-1.98915600
H	-5.01556400	-0.18239300	1.74539400
C	-5.46731100	0.07906300	0.79480400
C	-6.66544400	0.75396400	-1.64431500
H	-5.11061800	2.30106700	-3.22619900
H	-2.85020400	3.11388600	-2.69864200
C	-7.35137400	-0.01272200	-0.73074400

C	-6.74382600	-0.34781900	0.50296800
H	-7.12131800	1.02172900	-2.59418500
H	-8.35717800	-0.35884100	-0.95049700
H	-7.29089900	-0.94676600	1.22577900
C	-2.78979600	1.04057700	1.49176300
C	-3.14480200	1.93576000	2.57043100
C	-1.92707400	-0.02676100	1.74494000
C	-4.01184100	3.04909300	2.37581200
C	-2.62268300	1.72122800	3.88605700
C	-1.39338800	-0.19517200	3.06157800
C	-4.34200100	3.88836400	3.41802100
H	-4.41709300	3.23531200	1.38843600
C	-2.98375900	2.59991700	4.94059200
C	-1.73846400	0.63245700	4.09589500
H	-0.69344500	-1.00200800	3.24685400
C	-3.82728900	3.66403100	4.71553600
H	-5.00541000	4.72997300	3.24076400
H	-2.57654700	2.41634800	5.93160700
H	-1.32644300	0.46828400	5.08838900
H	-4.09678800	4.33186200	5.52859800
C	-1.34411100	2.70811100	-0.44347100
H	-1.43416900	3.35246900	0.44095500
H	-0.69145200	1.88001600	-0.14291700
C	-0.66419700	3.48227100	-1.55369300
C	-0.81013300	4.87272600	-1.65263000
C	0.11969900	2.82215500	-2.51235600
C	-0.19615300	5.58870000	-2.68203500
H	-1.41040900	5.39891500	-0.91377800
C	0.73340400	3.53588700	-3.54403200
H	0.26079900	1.74564100	-2.44847200
C	0.57724700	4.92103600	-3.63300800
H	-0.31937000	6.66690800	-2.73835000
H	1.33777100	3.00654000	-4.27534500
H	1.05804500	5.47562100	-4.43396500
C	-2.38750000	-1.52520900	-0.86221200
C	-3.46065800	-2.41631600	-0.70039400
C	-2.19541900	-0.92574500	-2.11674600
C	-4.32812900	-2.69618000	-1.75446400
H	-3.62338600	-2.91441600	0.24758300
C	-3.05610300	-1.19484500	-3.17970400
H	-1.35528500	-0.26257700	-2.27813100
C	-4.11185900	-2.07556700	-2.97848400
H	-5.16004100	-3.38184600	-1.63782800
H	-2.91723400	-0.73064000	-4.14979300

C	-1.14471400	-2.79910000	1.40605700
C	-2.15533700	-3.16601700	2.31255400
C	-0.10214700	-3.70563000	1.15362400
C	-2.13572500	-4.40597200	2.94866500
H	-2.95890700	-2.47405800	2.54340300
C	-0.07354000	-4.95070900	1.78267800
H	0.68890700	-3.43698500	0.46285700
C	-1.09099400	-5.28066000	2.66867000
H	-2.90721400	-4.69667300	3.65354000
H	0.72774500	-5.65750600	1.59648700
P	-1.17445300	-1.19109600	0.49130700
F	-4.94492200	-2.34458700	-4.00437300
F	-1.06518900	-6.48069400	3.28251800
Pt	1.01739800	-0.61162200	-0.11865500
C	5.89635600	0.66912600	0.35229100
C	6.01396800	-0.06194400	1.54877200
C	7.03224800	0.76509500	-0.47108500
C	7.21740000	-0.67170200	1.90880900
H	5.15095100	-0.16685700	2.20102000
C	8.23862400	0.15609600	-0.11693400
H	6.97883600	1.31875000	-1.40512300
C	8.33317600	-0.56431500	1.07529300
H	7.28446700	-1.23038800	2.83869200
H	9.10252100	0.24349000	-0.77059800
H	9.27044900	-1.03872600	1.35337700
C	4.15584400	1.92293600	-1.93073600
H	3.23092100	2.47266700	-2.12817200
H	4.99416800	2.54779200	-2.25733400
H	4.14456100	0.99902600	-2.51319900

116

D-cis-r

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.052216

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3462.987267

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.161701

B	-0.97226000	1.15435300	-2.20223900
O	-1.08678100	2.44631000	-2.71041300
C	-1.28716300	2.37830300	-4.13285700
C	-0.97946200	0.91194500	-4.49621200
B	-3.42175100	1.55661600	0.32745900
O	-4.22666600	2.05695800	-0.68385800
C	-4.60894900	3.39052700	-0.32446500
O	-0.97118700	0.21919800	-3.23691900

O	-3.15749400	2.50453500	1.30393600
C	-3.65934600	3.76237400	0.83455200
C	-3.09897800	0.02718000	0.48281400
C	-2.02217900	-0.36909900	1.26710800
H	-0.62104500	3.09013400	-4.63064100
H	-2.32366500	2.65394100	-4.36127300
H	-1.73365200	0.46780900	-5.15311200
H	0.00384800	0.80222800	-4.97078000
H	-2.81758400	4.37938900	0.49751800
H	-4.50100300	4.04837300	-1.19173000
H	-4.16624100	4.28130600	1.65387700
C	-1.92363100	-1.48073600	2.24343100
H	-2.17885500	-1.04947000	3.22352200
H	-2.63006100	-2.29690800	2.05268500
H	-0.90600600	-1.86935800	2.32723200
H	-5.66099800	3.38718400	-0.01353700
Si	-4.40644900	-1.10522000	-0.32140700
C	-3.99289500	-2.87458300	-0.05823600
C	-3.74652700	-4.06281800	0.05482600
C	-3.43531300	-5.48098400	0.19036000
H	-2.54701000	-5.74143200	-0.39554400
H	-3.23979200	-5.74465000	1.23610200
H	-4.26791300	-6.10218100	-0.15929300
C	2.77790500	-2.29632900	-0.17797900
C	3.38658300	-1.27823600	0.55509100
C	4.72441800	-0.86393600	0.24692200
C	5.41832000	-1.47817800	-0.84629100
C	4.76389800	-2.49880400	-1.57915300
C	3.48938600	-2.89414100	-1.25147100
H	4.90039100	0.60545900	1.83089000
C	5.40542500	0.14083400	0.99087900
C	6.73849000	-1.05687300	-1.16098100
H	5.28753200	-2.97033200	-2.40708400
H	3.00855500	-3.68115200	-1.82128900
C	7.36356100	-0.07716500	-0.42439800
C	6.68823900	0.52240500	0.66571600
H	7.24791800	-1.52801600	-1.99782000
H	8.37386700	0.23481500	-0.67282500
H	7.18814800	1.28916500	1.25106600
C	2.69578100	-0.68829800	1.75216400
C	2.96595900	-1.31669300	3.02696400
C	1.81034100	0.38708700	1.69747100
C	3.85938500	-2.41821900	3.15275800
C	2.32684700	-0.83770100	4.21480100

C	1.15402500	0.81930300	2.89384900
C	4.10767100	-3.00088600	4.37731200
H	4.35261000	-2.80062500	2.26708700
C	2.60335900	-1.45614800	5.46135300
C	1.41167700	0.24233400	4.10707700
H	0.42186700	1.61712600	2.83305600
C	3.47735200	-2.51685800	5.54590400
H	4.79551900	-3.83884600	4.44431600
H	2.10750100	-1.07592200	6.35081300
H	0.90594600	0.59906400	5.00065300
H	3.68185400	-2.98339700	6.50518300
C	1.37095600	-2.77653800	0.18754300
H	1.40201400	-3.16952500	1.21241900
H	0.69943600	-1.91061500	0.22342000
C	0.76498100	-3.82227200	-0.72587600
C	1.02677600	-5.18598400	-0.52837500
C	-0.07110700	-3.44878700	-1.78822000
C	0.47927900	-6.15252200	-1.37361200
H	1.66740900	-5.49147900	0.29581900
C	-0.62246100	-4.41356600	-2.63423700
H	-0.30554000	-2.39932900	-1.95087400
C	-0.34712100	-5.76793200	-2.43267800
H	0.69597800	-7.20392600	-1.20449200
H	-1.27264200	-4.10397500	-3.44743000
H	-0.77408400	-6.51775300	-3.09300900
C	2.39492700	1.18080100	-1.19373300
C	3.50893900	2.03512100	-1.22823300
C	2.17573900	0.31168600	-2.27300000
C	4.39083300	2.01874500	-2.30692200
H	3.69313000	2.72884700	-0.41603900
C	3.05027700	0.28391900	-3.35768500
H	1.30544400	-0.33309500	-2.27922900
C	4.14564300	1.13935600	-3.35453000
H	5.25587500	2.67145600	-2.34306200
H	2.89336100	-0.38847800	-4.19386600
C	1.23327700	3.04785800	0.64067100
C	2.11441400	3.55629400	1.60801800
C	0.40855300	3.94284200	-0.06339100
C	2.16875000	4.92359900	1.88176300
H	2.76022500	2.88612800	2.16513900
C	0.45958200	5.31145200	0.19746600
H	-0.26386300	3.56892900	-0.82893400
C	1.33632800	5.77904400	1.17031800
H	2.84043500	5.32679200	2.63195200

H	-0.16740500	6.01359800	-0.34171000
P	1.16573900	1.25869200	0.17940100
F	4.99225400	1.12121000	-4.40401000
F	1.38231200	7.10098800	1.43022700
Pt	-0.98834200	0.61550800	-0.18243000
C	-6.09078200	-0.76129900	0.47276400
C	-6.19455700	-0.20677400	1.76107600
C	-7.28667000	-1.06586500	-0.20288800
C	-7.43705300	0.03100500	2.35285700
H	-5.29179000	0.05008400	2.31043900
C	-8.53196400	-0.83110900	0.38217800
H	-7.24986900	-1.49218400	-1.20263300
C	-8.60971300	-0.28146000	1.66357700
H	-7.48919800	0.46065400	3.34992200
H	-9.44103800	-1.07451500	-0.16165200
H	-9.57822700	-0.09691800	2.12066300
C	-4.45946000	-0.79752600	-2.17917200
H	-3.45310200	-0.89275200	-2.59904700
H	-5.11231900	-1.52079900	-2.67905600
H	-4.82038900	0.21344100	-2.38351200

116

F-cis-s

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.092839

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.028535

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.201961

B	-0.91566100	2.16800200	-1.57506200
O	-1.06104000	3.54481700	-1.45828500
C	-0.97529800	4.13334600	-2.76567000
C	-1.00814000	2.93211300	-3.73792900
B	-2.63255900	-0.90034400	1.74657800
O	-3.05446200	-1.59073100	2.85975000
C	-1.91836100	-1.88172400	3.68127800
O	-0.83117100	1.77968800	-2.90306000
O	-1.26123300	-0.60482800	1.83315200
C	-0.80317200	-0.96070000	3.15097300
C	-5.70120700	-2.37048400	1.60427600
H	-5.66826100	-1.96282500	2.61785800
H	-6.71648500	-2.72927100	1.40457700
H	-5.02017200	-3.22572000	1.56852600
C	-3.46584400	-0.43039600	0.55050700
C	-2.85700700	0.44714500	-0.31886400
C	-6.50166500	0.34528100	0.41519800

C	-7.72019200	0.28933800	-0.28517100
C	-6.27428000	1.46094000	1.24119100
C	-8.67478200	1.30089100	-0.16230500
H	-7.91899600	-0.55112400	-0.94595200
C	-7.22527300	2.47518500	1.36990900
H	-5.33466500	1.54409500	1.78262000
C	-8.42960800	2.39647500	0.66786600
H	-9.60763000	1.23659400	-0.71681200
H	-7.02482300	3.32826600	2.01313900
H	-9.17037700	3.18604000	0.76348800
H	-0.04243900	4.70471800	-2.83996100
H	-1.81445000	4.82082500	-2.90965700
H	-1.96741000	2.84833300	-4.26280000
H	-0.20710000	2.96698800	-4.48304700
H	-0.69619400	-0.04882500	3.74877800
H	-2.16411700	-1.68760400	4.72953700
H	0.16823500	-1.45155900	3.08282300
C	-3.60140000	1.03214200	-1.49466800
H	-3.58771300	2.12736200	-1.43123100
H	-3.09412300	0.76609700	-2.42796700
H	-4.64477200	0.71522800	-1.56628200
H	-1.66087000	-2.94229600	3.57337500
Si	-5.23436300	-1.06418800	0.32007100
C	-5.42587800	-1.87633100	-1.32675700
C	-5.56047500	-2.42575800	-2.40641200
C	-5.72052000	-3.07239100	-3.70515700
H	-6.19332200	-2.39699500	-4.42747500
H	-4.75187900	-3.37487600	-4.11939900
H	-6.34582500	-3.96951100	-3.62993900
C	2.08919000	-2.26253300	-0.83419500
C	3.10783000	-1.54450000	-0.21071600
C	4.37859600	-1.37678300	-0.86141600
C	4.57365400	-1.91743300	-2.17375100
C	3.49904500	-2.60407000	-2.79564000
C	2.30168100	-2.77036300	-2.14547400
H	5.34583800	-0.29129100	0.74692400
C	5.47257900	-0.70455600	-0.24778000
C	5.83231600	-1.76304200	-2.81374900
H	3.64189500	-3.00888400	-3.79448800
H	1.49605500	-3.31639500	-2.62539500
C	6.86983200	-1.10987000	-2.18830200
C	6.68453800	-0.57813500	-0.89069900
H	5.96144800	-2.17589200	-3.81109800
H	7.82873900	-1.00114400	-2.68659300

H	7.50553800	-0.06488100	-0.39788600
C	2.94531400	-1.04524200	1.19902600
C	3.44426700	-1.90766400	2.24608000
C	2.34726600	0.17202000	1.53967100
C	4.05219500	-3.16580500	1.96477200
C	3.33358100	-1.51576500	3.61926000
C	2.22373600	0.52032000	2.92118300
C	4.52113100	-3.97457300	2.97647900
H	4.14623700	-3.48713500	0.93474400
C	3.83038900	-2.36883700	4.64046000
C	2.70900000	-0.28080100	3.92194000
H	1.73466400	1.44885900	3.19017400
C	4.41336500	-3.57533300	4.32928600
H	4.97966200	-4.92847900	2.73277400
H	3.73706500	-2.04913400	5.67518000
H	2.60847600	0.02232200	4.96113100
H	4.78879000	-4.22239200	5.11661100
C	0.74139700	-2.47133700	-0.15957100
H	0.88827900	-2.45845300	0.92547900
H	0.10836500	-1.59885500	-0.37315300
C	-0.02545700	-3.72561900	-0.53329100
C	0.53380400	-5.00126800	-0.36174300
C	-1.34139600	-3.63071400	-1.00519400
C	-0.20191300	-6.14878900	-0.65650900
H	1.55257900	-5.09300800	0.00717300
C	-2.08369400	-4.77886800	-1.29370100
H	-1.79523300	-2.65136000	-1.13194400
C	-1.51520100	-6.04129400	-1.12292100
H	0.24763000	-7.12845000	-0.51747800
H	-3.10694400	-4.67695600	-1.64421800
H	-2.08952100	-6.93594300	-1.34702300
C	2.51090400	1.48857600	-1.18682800
C	3.69108000	2.24432800	-1.28077600
C	2.03164400	0.84689500	-2.34022900
C	4.38151500	2.35198500	-2.48610400
H	4.07681000	2.77211600	-0.41731200
C	2.71163600	0.94536100	-3.55257300
H	1.11227800	0.27746200	-2.29783600
C	3.87931100	1.69572800	-3.60400700
H	5.29337400	2.93327900	-2.56806300
H	2.34628200	0.45058500	-4.44544700
C	1.82971500	2.99989600	1.18305400
C	3.04899900	3.31793200	1.81102700
C	0.81860300	3.97378600	1.15141000

C	3.26041400	4.56993100	2.38382300
H	3.83837600	2.57601600	1.87826200
C	1.01838100	5.23329100	1.72004400
H	-0.12578300	3.75589300	0.66590200
C	2.23625300	5.51070100	2.32603400
H	4.19493300	4.82155400	2.87365900
H	0.24234400	5.99077000	1.69908000
P	1.51143300	1.36842900	0.36479000
F	4.54020500	1.80150300	-4.77429300
F	2.43482200	6.72194600	2.88160000
Pt	-0.86680200	0.92322300	-0.01669100

116

F-cis-r

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.087749

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.022553

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.200562

B	0.51511600	-0.68398300	-2.77906500
O	0.62641300	-1.97481500	-3.27113500
C	0.45703200	-1.92654000	-4.69840900
C	-0.10268900	-0.51439700	-4.97329100
B	3.62659400	-1.11847200	0.01881200
O	4.34300200	-2.19412800	-0.46991300
C	4.28333500	-3.25406100	0.49214700
O	0.15340500	0.22068200	-3.76371700
O	2.96966100	-1.42482300	1.20222400
C	3.17505800	-2.82064600	1.47743300
C	3.64544200	0.28026700	-0.66618300
C	2.51769700	0.75636700	-1.26725000
H	-0.22340900	-2.72375700	-5.01198900
H	1.43019900	-2.08815100	-5.17622600
H	0.38804300	-0.01528500	-5.81390600
H	-1.18378500	-0.52811900	-5.15688200
H	2.23622300	-3.35860400	1.30331700
H	4.05568100	-4.19719700	-0.01400300
H	3.46436800	-2.94489700	2.52551500
C	2.45350500	2.02951500	-2.07656100
H	1.68647000	2.70330100	-1.67758000
H	3.40080300	2.57811400	-2.10057300
H	2.15077700	1.80163200	-3.10462200
H	5.26097100	-3.34208000	0.98078200
Si	5.32236300	1.16854000	-0.64876100
C	5.14347900	2.92240400	-0.12191500

C	5.02236900	4.08268000	0.22969000
C	4.86937900	5.47333800	0.64289500
H	4.26865100	6.03587800	-0.08091400
H	4.36864800	5.54413500	1.61522400
H	5.84142400	5.97219700	0.73023600
C	-3.15437200	2.06674800	0.25519100
C	-3.44291500	0.98627800	1.08878200
C	-4.75932100	0.42029700	1.11432200
C	-5.76813600	0.94527700	0.24216700
C	-5.43582500	2.03055900	-0.60607800
C	-4.17366200	2.57369800	-0.59362200
H	-4.36728400	-1.04836500	2.65923900
C	-5.11505500	-0.65184500	1.98060100
C	-7.06880500	0.37302600	0.25542100
H	-6.19908700	2.43436400	-1.26665200
H	-3.94212200	3.41133500	-1.24213100
C	-7.37567800	-0.66856800	1.10063300
C	-6.38703700	-1.18044800	1.97513800
H	-7.82106000	0.77864800	-0.41644800
H	-8.37418500	-1.09601900	1.10362100
H	-6.63611400	-1.99547400	2.64905100
C	-2.39438000	0.46899800	2.03144300
C	-2.34831700	1.05493500	3.35011900
C	-1.44846100	-0.49285700	1.67983400
C	-3.30159700	2.02167900	3.78076200
C	-1.31799900	0.67523900	4.26973300
C	-0.40318500	-0.82296800	2.60113000
C	-3.24090900	2.56888200	5.04389200
H	-4.08795400	2.32503200	3.09986900
C	-1.28136000	1.25765600	5.56390300
C	-0.34186800	-0.26373600	3.84998000
H	0.37468200	-1.51493500	2.29652600
C	-2.22293200	2.18504900	5.94764300
H	-3.98228000	3.30181000	5.34876200
H	-0.48986200	0.95789300	6.24580200
H	0.46531400	-0.52872300	4.52749200
H	-2.18577200	2.62513200	6.93989000
C	-1.75516400	2.68503300	0.24351200
H	-1.43328200	2.83227600	1.28077600
H	-1.04964100	1.95599500	-0.18104300
C	-1.61256300	3.99151200	-0.50895900
C	-1.95983500	5.20871700	0.09477400
C	-1.12658000	4.01322600	-1.82381300
C	-1.82784500	6.41431200	-0.59476700

H	-2.33314100	5.20894100	1.11628000
C	-0.99216100	5.21889000	-2.51664900
H	-0.84157300	3.08043000	-2.30456700
C	-1.34326800	6.42304200	-1.90484300
H	-2.09835700	7.34734400	-0.10784600
H	-0.60747000	5.21526400	-3.53275800
H	-1.23609100	7.36141300	-2.44165400
C	-2.71448100	-1.33566400	-1.00258600
C	-3.72503700	-2.29069600	-0.80303600
C	-2.82312900	-0.45276200	-2.08883100
C	-4.82572700	-2.35631600	-1.65380700
H	-3.65521600	-2.99808300	0.01539800
C	-3.92005300	-0.50682800	-2.94785300
H	-2.03851500	0.27275100	-2.27442800
C	-4.90464300	-1.45881700	-2.71294200
H	-5.61493900	-3.08518300	-1.50685500
H	-4.01835400	0.17427500	-3.78605500
C	-0.94801500	-3.07543800	0.43355700
C	-1.50313200	-3.69146200	1.56648800
C	-0.20106500	-3.85519000	-0.46769200
C	-1.32158100	-5.05435000	1.80288700
H	-2.07258800	-3.10526000	2.28040300
C	-0.01924100	-5.22032600	-0.24505000
H	0.23631100	-3.39491500	-1.34952300
C	-0.58166700	-5.79639000	0.88898200
H	-1.74052600	-5.54159200	2.67679300
H	0.55207300	-5.83498400	-0.93249100
P	-1.18526500	-1.29136100	0.02189000
F	-5.96490900	-1.52086700	-3.54297600
F	-0.40137900	-7.11324600	1.11234500
Pt	0.78139100	-0.23568800	-0.86697300
C	6.46752000	0.34659500	0.62354800
C	6.66122400	0.90427900	1.90021400
C	7.15949700	-0.84276700	0.32277800
C	7.50065800	0.30081800	2.83929300
H	6.15497400	1.83090000	2.15722300
C	8.00239900	-1.44973300	1.25620100
H	7.03324100	-1.31081400	-0.64954700
C	8.17412100	-0.87887000	2.51939400
H	7.63251100	0.75445800	3.81834200
H	8.53010200	-2.36380900	0.99547900
H	8.83177700	-1.34825200	3.24640600
C	6.16302100	1.12147600	-2.34434000
H	5.55275700	1.63119600	-3.09613300

H	7.14423000	1.60638600	-2.31137100
H	6.30166300	0.08719700	-2.67676500

116

F-trans-s

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.084449

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.019562

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.195128

B	1.25158700	-0.62741600	-2.62508800
O	1.46975400	-1.94780100	-2.98174700
C	1.48781600	-2.02637000	-4.41701000
C	0.92180200	-0.66979400	-4.88724600
B	4.85688800	2.52390900	-0.46362900
O	5.34034500	2.99418200	0.74809100
C	6.27967800	4.04553200	0.49123200
O	0.98603200	0.17089700	-3.72430900
O	5.34715100	3.25188700	-1.52968000
C	6.13274100	4.33822200	-1.02131100
C	3.90725900	1.28906600	-0.53626600
C	2.67766700	1.36969900	-1.12761100
H	0.88181400	-2.87739200	-4.74231200
H	2.52043300	-2.18180200	-4.75116400
H	1.50491200	-0.21950300	-5.69580700
H	-0.12316300	-0.74923100	-5.21042600
H	5.60667000	5.28113400	-1.21295600
H	6.04015900	4.91084600	1.11730900
H	7.09396500	4.36766600	-1.54406600
C	2.22549000	2.59956500	-1.89269900
H	1.36564200	3.06822000	-1.39742400
H	3.01484100	3.34900900	-2.00579700
H	1.88174400	2.30354500	-2.88871900
H	7.28666300	3.69827200	0.75222300
Si	4.57464500	-0.25249200	0.32680700
C	4.33316800	-1.77983500	-0.66679700
C	4.29529900	-2.80125500	-1.32972400
C	4.21567500	-4.01076100	-2.14025100
H	3.24518100	-4.06897500	-2.64540400
H	4.99789000	-4.02656000	-2.90822900
H	4.33942000	-4.91258300	-1.52885400
C	-3.18884600	1.74399700	-0.33566300
C	-3.40704300	0.68271600	0.53952400
C	-4.60284900	-0.10422900	0.43742700
C	-5.54811600	0.18146800	-0.60057700

C	-5.28256700	1.25593900	-1.48796500
C	-4.14503100	2.01211100	-1.35298900
H	-4.19939200	-1.38065400	2.13996400
C	-4.89789900	-1.16500200	1.33849300
C	-6.72504400	-0.60663200	-0.70814000
H	-6.00018700	1.47814800	-2.27382600
H	-3.96509900	2.84396900	-2.02640000
C	-6.97502700	-1.63108000	0.17675300
C	-6.05219100	-1.90687600	1.21332900
H	-7.42942600	-0.38139300	-1.50499300
H	-7.87982000	-2.22505400	0.08557100
H	-6.25782800	-2.70915200	1.91651100
C	-2.44333000	0.42012600	1.66137100
C	-2.69478400	1.10306800	2.90845000
C	-1.31696900	-0.39352000	1.54429700
C	-3.84240800	1.92497900	3.10278200
C	-1.77200700	0.97488800	3.99586700
C	-0.39684700	-0.48429700	2.63710700
C	-4.05967400	2.57483700	4.29847700
H	-4.55650500	2.03284400	2.29517300
C	-2.02280500	1.65860600	5.21495300
C	-0.61545300	0.17470100	3.81811200
H	0.50115900	-1.08512400	2.53444200
C	-3.14266200	2.44351200	5.36743300
H	-4.94490800	3.19204300	4.42203000
H	-1.30793900	1.55035400	6.02645800
H	0.10880600	0.09181300	4.62298000
H	-3.32483900	2.96283500	6.30378800
C	-1.92883300	2.60145100	-0.25327500
H	-1.52609900	2.54653800	0.76208600
H	-1.15712700	2.15523800	-0.89619300
C	-2.11664800	4.05786300	-0.63275600
C	-2.80642700	4.93105000	0.22212400
C	-1.60248600	4.56635300	-1.83214300
C	-2.97852300	6.27287500	-0.11448800
H	-3.20461100	4.55271200	1.16064500
C	-1.77311300	5.91103200	-2.17283200
H	-1.05721200	3.90512900	-2.50124600
C	-2.46286400	6.76801000	-1.31549000
H	-3.51198800	6.93496900	0.56217200
H	-1.36320100	6.28647500	-3.10642100
H	-2.59494200	7.81409800	-1.57698900
C	-2.01354000	-1.64450200	-1.18216100
C	-2.86400900	-2.75444000	-1.05167700

C	-2.11895300	-0.84590100	-2.33234700
C	-3.80604200	-3.05539400	-2.03300800
H	-2.78913700	-3.40040400	-0.18466400
C	-3.05785600	-1.13409400	-3.32162700
H	-1.45522900	0.00199500	-2.46287900
C	-3.88792300	-2.23590900	-3.15266800
H	-4.47036200	-3.90733100	-1.94008500
H	-3.15308100	-0.51935500	-4.21001700
C	-0.26413700	-2.95451200	0.68339000
C	-0.94374300	-3.55964700	1.75317600
C	0.76463800	-3.66464600	0.04247700
C	-0.61237100	-4.84640800	2.17649900
H	-1.72966900	-3.02182300	2.27369800
C	1.10051300	-4.95467900	0.45294900
H	1.30730100	-3.20492700	-0.77729600
C	0.40636600	-5.52335000	1.51449100
H	-1.12546400	-5.32356200	3.00457400
H	1.89366700	-5.51475400	-0.03031000
P	-0.67945600	-1.27779300	0.03553800
F	-4.79424100	-2.52390200	-4.10832800
F	0.73252800	-6.76698100	1.91969900
Pt	1.19386800	0.02236900	-0.74843900
C	3.83759700	-0.53401000	2.05322400
C	3.42902100	-1.80496000	2.49644000
C	3.77462300	0.53242400	2.97164700
C	2.98367800	-2.00850200	3.80575600
H	3.46451700	-2.64638500	1.80957800
C	3.33436100	0.33373500	4.28165400
H	4.08477900	1.52799600	2.66179400
C	2.94040800	-0.93912100	4.70367100
H	2.67785500	-3.00144000	4.12562100
H	3.30372600	1.17053400	4.97501100
H	2.60871800	-1.09798300	5.72682900
C	6.45154800	-0.07687600	0.54419400
H	6.94465100	0.10023500	-0.41837500
H	6.69264100	0.75461500	1.21263800
H	6.87003500	-0.99401500	0.97059200

116

F-trans-r

imaginary frequencies no

E(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.082029

H(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.01707

G(B3LYP/LanL2DZ(Pd),6-31G(d,p))=-3463.192686

B	1.02508900	-1.15743400	-2.26115300
O	1.31136200	-2.50981200	-2.32550700
C	1.39920400	-2.88023600	-3.71234500
C	0.80082800	-1.67857400	-4.47418700
B	4.70925200	2.13153500	-0.82551300
O	4.91704200	3.21407200	0.00670100
C	6.08316200	3.91257900	-0.45033400
O	0.77783100	-0.61455500	-3.50857100
O	5.57106400	2.12117000	-1.90168800
C	6.38653600	3.29953200	-1.83803500
C	3.65033000	1.01843300	-0.53331400
C	2.42976000	1.04302700	-1.13914800
H	0.84402000	-3.80874100	-3.87626800
H	2.45179500	-3.04935300	-3.96757600
H	1.40228900	-1.37515600	-5.33593600
H	-0.22438200	-1.87257300	-4.81135900
H	6.10867600	3.97073700	-2.66003200
H	5.87325400	4.98606700	-0.49398800
H	7.43812500	3.02165600	-1.95877400
C	2.09332000	2.10223500	-2.17506900
H	1.29039900	2.75792600	-1.81524700
H	2.95413600	2.73293800	-2.43173200
H	1.73008600	1.63252500	-3.09429100
H	6.89739000	3.74125500	0.26335200
Si	4.20824700	-0.29371000	0.70387900
C	4.21372900	-1.96606700	-0.05904800
C	4.24937800	-3.06808100	-0.57704700
C	4.26179500	-4.38090900	-1.21206200
H	3.28769100	-4.59603300	-1.66561500
H	5.01915500	-4.43263000	-2.00298200
H	4.48471800	-5.17541400	-0.49017300
C	-3.28065900	1.80162300	-0.51343800
C	-3.66540700	0.84809600	0.42503800
C	-4.90669700	0.14090700	0.27023600
C	-5.71896300	0.38847600	-0.88317700
C	-5.28036600	1.34584800	-1.83476000
C	-4.10653100	2.03091000	-1.64868200
H	-4.77963900	-0.98740700	2.11554900
C	-5.37575500	-0.79969800	1.22892200
C	-6.94187600	-0.31631000	-1.04008200
H	-5.89648500	1.53732100	-2.70974800
H	-3.79606200	2.77922200	-2.37133200
C	-7.36332700	-1.22376300	-0.09443000
C	-6.57175000	-1.46168400	1.05338000

H	-7.54410100	-0.12092600	-1.92379600
H	-8.30234500	-1.75398900	-0.22401300
H	-6.91110600	-2.17128000	1.80286800
C	-2.84209600	0.62203600	1.66121600
C	-3.17798500	1.40718500	2.82524200
C	-1.77142200	-0.26990200	1.72381200
C	-4.27654800	2.31452500	2.83408300
C	-2.39472700	1.29554800	4.01863100
C	-0.99129900	-0.34430100	2.92083700
C	-4.57839400	3.05795200	3.95465400
H	-4.88572500	2.41388400	1.94368400
C	-2.72984200	2.07560500	5.15674000
C	-1.28935500	0.40805900	4.02615700
H	-0.14216200	-1.01769000	2.95895600
C	-3.79973100	2.94043700	5.12960200
H	-5.42442600	3.73885000	3.93625700
H	-2.12074500	1.97656900	6.05144900
H	-0.67788400	0.32912200	4.92109000
H	-4.04780200	3.53316500	6.00515500
C	-1.98378800	2.59367400	-0.38330300
H	-1.61043300	2.50849600	0.64071300
H	-1.21909500	2.12190700	-1.01603400
C	-2.10147000	4.06223200	-0.74906800
C	-2.79733600	4.94938600	0.08623500
C	-1.51551200	4.56659200	-1.91677600
C	-2.90450700	6.30077400	-0.23867200
H	-3.25152600	4.57559600	1.00063300
C	-1.62133300	5.92081300	-2.24566900
H	-0.96574300	3.89427600	-2.57108200
C	-2.31718100	6.79189200	-1.40790100
H	-3.44355000	6.97345800	0.42297900
H	-1.15619800	6.29250100	-3.15451600
H	-2.39871000	7.84546000	-1.65972000
C	-2.34214900	-1.76510300	-0.90180100
C	-3.24930100	-2.81613600	-0.69027200
C	-2.34302900	-1.11567900	-2.14733600
C	-4.14523200	-3.20203100	-1.68474400
H	-3.25632400	-3.35354200	0.25055100
C	-3.23440700	-1.49079800	-3.15151500
H	-1.63178700	-0.32042000	-2.34119300
C	-4.12401800	-2.52823400	-2.90040800
H	-4.85215500	-4.00950000	-1.52959500
H	-3.24695500	-0.99073100	-4.11377800
C	-0.68258700	-2.88872900	1.17754500

C	-1.50838100	-3.43967000	2.17347100
C	0.46948000	-3.59045900	0.78713400
C	-1.20384600	-4.66644300	2.75986500
H	-2.38901800	-2.90208200	2.51125200
C	0.78393100	-4.82036500	1.36666100
H	1.12480000	-3.17443600	0.02925400
C	-0.05910400	-5.33830600	2.34152100
H	-1.82975000	-5.10061300	3.53207700
H	1.67440500	-5.36862900	1.07946800
P	-1.05755400	-1.28949300	0.33454400
F	-4.98523400	-2.90011100	-3.86852300
F	0.24208400	-6.52344000	2.90781800
Pt	0.86358100	-0.13445600	-0.56223700
C	5.99820400	0.06250600	1.23539900
C	7.07380700	-0.73527200	0.80678000
C	6.29170100	1.14144000	2.09284700
C	8.38481500	-0.46804400	1.20819300
H	6.87880700	-1.58107800	0.15311900
C	7.59981500	1.41404800	2.49828500
H	5.49208100	1.78962000	2.44206700
C	8.65145400	0.60821200	2.05547900
H	9.19719700	-1.10144500	0.86098500
H	7.79752400	2.25070600	3.16374700
H	9.67024600	0.81685100	2.37158800
C	3.14301100	-0.33304600	2.26874600
H	2.11242800	-0.59995700	2.01147500
H	3.52257000	-1.06904300	2.98541000
H	3.12904600	0.64848200	2.75478300

28

A1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-793.070898

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-793.05317

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-793.116882

E(M06L/def2TZVP)=-793.118361473

Si	-0.66058500	0.05302200	0.64797700
C	1.14314400	-0.03192500	0.13302500
C	1.97192100	1.08798300	0.29004100
C	1.71283500	-1.20481300	-0.37510800
C	3.31994700	1.03703100	-0.04259900
H	1.55415100	2.01879100	0.66935000
C	3.06194900	-1.26064000	-0.71033800
H	1.08686500	-2.08322400	-0.51435400

C	3.86777000	-0.14031100	-0.54324300
H	3.94456400	1.91620800	0.08447900
H	3.48477800	-2.17962600	-1.10506200
H	4.92029200	-0.18179600	-0.80607700
C	-0.79278300	0.18930800	2.50836000
H	-0.26489500	1.07867300	2.86366500
H	-1.83414500	0.26512400	2.82942800
H	-0.34826300	-0.68233800	2.99521900
C	-1.42720800	1.52870200	-0.10129600
C	-1.91152000	2.53343400	-0.58322400
C	-1.50342100	-1.45546400	0.06783300
C	-2.04234400	-2.47819200	-0.30614300
C	-2.49573500	3.72088700	-1.16271400
H	-3.55868800	3.79971000	-0.91782800
H	-2.00421800	4.62603200	-0.79488900
H	-2.40610600	3.71572400	-2.25253600
C	-2.69088700	-3.68831600	-0.75560500
H	-2.16923000	-4.57797800	-0.39163000
H	-3.72289200	-3.74115600	-0.39787100
H	-2.71603500	-3.74255300	-1.84750300

18

B1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-507.916838

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-507.90651

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-507.953648

E(M06L/def2TZVP)=-507.973038208

B	-0.83906100	-0.00004800	0.00000000
B	0.83906000	-0.00004500	-0.00000200
O	1.59402500	1.12841000	-0.17839100
O	1.59410100	-1.12844700	0.17839000
O	-1.59410500	-1.12847600	-0.17821100
O	-1.59402500	1.12843800	0.17821000
C	-2.97330400	0.74528200	0.18124700
C	-2.97335700	-0.74522200	-0.18124900
C	2.97335700	-0.74520700	0.18132400
C	2.97330600	0.74526500	-0.18131800
H	-3.51611400	-1.36333500	0.53914300
H	-3.51601700	1.36343300	-0.53914700
H	-3.38891300	0.94068100	1.17515700
H	-3.38897800	-0.94059100	-1.17516000
H	3.38902800	-0.94048900	1.17523000
H	3.51606800	-1.36339500	-0.53904000

H	3.38897000	0.94057500	-1.17522200
H	3.51597200	1.36348900	0.53904800

47

PtL3

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-1498.807304

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-1498.781117

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-1498.865899

E(M06L/def2TZVP)=-1499.17359209

P	0.07548500	-0.00213700	0.45518200
Pt	0.27913600	0.17927000	2.56752000
C	-0.69199500	1.43687600	-0.36362500
C	-1.70824600	2.12713800	0.29747300
C	-0.33657300	1.84729000	-1.65505600
C	-2.37176100	3.18791400	-0.30689300
H	-1.96765500	1.82869600	1.31080200
C	-0.98328100	2.90694000	-2.26584700
H	0.45968800	1.33497500	-2.18734900
C	-2.00913900	3.58208300	-1.59724000
H	-3.15497700	3.70417600	0.23483800
H	-0.71109800	3.23694600	-3.26258500
C	1.64589500	-0.23383800	-0.44490900
C	1.75524400	-1.05570900	-1.57403700
C	2.77433500	0.46947300	-0.02231400
C	2.95232700	-1.16309600	-2.25946900
H	0.89439800	-1.62270700	-1.91724300
C	3.98031800	0.37755800	-0.70573000
H	2.70060300	1.08828300	0.86913800
C	4.07211700	-0.44299400	-1.83284500
H	3.04958600	-1.80146300	-3.13087500
H	4.83910000	0.93444600	-0.35067100
C	-0.94475500	-1.41439500	-0.08850600
C	-1.89514100	-1.31862700	-1.10250300
C	-0.74382300	-2.66090900	0.52381500
C	-2.63262400	-2.42922700	-1.50751300
H	-2.07521800	-0.36439300	-1.58894600
C	-1.46066400	-3.77114700	0.12637800
H	-0.01904400	-2.74029300	1.33065600
C	-2.41483600	-3.66196800	-0.89319200
H	-3.36988800	-2.32059400	-2.29371200
H	-1.31337000	-4.73832900	0.59420700
O	5.19866600	-0.61152800	-2.57010300
O	-3.07473700	-4.80562900	-1.20533800

O	-2.58259800	4.60634200	-2.27788300
C	-4.05148400	-4.73565300	-2.22365200
H	-4.45982800	-5.74005500	-2.32040800
H	-4.85933400	-4.04181400	-1.96250900
H	-3.61538200	-4.43020800	-3.18219200
C	-3.61462000	5.32108000	-1.62898900
H	-3.93494200	6.09097000	-2.32886400
H	-4.46703800	4.67426400	-1.39044800
H	-3.25930800	5.79712700	-0.70767400
C	6.35137900	0.09976800	-2.16722600
H	7.13272200	-0.16357300	-2.87799500
H	6.18837000	1.18354200	-2.19637600
H	6.67103300	-0.18581400	-1.15821900

65

Cplx3

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.774326

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.737713

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.845673

E(M06L/def2TZVP)=-2007.19134048

P	-0.61577900	-0.08512000	0.09976600
C	-1.23638200	1.63087900	0.00600400
C	-0.49859800	2.57814200	-0.70486400
C	-2.42927900	2.03773600	0.62061000
C	-0.91465400	3.90322000	-0.78752500
H	0.40578500	2.25933500	-1.22077700
C	-2.85411700	3.35088600	0.54731000
H	-3.03957400	1.31007000	1.15033500
C	-2.09639000	4.29468800	-0.15550400
H	-0.32592300	4.61214000	-1.35789900
H	-3.77732200	3.67545700	1.01499500
C	-2.15934600	-1.05183200	0.22957400
C	-2.61522500	-1.62682500	1.42103000
C	-2.94108700	-1.19397700	-0.91802400
C	-3.81912800	-2.31009000	1.46366500
H	-2.01947100	-1.54139900	2.32530700
C	-4.15367400	-1.86949200	-0.88877100
H	-2.59183800	-0.76830800	-1.85614300
C	-4.60007500	-2.43013300	0.31137600
H	-4.18000600	-2.76032500	2.38205000
H	-4.73707600	-1.95876000	-1.79721700
C	0.16174800	-0.21543500	1.74164500
C	-0.24766500	0.55621800	2.83878000

C	1.21539900	-1.11227600	1.91553700
C	0.37470000	0.42935400	4.06650000
H	-1.05265100	1.27736500	2.72767100
C	1.84355100	-1.25676900	3.14614600
H	1.57105300	-1.68325700	1.06098400
C	1.42582000	-0.48120800	4.22781400
H	0.07293300	1.02753900	4.91916500
H	2.67158700	-1.94825900	3.24036200
O	-5.76691800	-3.10838700	0.45514000
O	1.97646300	-0.52844200	5.46669600
O	-2.60001500	5.55399700	-0.17631500
C	3.04904300	-1.42748500	5.66654700
H	3.34471000	-1.31760400	6.70859100
H	2.74498800	-2.46507300	5.48567200
H	3.90231300	-1.18849300	5.02151700
C	-1.87267500	6.53343200	-0.88994300
H	-2.43240600	7.46118600	-0.78528900
H	-0.86663000	6.67049300	-0.47663200
H	-1.79003800	6.28003700	-1.95322000
C	-6.58319700	-3.24951500	-0.68947600
H	-7.46174900	-3.80563700	-0.36715300
H	-6.89766400	-2.27647800	-1.08483100
H	-6.07457300	-3.80948600	-1.48290400
Pt	0.73800100	-0.61457100	-1.53357900
C	2.94648800	2.02949200	0.81347700
C	3.10787500	2.76185000	-0.51542800
H	1.91623400	2.09174800	1.19541000
H	3.62412700	2.38173800	1.59588500
H	2.36247300	3.54899900	-0.66647400
H	4.10388100	3.20908400	-0.62755800
C	2.65902900	-2.56314100	-3.22344400
C	2.97920300	-3.22516500	-1.89075600
H	1.75547600	-2.94244600	-3.70336100
H	3.49239300	-2.61769500	-3.93232400
H	2.07042800	-3.60845700	-1.40678000
H	3.70747200	-4.03546600	-1.97415500
B	3.05302700	0.51955600	-0.86270500
B	3.04174200	-0.98102900	-1.58471600
O	3.23926300	0.67039100	0.50086700
O	2.94195200	1.74677900	-1.50687100
O	3.51917500	-2.17638100	-1.08637900
O	2.47153600	-1.17204000	-2.88928500

65

TSO1C1

imaginary frequencies -79.81

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.765205

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.728715

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.837176

E(M06L/def2TZVP)=-2007.18327688

P	-0.76318300	-0.03824700	0.10415000
C	-1.30874200	1.28940600	-1.02648900
C	-0.35827500	1.92248900	-1.83005500
C	-2.63951900	1.72440700	-1.09847300
C	-0.71209700	2.96689900	-2.67660600
H	0.67194200	1.57180800	-1.81116800
C	-3.00419200	2.76039700	-1.93849000
H	-3.40288600	1.23354100	-0.50025000
C	-2.04126800	3.39080100	-2.73364200
H	0.04922300	3.42832900	-3.29435400
H	-4.03240400	3.09893300	-2.00576200
C	-2.27941200	-1.02701800	0.34660900
C	-2.86788300	-1.23790200	1.59896000
C	-2.84863800	-1.65160800	-0.76556200
C	-3.99418000	-2.03215400	1.72984000
H	-2.44007200	-0.77497600	2.48317000
C	-3.98252200	-2.44451500	-0.65056900
H	-2.39777400	-1.51438100	-1.74560300
C	-4.56203300	-2.63802700	0.60676200
H	-4.45628700	-2.19973300	2.69645100
H	-4.40115300	-2.90905600	-1.53530200
C	-0.50432100	0.80254300	1.70160700
C	-1.38334800	1.78763700	2.17554300
C	0.60519600	0.47070000	2.47689800
C	-1.15968500	2.41389300	3.38642100
H	-2.24908600	2.07395000	1.58422100
C	0.84343300	1.09466400	3.69718700
H	1.30987600	-0.26436500	2.09814400
C	-0.04224900	2.06922500	4.15740900
H	-1.83002200	3.17989800	3.76081100
H	1.72190800	0.82032900	4.26843900
O	-5.66534000	-3.39447100	0.83598000
O	0.09289200	2.74265900	5.32743300
O	-2.49804600	4.38884400	-3.53164000
C	1.20796600	2.42335600	6.13518300
H	1.13244500	3.05646900	7.01752800
H	1.19568200	1.37169500	6.44357300
H	2.15312600	2.63273500	5.62084100

C	-1.55963100	5.02833900	-4.37315900
H	-2.11752500	5.77518700	-4.93540300
H	-0.77188900	5.52642900	-3.79595700
H	-1.09682200	4.32172500	-5.07171600
C	-6.26163200	-4.02947100	-0.27638600
H	-7.11621900	-4.58043300	0.11248300
H	-6.61002000	-3.30220900	-1.01925500
H	-5.57157800	-4.73042100	-0.76045400
Pt	1.10223900	-1.00762900	-0.61148900
C	3.41689100	2.02676800	0.44162700
C	3.63878900	2.16309400	-1.06400100
H	2.48031100	2.51060900	0.75810100
H	4.23380900	2.43693100	1.04218300
H	3.10448500	3.01432400	-1.49946200
H	4.70119800	2.25902200	-1.32413500
C	3.66173700	-3.77972500	-1.59711500
C	4.55925000	-3.54500300	-0.38297000
H	2.86067400	-4.49953700	-1.39864800
H	4.20563800	-4.10449900	-2.48685800
H	4.47143100	-4.32640600	0.37544600
H	5.61703700	-3.44796900	-0.65302500
B	2.93015500	0.05428800	-0.55494600
B	3.28122900	-1.70893300	-0.74397700
O	3.31549500	0.62554400	0.66285800
O	3.13338300	0.94997700	-1.61575500
O	4.11175600	-2.30340400	0.17346900
O	3.06727200	-2.49803600	-1.85718800

65

C1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.778141

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.740972

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2006.850945

E(M06L/def2TZVP)=-2007.19422333

P	0.87405700	-0.03299400	-0.04436000
C	1.42488100	0.22375600	1.67374900
C	0.44651900	0.47584800	2.63972100
C	2.76753800	0.19029400	2.06908700
C	0.79279000	0.69926200	3.96692500
H	-0.60138400	0.50265700	2.34688900
C	3.12170500	0.40129200	3.39004700
H	3.54411500	-0.00787200	1.33558900
C	2.13629700	0.65827600	4.34805600

H	0.01193300	0.89286700	4.69225600
H	4.15778300	0.37284800	3.70905800
C	2.36977200	-0.63391500	-0.89718800
C	3.25271700	0.20830100	-1.58547700
C	2.65982100	-1.99823900	-0.84940400
C	4.38497500	-0.29803900	-2.19700900
H	3.04600000	1.27318600	-1.64454200
C	3.79867600	-2.52074200	-1.45010000
H	1.98471800	-2.67330600	-0.32771300
C	4.66826400	-1.66591800	-2.13166900
H	5.07166500	0.34555400	-2.73614200
H	3.99341200	-3.58479000	-1.39274100
C	0.63460200	1.65771200	-0.68392600
C	1.16707900	2.79702700	-0.06600800
C	-0.14465900	1.82442100	-1.82974700
C	0.92692500	4.05885100	-0.57954700
H	1.76841700	2.69447900	0.83320200
C	-0.39339200	3.08635200	-2.35665700
H	-0.58868800	0.95398600	-2.30587200
C	0.14094900	4.21230400	-1.72708300
H	1.32961600	4.94800600	-0.10637900
H	-1.01502000	3.17793200	-3.23923700
O	5.80094800	-2.06448700	-2.76156500
O	-0.05180000	5.48957000	-2.14347500
O	2.58267900	0.85093800	5.61520600
C	-0.86750000	5.68470900	-3.28101200
H	-0.90690200	6.76026600	-3.44404600
H	-0.44653900	5.19996800	-4.16968300
H	-1.88409200	5.30690600	-3.11778600
C	1.61656700	1.11046200	6.61345200
H	2.16925800	1.23353700	7.54329000
H	1.05483500	2.02852200	6.40462300
H	0.91162500	0.27780300	6.72109200
C	6.11650000	-3.44192900	-2.72545800
H	7.04539800	-3.55324800	-3.28188100
H	6.26722100	-3.79526300	-1.69864200
H	5.33672700	-4.04777500	-3.20129700
Pt	-1.25490000	-1.23742500	-0.17026000
C	-3.82716100	2.02182900	-0.69884700
C	-3.32787900	2.25669000	0.72907800
H	-3.66010500	2.88140400	-1.35565400
H	-4.89199700	1.76162100	-0.72947600
H	-2.61059400	3.08582600	0.78837900
H	-4.13437500	2.44918000	1.44167700

C	-5.27553700	-2.77289100	-0.19102600
C	-4.42514000	-4.04390400	-0.25828100
H	-5.99843700	-2.78310700	0.62983700
H	-5.82344400	-2.58723400	-1.12286700
H	-4.48540600	-4.63639300	0.66272600
H	-4.69052200	-4.69459600	-1.09643000
B	-2.46249500	0.32894000	-0.08266200
B	-3.06076100	-2.21125100	-0.19463500
O	-3.06848400	0.91108300	-1.17419400
O	-2.66041800	1.04424600	1.08319000
O	-3.08452400	-3.57893500	-0.42508200
O	-4.33832800	-1.71593800	0.01390600

93

(*S*)-Cplx4

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.884445

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.829768

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.977873

E(M06L/def2TZVP)=-2800.34693571

P	1.69129000	0.35101500	0.22491700
Pt	-0.53146900	-0.26948900	-0.35950500
C	1.82632000	1.08825500	1.88567600
C	3.07007600	1.33482900	2.48903400
C	0.67087000	1.38210500	2.60807900
C	3.14978500	1.88417500	3.75355300
C	0.73526400	1.93149100	3.88456400
C	1.97982800	2.18933300	4.46052900
C	2.95913200	-0.96308200	0.28202600
C	2.71583700	-2.06900200	1.11175100
C	4.13441900	-0.93837000	-0.46382100
C	3.62103400	-3.10825400	1.19265800
C	5.05363100	-1.98463300	-0.39622700
C	4.79767600	-3.07541000	0.43442200
O	2.16211900	2.72128100	5.69336900
C	2.37051900	1.56617700	-0.94742100
C	2.18941600	1.28925000	-2.31373800
C	2.97715700	2.76539600	-0.58512200
C	2.62238600	2.17761000	-3.27708300
C	3.40474700	3.67686600	-1.54923800
C	3.23151000	3.38200400	-2.90127300
O	5.61772800	-4.14903500	0.57217900
O	3.61071200	4.19182100	-3.92175100
C	6.81153300	-4.15334600	-0.18279400

C	1.00538000	3.02986000	6.44620700
C	4.21870000	5.42178900	-3.58489400
B	0.26579600	-2.11716900	-0.91457900
B	-1.83653300	-1.90074500	-0.36129600
H	3.98576700	1.08116900	1.96000600
H	-0.29859200	1.16189400	2.16547800
H	4.10530400	2.07796300	4.22859800
H	-0.18286800	2.14101800	4.41949900
H	1.79635100	-2.11655100	1.68923900
H	4.34522800	-0.09581900	-1.11600100
H	3.43955300	-3.96559400	1.83198700
H	5.95631100	-1.93625700	-0.99332900
H	1.69539900	0.36502100	-2.60851900
H	3.10662100	3.01555500	0.46400600
H	2.48920800	1.97380700	-4.33391000
H	3.86402200	4.60631700	-1.23441100
H	7.45995200	-3.30935300	0.08051600
H	6.60897200	-4.12366300	-1.26005500
H	7.32028400	-5.08473100	0.06017800
H	0.40531800	2.13531800	6.64816100
H	0.37963200	3.77204200	5.93714900
H	1.35987000	3.44436000	7.38803400
H	5.14712200	5.27328400	-3.02073300
H	3.54489300	6.05994600	-3.00113600
H	4.44868700	5.91369300	-4.52840800
O	-2.23129700	-2.45854600	0.83150900
O	-2.50376000	-2.45142400	-1.44443800
O	1.05518500	-2.08557300	-2.05859600
O	0.29969700	-3.37502800	-0.32646100
Si	-3.98202300	0.77976500	-1.10607900
C	-4.12584500	0.07818800	-2.82739500
H	-3.64513500	-0.90128000	-2.87348300
H	-5.17219000	-0.02044100	-3.12989200
H	-3.63486700	0.73699600	-3.54741600
C	-2.23431800	1.03610700	-0.62325300
C	-1.22230400	1.76861800	-0.37101300
C	-4.79282100	2.42319700	-1.05589800
C	-5.31874300	3.51817300	-1.00093000
C	-4.83595300	-0.31732600	0.16045500
C	-5.96902700	-1.06838900	-0.17959300
C	-4.42167900	-0.32876100	1.49882100
C	-6.67316000	-1.79017200	0.77972700
H	-6.31427700	-1.08697500	-1.21140000
C	-5.12168900	-1.04446400	2.46282000

H	-3.52599600	0.21901300	1.78419300
C	-6.25367200	-1.77196600	2.10616900
H	-7.55023800	-2.36323700	0.49382600
H	-4.77998300	-1.04313000	3.49345700
H	-6.80266800	-2.33002500	2.85885900
C	-0.64817600	3.11099700	-0.22929500
H	0.02481100	3.32673200	-1.06593700
H	-1.43219300	3.87477100	-0.21423100
H	-0.04827700	3.20805300	0.68142000
C	-5.94956200	4.81721600	-0.93946400
H	-6.73857100	4.84051800	-0.18212300
H	-5.22766700	5.59937000	-0.68644100
H	-6.40370300	5.08655600	-1.89754200
C	1.77254100	-3.31788400	-2.13994200
C	1.03921800	-4.24894100	-1.17912500
C	-3.31475000	-3.52637200	-0.96678500
C	-3.21553000	-3.45607200	0.56255700
H	0.33575900	-4.91379200	-1.69649500
H	1.71344900	-4.86219900	-0.57383900
H	1.77428800	-3.67346600	-3.17382900
H	2.81071900	-3.14075300	-1.82868100
H	-4.16096400	-3.15966200	1.02884100
H	-2.89075200	-4.40249500	1.00738500
H	-4.33889600	-3.39253600	-1.33262800
H	-2.92401800	-4.46675000	-1.37319800

93

(*S*)-TSC1D1

imaginary frequencies -149.87

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.870757

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.817326

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.961336

E(M06L/def2TZVP)=-2800.33583864

P	1.83607900	0.32969200	0.11050600
Pt	-0.41320800	-0.15657700	-0.14247800
C	2.26393800	1.43472700	1.49642000
C	3.59596900	1.77169200	1.78591700
C	1.26445600	1.89817200	2.34655200
C	3.90620100	2.57176500	2.86721200
C	1.56119200	2.69968900	3.44562600
C	2.88752700	3.04417100	3.70519000
C	2.91393600	-1.10913400	0.44182600
C	2.48285400	-2.03094700	1.40722700
C	4.13579300	-1.32682100	-0.18684800

C	3.25146600	-3.13202500	1.73050400
C	4.91885100	-2.43766600	0.12500300
C	4.47789100	-3.34368200	1.08936200
O	3.29453400	3.81756000	4.74152000
C	2.53744200	1.09078500	-1.38569400
C	2.44799400	0.35272600	-2.57995300
C	3.07045900	2.37593000	-1.43344900
C	2.90915200	0.88049500	-3.76867400
C	3.53086600	2.92009800	-2.63152200
C	3.45655900	2.16870700	-3.80388700
O	5.15581800	-4.45865000	1.46635100
O	3.87940500	2.59540700	-5.02126200
C	6.39681600	-4.70484600	0.83867800
C	2.29967100	4.30204900	5.62117100
C	4.43022200	3.89340700	-5.09971700
B	0.13989500	-2.13384200	-0.55410200
B	-2.19889300	-1.25807400	0.01027900
H	4.39787400	1.39222300	1.15682200
H	0.23559500	1.60738000	2.14878800
H	4.93090300	2.84021400	3.09937800
H	0.75937900	3.03694400	4.09140800
H	1.51817200	-1.89011700	1.88883000
H	4.48698400	-0.63105800	-0.94399600
H	2.92260300	-3.85179700	2.47246800
H	5.86147200	-2.58293400	-0.38905800
H	2.00540600	-0.64110600	-2.55929700
H	3.12854300	2.97650800	-0.53070300
H	2.84805900	0.32008400	-4.69524800
H	3.93851900	3.92384900	-2.63547700
H	7.11377700	-3.89724300	1.02851500
H	6.28434200	-4.83260400	-0.24453700
H	6.77670900	-5.62927400	1.27018200
H	1.76457100	3.48326200	6.11567900
H	1.57514500	4.93823000	5.09943900
H	2.82172100	4.89382500	6.37105400
H	5.32318300	3.99284700	-4.47122500
H	3.70265000	4.66040400	-4.80888400
H	4.70819500	4.04187900	-6.14182000
O	-2.58664000	-1.67647500	1.26359800
O	-2.85142600	-1.95765300	-1.00252600
O	0.99114700	-2.44748500	-1.61017500
O	-0.20162900	-3.28492400	0.14870300
Si	-4.09192700	0.82635000	-0.96363100
C	-4.08438200	0.41401300	-2.78186400

H	-3.74521900	-0.61112300	-2.94021900
H	-5.08108300	0.53330100	-3.21585800
H	-3.40488700	1.08291500	-3.31486600
C	-2.37763300	0.74325500	-0.23792100
C	-1.47853300	1.66112900	-0.00598100
C	-4.60644300	2.57051800	-0.73605000
C	-4.98731700	3.71466800	-0.58172000
C	-5.33215700	-0.21801700	-0.01587700
C	-6.09589300	-1.20712200	-0.64445200
C	-5.54415700	0.00421100	1.35220100
C	-7.03364100	-1.95377300	0.06357500
H	-5.95030500	-1.40706300	-1.70388500
C	-6.47819800	-0.73673400	2.06524400
H	-4.95849500	0.76255500	1.86728500
C	-7.22538800	-1.71939500	1.42055200
H	-7.61476500	-2.71848600	-0.44372100
H	-6.62269100	-0.55319500	3.12573000
H	-7.95612200	-2.30002600	1.97569000
C	-1.31464900	3.11455300	0.13442400
H	-0.46824300	3.47127700	-0.46093400
H	-2.21688400	3.66401800	-0.15465700
H	-1.08228500	3.37206000	1.17334600
C	-5.42386800	5.07981700	-0.39705200
H	-6.21361000	5.14758100	0.35651800
H	-4.59833800	5.71890700	-0.06856900
H	-5.81683200	5.50167800	-1.32640900
C	1.37528100	-3.81762300	-1.50143900
C	0.39480700	-4.41306900	-0.49190600
C	-3.42674100	-3.11439200	-0.39451200
C	-3.44491200	-2.80767200	1.10682000
H	-0.39132900	-5.00862300	-0.97387000
H	0.88407300	-5.04094100	0.25943700
H	1.32483800	-4.29253400	-2.48548800
H	2.41378400	-3.86435200	-1.14712600
H	-4.44673000	-2.55391200	1.47201700
H	-3.05144500	-3.63446900	1.70562400
H	-4.42411800	-3.28783000	-0.80860500
H	-2.79432100	-3.97912300	-0.62766300

93

(*S*)-D1

imaginary frequencies -9.28

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.878945

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.825758

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.970226

E(M06L/def2TZVP)=-2800.34210002

P	-1.82976600	-0.21746700	0.17557300
Pt	0.41119200	-0.00627900	0.08571000
C	-2.49185000	-0.85357600	1.75228100
C	-3.86141500	-0.78060500	2.04980400
C	-1.63675200	-1.42389700	2.69219100
C	-4.35663000	-1.27903900	3.23861100
C	-2.12114200	-1.92674600	3.89609900
C	-3.48720200	-1.85805100	4.17168300
C	-2.81769200	1.29780100	-0.08214000
C	-2.43730700	2.45329800	0.61637900
C	-3.92239500	1.36547800	-0.92664300
C	-3.14044700	3.63239700	0.47512400
C	-4.63931000	2.55070100	-1.08327000
C	-4.24835200	3.68975400	-0.37950400
O	-4.06750300	-2.31180300	5.31017900
C	-2.42768600	-1.36333600	-1.10566700
C	-2.06660100	-1.10786800	-2.44028700
C	-3.19068500	-2.49345400	-0.82279700
C	-2.48030000	-1.95049700	-3.45201200
C	-3.60439700	-3.35462400	-1.83716100
C	-3.25311900	-3.08105400	-3.15851900
O	-4.86669700	4.89575300	-0.46066000
O	-3.60553100	-3.84543500	-4.22346700
C	-5.97955800	4.99671700	-1.32511000
C	-3.22276300	-2.89196900	6.28389700
C	-4.38309600	-4.99666300	-3.96859600
B	0.08885500	1.67878600	-1.10200800
B	2.45695800	1.04848000	0.96271600
H	-4.54543500	-0.32234300	1.33991400
H	-0.57061000	-1.45513500	2.47642100
H	-5.41273900	-1.22727300	3.47994500
H	-1.42846200	-2.35412200	4.61092200
H	-1.56155200	2.42085500	1.25964800
H	-4.23362800	0.48603000	-1.48339000
H	-2.85119100	4.53132100	1.00886300
H	-5.48998600	2.57288200	-1.75369400
H	-1.45572500	-0.23870200	-2.67217500
H	-3.47046100	-2.71906000	0.20170300
H	-2.21049900	-1.76367900	-4.48583800
H	-4.19528400	-4.22648800	-1.58438100
H	-6.78963200	4.32252600	-1.02255300
H	-5.70515000	4.77880300	-2.36408500

H	-6.32560700	6.02642900	-1.25478200
H	-2.48139800	-2.17466900	6.65429100
H	-2.70171100	-3.77349600	5.89245800
H	-3.87075700	-3.19357900	7.10493700
H	-5.34629800	-4.74167500	-3.51057400
H	-3.85650100	-5.70559200	-3.31868000
H	-4.56005400	-5.46256400	-4.93639200
O	1.99564200	1.42538300	2.21127300
O	3.09336200	2.08625300	0.30032400
O	-0.36232900	1.72203000	-2.41561300
O	0.33537000	2.96397400	-0.62723400
Si	3.97649300	-0.57898500	-0.84026200
C	3.46570300	0.41232000	-2.33886200
H	3.29430500	1.45474300	-2.05960000
H	4.22427100	0.37232000	-3.12531900
H	2.52666100	0.02035900	-2.73956800
C	2.58667100	-0.42249800	0.43843000
C	1.71266900	-1.41679700	0.81511400
C	4.17560500	-2.33690500	-1.30660000
C	4.28790200	-3.50224100	-1.63341500
C	5.61362100	0.00858600	-0.12767300
C	6.07650900	1.31495800	-0.33478700
C	6.39537000	-0.84330900	0.66440900
C	7.27048000	1.75356000	0.22752900
H	5.48818200	2.00099200	-0.93789100
C	7.58736400	-0.40880400	1.23307800
H	6.06674800	-1.86757500	0.83246100
C	8.02770500	0.89260100	1.01520400
H	7.61279900	2.76903600	0.04942800
H	8.17636900	-1.08636600	1.84415600
H	8.96011400	1.23359500	1.45506600
C	1.94669200	-2.86247600	0.98713000
H	1.47508600	-3.40673400	0.15993900
H	3.00087700	-3.15336200	1.04292900
H	1.43171700	-3.20963000	1.88996300
C	4.40077600	-4.89593200	-1.99640600
H	5.44157300	-5.23153100	-1.98065300
H	3.83835900	-5.52994500	-1.30325300
H	4.00970500	-5.07959500	-3.00113200
C	-0.58389400	3.08988900	-2.76959100
C	0.16890600	3.88403800	-1.70686900
C	3.06326100	3.22627400	1.15180600
C	2.08806000	2.84841600	2.26928000
H	1.15979200	4.20945900	-2.05246000

H	-0.38141700	4.76281800	-1.35740400
H	-0.22334600	3.26951200	-3.78583500
H	-1.66338500	3.28814400	-2.74101400
H	2.42984700	3.14815600	3.26375500
H	1.09354200	3.27448400	2.09259700
H	4.07940300	3.41757200	1.52149200
H	2.72833600	4.09639200	0.57968400

93

(*S*)-Cplx5

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.882815

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.828544

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.975496

E(M06L/def2TZVP)=-2800.34580282

P	0.82082500	0.71404000	0.35708900
Pt	0.22427600	-1.37300800	-0.67304400
C	2.53107700	1.35041200	0.19868200
C	3.45490200	1.33066300	1.24871500
C	2.93710500	1.87130200	-1.03168900
C	4.73498400	1.83143100	1.07876300
C	4.21742200	2.38167300	-1.21522500
C	5.12450700	2.36461000	-0.15290200
C	-0.13532600	2.19752100	-0.09705800
C	-1.21461200	2.06846200	-0.97774200
C	0.18815000	3.47461700	0.36997100
C	-1.97793300	3.16115100	-1.34528100
C	-0.56971200	4.58396600	0.01351000
C	-1.66482500	4.42672700	-0.84301400
O	6.39817300	2.83289500	-0.22078200
C	0.62692000	0.45414000	2.15071500
C	0.97596500	-0.81041500	2.65466300
C	0.14528100	1.41317600	3.03787400
C	0.84827300	-1.09449700	4.00023000
C	0.00021900	1.13422000	4.39396200
C	0.35320900	-0.12524200	4.87985200
O	-2.46736400	5.44083500	-1.25141300
O	0.24782700	-0.50571300	6.17808000
C	-2.17908200	6.73729100	-0.77066100
C	6.83241700	3.35227100	-1.46024500
C	-0.27100600	0.43782000	7.09215400
B	2.23526000	-1.39575300	-1.24505700
O	2.63709900	-0.90251600	-2.47086000
C	4.05686300	-1.01382200	-2.55020100

C	4.50880800	-1.29273300	-1.11625900
B	1.15671400	-3.21373600	-0.95194000
O	1.36176800	-4.01377900	0.15799600
C	2.02953700	-5.19539400	-0.28147800
O	3.32067600	-1.70396500	-0.43619200
O	1.45291300	-3.88150200	-2.12802700
C	1.79373900	-5.22831400	-1.79022100
H	3.17038700	0.92071100	2.21310200
H	2.24256800	1.87885600	-1.86794000
H	5.45556500	1.82177500	1.88948300
H	4.49442700	2.78619600	-2.18164000
H	-1.44939000	1.08762300	-1.38197500
H	1.05389700	3.61296000	1.01349200
H	-2.82136700	3.05373500	-2.02009800
H	-0.29694300	5.56021900	0.39632100
H	1.34069100	-1.57567500	1.97201900
H	-0.15461900	2.39106000	2.67384500
H	1.11140200	-2.06884300	4.39696700
H	-0.39561500	1.89624900	5.05436300
H	-1.18185200	7.07234200	-1.08019900
H	-2.24948000	6.78948300	0.32220600
H	-2.92809000	7.39497700	-1.20824200
H	6.24035700	4.22294000	-1.76593700
H	6.78807800	2.59611100	-2.25352400
H	7.86742800	3.65717500	-1.31511200
H	-1.29242900	0.73660900	6.82858800
H	0.35875600	1.33339000	7.15162900
H	-0.28194100	-0.05551900	8.06264400
C	-1.52794100	-2.49062200	-0.94285800
C	-1.93771000	-1.38683000	-0.43588800
H	4.47312700	-0.08545800	-2.95497200
H	4.30692000	-1.83264600	-3.23686300
H	5.25975500	-2.08502900	-1.04529800
H	4.90408700	-0.39742300	-0.62206600
H	2.67325500	-5.53507100	-2.36215000
H	3.09515800	-5.11039800	-0.03148700
H	0.95916600	-5.88443500	-2.06922100
H	1.62167300	-6.06471600	0.24183300
C	-1.84261400	-3.84901700	-1.40078900
H	-1.35043100	-4.59031700	-0.76246000
H	-2.92171100	-4.02803500	-1.36938100
H	-1.48153000	-4.01797400	-2.41917300
Si	-3.40607800	-0.55797100	0.27285600
C	-2.99005600	0.45445700	1.78853600

H	-2.40177800	1.33789000	1.52284900
H	-3.89817300	0.79212700	2.29590400
H	-2.40826100	-0.13571800	2.50171800
C	-4.61512400	-1.85171100	0.73969100
C	-5.41490400	-2.72132100	1.02744100
C	-4.21298900	0.54712000	-1.02484600
C	-3.95396900	0.38595500	-2.39146700
C	-5.09231600	1.56819800	-0.64227000
C	-4.54788400	1.21318700	-3.34000000
H	-3.26327800	-0.39119500	-2.71426100
C	-5.68948800	2.39867600	-1.58438800
H	-5.31238800	1.72453000	0.41184300
C	-5.41766000	2.22199300	-2.93741300
H	-4.32909200	1.07343600	-4.39459800
H	-6.36334700	3.18784500	-1.26409600
H	-5.87906800	2.87115600	-3.67545200
C	-6.36495500	-3.75349200	1.37532100
H	-7.08203900	-3.40020400	2.12190800
H	-6.93525800	-4.08088100	0.50126200
H	-5.86363500	-4.63262400	1.79074100

93

(*S*)-TSC1D2

imaginary frequencies -134.15

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.864095

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.810414

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.956745

E(M06L/def2TZVP)=-2800.32912352

P	1.01352500	0.71247200	0.32595100
Pt	0.01064400	-1.10494400	-0.61033400
C	2.80961500	0.90585400	0.07455000
C	3.74232400	0.80717900	1.11164200
C	3.27618500	1.10908900	-1.22551400
C	5.09906600	0.91816700	0.85736900
C	4.63378200	1.22795300	-1.49394800
C	5.55381800	1.13139400	-0.44646300
C	0.36425300	2.34818900	-0.14620100
C	-0.91536800	2.43848800	-0.70577200
C	1.09044900	3.52470300	0.04524600
C	-1.46693900	3.65989400	-1.04115900
C	0.55135400	4.76259900	-0.28786500
C	-0.73577400	4.83342200	-0.82937400
O	6.90026800	1.22379000	-0.59702700
C	0.80658100	0.59143200	2.13145400

C	0.83735100	-0.68135900	2.72539900
C	0.59535400	1.70278300	2.94335900
C	0.67251700	-0.82503400	4.08872100
C	0.41483000	1.56841900	4.31706000
C	0.45588900	0.29890300	4.89517700
O	-1.35211500	5.98690100	-1.18816400
O	0.29014200	0.05074900	6.21846100
C	-0.64254100	7.19341700	-0.99803700
C	7.39429900	1.41906300	-1.90587000
C	0.05472600	1.15839400	7.06305100
B	1.86807100	-1.72963000	-1.29252200
O	2.37421900	-1.57258700	-2.56979700
C	3.60571000	-2.28777200	-2.65897200
C	3.96898300	-2.62892200	-1.21294100
B	-0.14067200	-3.24423500	-0.52889300
O	0.03764800	-3.78986600	0.73082000
C	0.83169900	-4.96541900	0.57071400
O	2.76343400	-2.41745300	-0.47751900
O	0.26271200	-4.10734300	-1.53544100
C	0.71988800	-5.30784800	-0.91730400
H	3.40452100	0.63709400	2.12974300
H	2.56966400	1.15679500	-2.04988800
H	5.83091000	0.83999800	1.65392500
H	4.96275800	1.38687800	-2.51403800
H	-1.47560900	1.52636200	-0.88904200
H	2.09640200	3.47938000	0.45539100
H	-2.45873900	3.72659400	-1.47669000
H	1.13991500	5.65827400	-0.12883600
H	0.96922100	-1.56166300	2.09926400
H	0.54819500	2.69560600	2.50512100
H	0.68869400	-1.80298500	4.55735900
H	0.23697600	2.45167400	4.91846000
H	0.28393500	7.21463900	-1.58381500
H	-0.40057700	7.35842900	0.05860000
H	-1.30133200	7.98886600	-1.34206300
H	7.02909200	2.35665400	-2.34130800
H	7.12101100	0.58927000	-2.56921900
H	8.47829400	1.46400600	-1.81719600
H	-0.86550900	1.68749100	6.78838300
H	0.89210200	1.86601000	7.04436900
H	-0.05053800	0.75505400	8.06865200
C	-1.75335700	-2.40544000	-0.73036900
C	-2.10021800	-1.24274000	-0.22091000
H	4.35666800	-1.66200800	-3.15304600

H	3.45028700	-3.18368500	-3.27322100
H	4.29825800	-3.66570500	-1.08548800
H	4.75003300	-1.97069100	-0.81149600
H	1.67642400	-5.60123400	-1.36112800
H	1.86241000	-4.73195300	0.86037800
H	-0.00599500	-6.10852400	-1.11154500
H	0.44975800	-5.75243100	1.22674800
C	-2.55930100	-3.49227900	-1.39050900
H	-2.43645700	-4.45820000	-0.88985700
H	-3.61684500	-3.21837400	-1.36103500
H	-2.24307000	-3.62944500	-2.42761600
Si	-3.58996500	-0.31355500	0.29310900
C	-3.20278400	0.69295200	1.82261000
H	-2.41736800	1.42466900	1.60815200
H	-4.08135400	1.23162900	2.18822900
H	-2.84363200	0.05065800	2.63147200
C	-5.00461900	-1.42364500	0.64502800
C	-5.92347900	-2.19188400	0.85736300
C	-4.07716900	0.83090900	-1.12511800
C	-3.56360900	0.64812100	-2.41574700
C	-4.95894100	1.89999500	-0.91699800
C	-3.91267300	1.50100800	-3.45786500
H	-2.86353300	-0.16523200	-2.60004300
C	-5.31525900	2.75361600	-1.95554900
H	-5.37747900	2.06991000	0.07299200
C	-4.78973600	2.55613000	-3.22896000
H	-3.49627500	1.34486200	-4.44840200
H	-6.00004000	3.57647400	-1.77203100
H	-5.06235800	3.22468300	-4.04004500
C	-7.01735400	-3.10135100	1.11273300
H	-7.80327000	-2.62384100	1.70508700
H	-7.47313900	-3.44770300	0.18058800
H	-6.68079300	-3.98444500	1.66360200

93

(*S*)-D2

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.876029

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.821906

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.969526

E(M06L/def2TZVP)=-2800.33813348

P	1.04504900	0.48405900	0.41749700
Pt	-0.56716700	-0.86838100	-0.30165200

C	2.65276000	-0.32783000	0.69541500
C	3.03442800	-0.80970500	1.95337400
C	3.50138700	-0.56270600	-0.38752700
C	4.22107200	-1.50127600	2.11926400
C	4.69781500	-1.25086500	-0.23569500
C	5.06091500	-1.72966800	1.02608500
C	1.41836200	1.92445100	-0.61593400
C	0.45862700	2.39451400	-1.52333300
C	2.62860000	2.60837600	-0.50183000
C	0.70719100	3.51989100	-2.28472100
C	2.89258500	3.73839900	-1.26800000
C	1.92469000	4.19808000	-2.16427400
O	6.20236900	-2.41347100	1.28927300
C	0.58507800	1.14432600	2.05944300
C	-0.05624500	0.28914800	2.97095000
C	0.83967000	2.45904500	2.44371800
C	-0.39811100	0.73135700	4.23250400
C	0.47622100	2.92284800	3.70550200
C	-0.13708000	2.05479500	4.60916200
O	2.07592500	5.28455400	-2.96222900
O	-0.52454200	2.39722700	5.86255000
C	3.29745900	5.98925500	-2.87944000
C	7.07499900	-2.66653100	0.20716000
C	-0.29501700	3.72951700	6.27334800
B	0.68800200	-1.21336000	-1.91111000
O	0.76238800	-0.46936700	-3.07502000
C	1.54610500	-1.18983800	-4.02822100
C	2.15243400	-2.35932000	-3.24318500
B	-0.96150500	-3.34736700	0.29103400
O	-0.18034200	-3.27899100	1.43288000
C	1.02584300	-3.98271600	1.12256600
O	1.47308300	-2.35548800	-1.98849000
O	-0.53497500	-4.32188700	-0.58447600
C	0.64621000	-4.90451800	-0.03777700
H	2.39661200	-0.64216200	2.81578500
H	3.23134800	-0.18783200	-1.37228900
H	4.52417900	-1.87543000	3.09091200
H	5.33543200	-1.40794800	-1.09767700
H	-0.47991300	1.85644300	-1.64204600
H	3.38660700	2.25286800	0.19158900
H	-0.02637600	3.88855100	-2.99290000
H	3.84392400	4.24561100	-1.16302100
H	-0.30713000	-0.72533200	2.66516500
H	1.31628200	3.14719400	1.75219900

H	-0.89270800	0.07834800	4.94342100
H	0.67406800	3.95491300	3.96837200
H	4.14948100	5.35349800	-3.14781400
H	3.46121300	6.39933700	-1.87582200
H	3.22329500	6.80823500	-3.59265800
H	7.44486100	-1.73659300	-0.24070300
H	6.59130600	-3.26973900	-0.57008700
H	7.91479200	-3.22256800	0.62004700
H	-0.83602600	4.44509000	5.64316300
H	0.77267000	3.97814300	6.25989600
H	-0.66630400	3.79929100	7.29427900
C	-2.27409800	-2.53833800	0.00154000
C	-2.42360300	-1.25257800	0.46744900
H	2.30085900	-0.52057700	-4.45304500
H	0.89633800	-1.52572800	-4.84441100
H	2.00491500	-3.32668000	-3.73290600
H	3.22891900	-2.23296300	-3.06562300
H	1.41773500	-4.94675200	-0.81061400
H	1.79082400	-3.25437800	0.82082300
H	0.41922600	-5.92690900	0.29034200
H	1.37615900	-4.51467900	2.01117500
C	-3.29041300	-3.24197700	-0.87281000
H	-3.64481300	-4.16204400	-0.39360400
H	-4.15617000	-2.61168200	-1.08785000
H	-2.82952300	-3.55214100	-1.81634900
Si	-3.74612300	0.03258800	0.44248700
C	-3.62075600	1.04928600	2.00989900
H	-2.64630900	1.54614300	2.05649600
H	-4.40437600	1.80975500	2.06607100
H	-3.71110400	0.41638300	2.89647200
C	-5.46578000	-0.59076300	0.28122100
C	-6.58141200	-1.06331500	0.16925600
C	-3.35602900	1.14329300	-1.03884300
C	-2.96182200	0.59167900	-2.26724300
C	-3.42968800	2.53865000	-0.94869200
C	-2.66291300	1.39600100	-3.36081100
H	-2.87373300	-0.48848500	-2.36766400
C	-3.13374400	3.35159000	-2.04007200
H	-3.71925100	3.00378600	-0.00907400
C	-2.75373000	2.78071100	-3.24957800
H	-2.34771900	0.94327500	-4.29605400
H	-3.19541700	4.43191700	-1.94449900
H	-2.52206900	3.41234100	-4.10247700
C	-7.90787400	-1.62179600	0.03574500

H	-8.67853500	-0.89217900	0.30159700
H	-8.10216200	-1.94519300	-0.99120000
H	-8.04098100	-2.49232000	0.68494000

93

(*S*)-TSD1E1

imaginary frequencies -60.69

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.866736

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.813386

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.958976

E(M06L/def2TZVP)=-2800.32956139

P	-1.75950000	0.37781300	-0.05040400
Pt	0.12021900	-0.54626900	0.58208300
C	-1.57770300	1.65026000	-1.34024600
C	-2.68493700	2.42145400	-1.72913700
C	-0.37398500	1.82042300	-2.01954800
C	-2.57701500	3.35666200	-2.73859600
C	-0.25522600	2.75206600	-3.04611600
C	-1.35645200	3.52985100	-3.40411200
C	-2.99686700	-0.74529300	-0.78011700
C	-2.55359300	-1.71238500	-1.69422500
C	-4.36106700	-0.64593800	-0.52373500
C	-3.44814000	-2.55215600	-2.32587900
C	-5.27465600	-1.49218800	-1.14898700
C	-4.81875200	-2.44850100	-2.05601800
O	-1.34927400	4.47155600	-4.37865500
C	-2.58021800	1.16745500	1.35658600
C	-3.11326100	0.34069400	2.36118400
C	-2.58257800	2.54740200	1.54814800
C	-3.66494700	0.89126100	3.49940500
C	-3.13076400	3.11021600	2.69685000
C	-3.68021400	2.28082800	3.67540900
O	-5.61630700	-3.32274200	-2.71929600
O	-4.24081300	2.72087400	4.82852700
C	-7.00721700	-3.24063400	-2.48405800
C	-0.13694800	4.67220600	-5.07870700
C	-4.24639400	4.11529800	5.05885400
B	-0.83597100	-2.42204300	0.76346200
B	2.57466900	-1.05779600	-0.23842200
H	-3.64163100	2.28819000	-1.22962600
H	0.48598000	1.21889100	-1.73463900
H	-3.42212900	3.96536400	-3.04025400
H	0.69567700	2.86103600	-3.55311200
H	-1.48777500	-1.81206300	-1.88749200

H	-4.73045400	0.09401500	0.17995000
H	-3.11518400	-3.30385200	-3.03335300
H	-6.32930100	-1.39687000	-0.92058200
H	-3.06239700	-0.73936400	2.24300200
H	-2.14562600	3.20130700	0.79921900
H	-4.08000000	0.26755000	4.28356400
H	-3.12023100	4.18645700	2.81771900
H	-7.40655100	-2.25884600	-2.76457700
H	-7.25243700	-3.43843700	-1.43394100
H	-7.46540600	-4.00542500	-3.10865400
H	0.17848300	3.76505800	-5.60658200
H	0.66771600	4.99230300	-4.40680300
H	-0.33414200	5.45955000	-5.80391900
H	-4.82184500	4.64894400	4.29332100
H	-3.22919800	4.52268200	5.08961500
H	-4.71996000	4.25972400	6.02813900
O	2.63114500	-1.35191500	-1.57826200
O	2.54404500	-2.18772700	0.56102700
O	-1.97190800	-2.66503000	1.53609900
O	-0.46885200	-3.58215300	0.08306800
Si	4.36122000	0.92428400	0.90073600
C	4.43268900	1.31270700	2.73194600
H	4.06187700	0.46832300	3.31995800
H	5.45208600	1.53746400	3.05798600
H	3.80607400	2.17524800	2.97068800
C	2.63792100	0.37695100	0.37104200
C	1.48191900	1.05067200	0.60228800
C	4.89905500	2.39035100	-0.05394400
C	5.23334000	3.36640200	-0.69771900
C	5.51279300	-0.51237600	0.50232100
C	5.96513700	-1.38388100	1.50104100
C	5.84791200	-0.81464000	-0.82599000
C	6.72539400	-2.50731600	1.19177000
H	5.71734900	-1.18721200	2.54150400
C	6.60480000	-1.93754000	-1.14253300
H	5.50368300	-0.16196800	-1.62560900
C	7.04629800	-2.78678800	-0.13227500
H	7.06735200	-3.16615500	1.98462900
H	6.85420900	-2.14934100	-2.17827600
H	7.63958000	-3.66284200	-0.37644300
C	1.37273300	2.46405300	1.05666700
H	0.88459200	2.52193300	2.03688000
H	2.33332500	2.99504700	1.11137200
H	0.72631300	3.02734400	0.37138500

C	5.64035500	4.52781400	-1.45537900
H	6.69142800	4.46278000	-1.75139500
H	5.04730700	4.63834100	-2.36812800
H	5.51973100	5.44512800	-0.87164500
C	-2.46168800	-3.97650900	1.25585500
C	-1.33720200	-4.65083600	0.47073700
C	2.71017500	-3.32367200	-0.29887200
C	2.48257900	-2.77140400	-1.70646400
H	-0.77281800	-5.36869700	1.07902800
H	-1.69301900	-5.17168500	-0.42395100
H	-2.69946000	-4.48865500	2.19302900
H	-3.38566700	-3.88990700	0.66948000
H	3.20605500	-3.14165700	-2.43806700
H	1.46873800	-2.98510900	-2.06447100
H	3.72715000	-3.70813900	-0.15494800
H	1.98145300	-4.08612200	-0.02064600

93

(*S*)-E1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.884337

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.830968

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.97577

E(M06L/def2TZVP)=-2800.34755056

P	-1.68680200	0.36374800	-0.01657400
Pt	-0.08803600	-1.07054700	0.45798300
C	-1.21273800	1.57318200	-1.29757300
C	-2.15826300	2.48368200	-1.79632400
C	0.06302300	1.56644200	-1.85977100
C	-1.83018100	3.36672200	-2.80519400
C	0.40445600	2.44409700	-2.88346500
C	-0.54440000	3.34912500	-3.36087000
C	-3.24818300	-0.28740800	-0.71143700
C	-3.17179700	-1.11647200	-1.84076100
C	-4.50248400	0.01385300	-0.19295100
C	-4.31288700	-1.62771100	-2.42466900
C	-5.66402800	-0.49932200	-0.76941100
C	-5.57180700	-1.32324100	-1.88980100
O	-0.32765500	4.24080600	-4.35844000
C	-2.19976800	1.29047200	1.45763700
C	-2.58062700	0.53227400	2.57764200
C	-2.15098800	2.67624100	1.56974600
C	-2.91615900	1.15098300	3.76401700
C	-2.47686200	3.31076600	2.76627000

C	-2.86125000	2.54728700	3.86840900
O	-6.63234900	-1.88186200	-2.52661300
O	-3.19475400	3.05863000	5.07904400
C	-7.91837300	-1.59933500	-2.01366800
C	0.93555800	4.21473200	-4.99391700
C	-3.12056000	4.46144200	5.23491000
B	-1.48399200	-2.61349400	0.22514400
B	2.84029700	-1.70431300	0.48122300
H	-3.16922300	2.48806500	-1.39535500
H	0.80369400	0.86152700	-1.49007900
H	-2.55339000	4.07206600	-3.19896600
H	1.40487700	2.40779100	-3.29888500
H	-2.19789300	-1.37686100	-2.24884800
H	-4.59069500	0.65258600	0.68086200
H	-4.26266500	-2.27022200	-3.29718100
H	-6.62521000	-0.25120300	-0.33541600
H	-2.60026700	-0.55322300	2.50136100
H	-1.83480100	3.28061900	0.72467700
H	-3.20976000	0.57898800	4.63705000
H	-2.41870000	4.39052600	2.82900300
H	-8.13978900	-0.52612600	-2.04761900
H	-8.02857700	-1.95308000	-0.98168400
H	-8.62243700	-2.13035600	-2.65192200
H	1.13798900	3.23824200	-5.44843500
H	1.74427600	4.45744100	-4.29568200
H	0.89657500	4.97335400	-5.77354800
H	-3.80733500	4.98069800	4.55609900
H	-2.10299700	4.83240800	5.06586500
H	-3.41068600	4.66705600	6.26361400
O	3.83196600	-2.54724700	0.06536700
O	1.64470200	-2.44203600	0.70350400
O	-2.59579600	-2.76927100	1.04602000
O	-1.42442100	-3.63418400	-0.71705600
Si	4.37487600	0.81902400	0.84762700
C	4.78551400	1.41858800	2.57941700
H	4.87299800	0.57507800	3.27069500
H	5.73095500	1.96813600	2.59826000
H	4.00504500	2.07495600	2.97111900
C	2.81012500	-0.20875000	0.74847900
C	1.54002200	0.30582800	0.88693900
C	4.17748800	2.27138600	-0.26350200
C	3.96603500	3.21367100	-1.00240000
C	5.82330700	-0.18898600	0.19625200
C	6.67255200	-0.88629100	1.06343600

C	6.02229800	-0.35336200	-1.18043800
C	7.67158300	-1.72422800	0.57958600
H	6.55098000	-0.78102000	2.13955700
C	7.01712500	-1.18924800	-1.67209400
H	5.38124000	0.18207300	-1.87838000
C	7.84240700	-1.88142900	-0.79136400
H	8.31805700	-2.25596900	1.27203100
H	7.15096800	-1.30296900	-2.74413000
H	8.61984800	-2.53702400	-1.17251600
C	1.30416400	1.71277000	1.33463800
H	0.72552200	1.68922400	2.26771600
H	2.20412500	2.31617300	1.50722700
H	0.67555900	2.26338900	0.62388100
C	3.71406600	4.34620500	-1.86502400
H	4.02202000	4.14042400	-2.89553400
H	2.64944800	4.60413700	-1.88018900
H	4.26295900	5.23272600	-1.53393000
C	-3.39859100	-3.83687200	0.54044300
C	-2.52014500	-4.52878200	-0.50392200
C	1.81511700	-3.75256400	0.13977600
C	3.33454900	-3.88628400	0.06865700
H	-2.13208200	-5.49417300	-0.15673700
H	-3.03968000	-4.69381500	-1.45332100
H	-3.69047300	-4.49672500	1.36286900
H	-4.31015700	-3.41227200	0.10139800
H	3.74603500	-4.41332300	0.93736800
H	3.67393500	-4.39851200	-0.83442300
H	1.33213700	-4.48633700	0.78817000
H	1.32724200	-3.78083200	-0.83949800

93

(*S*)-F1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.913467

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.85984

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2800.006522

E(M06L/def2TZVP)=-2800.37198918

P	-1.97483200	0.36938800	-0.02342800
Pt	0.08844800	-0.74254100	-0.34689400
C	-2.25077800	1.86731100	-1.02185500
C	-3.51597800	2.46134300	-1.14518400
C	-1.17344400	2.45247000	-1.68654100
C	-3.68994700	3.61095500	-1.89026500
C	-1.33371900	3.61255300	-2.43856600

C	-2.59673700	4.19797100	-2.54001600
C	-3.49438700	-0.60022000	-0.30380300
C	-3.62341200	-1.25877100	-1.53688700
C	-4.51210500	-0.74154100	0.63506400
C	-4.74134500	-2.01761300	-1.82262800
C	-5.64171000	-1.51123400	0.36270300
C	-5.76139700	-2.14894700	-0.87253200
O	-2.86977300	5.32238200	-3.24545400
C	-2.07708000	0.92158700	1.70914200
C	-1.76560400	-0.02538400	2.70212500
C	-2.33152200	2.23442800	2.09756900
C	-1.72936200	0.33532000	4.03397700
C	-2.28357600	2.61266300	3.43838500
C	-1.98346200	1.66028100	4.41249500
O	-6.81623300	-2.91790400	-1.24419400
O	-1.90666200	1.91611300	5.74242700
C	-7.86425400	-3.07782200	-0.31017300
C	-1.79821400	5.93473800	-3.93590100
C	-2.14096700	3.24407600	6.16409500
B	-0.89001300	-2.46783600	-0.45483300
B	2.72834100	0.61664300	0.18907800
H	-4.37332500	2.00810600	-0.65330100
H	-0.19321700	1.98579700	-1.62366300
H	-4.66365400	4.07649300	-1.99638600
H	-0.47852600	4.03836600	-2.94937000
H	-2.82485600	-1.18479000	-2.27088600
H	-4.42969900	-0.25071900	1.60080800
H	-4.85070500	-2.52673900	-2.77424500
H	-6.41487200	-1.60376900	1.11589100
H	-1.54136100	-1.04961200	2.41010200
H	-2.55611700	2.98858300	1.34866500
H	-1.49086500	-0.38612100	4.80789100
H	-2.48057500	3.64372100	3.70627000
H	-8.32812200	-2.11778500	-0.05461500
H	-7.51575300	-3.56136300	0.61019600
H	-8.60386300	-3.71525800	-0.79139400
H	-1.36175100	5.26098700	-4.68187300
H	-1.01076500	6.26432700	-3.24814800
H	-2.22036200	6.80241500	-4.43961100
H	-3.15317600	3.57767100	5.90657700
H	-1.41471600	3.94024600	5.72815700
H	-2.02968700	3.24182400	7.24678400
O	3.50885100	1.40000300	0.99804600
O	1.46480300	1.21362300	-0.00577500

O	-1.08365000	-3.23236800	-1.59116000
O	-1.52209100	-3.02104900	0.65073300
Si	4.81041500	-1.25360800	-0.73343200
C	5.02830900	-1.90071200	-2.48538600
H	4.66862200	-1.16225400	-3.20804600
H	6.08589000	-2.08231200	-2.69560800
H	4.48469100	-2.82900400	-2.66923100
C	3.03310900	-0.76325700	-0.38302000
C	1.95001400	-1.58403000	-0.57912700
C	5.44565000	-2.49957800	0.44931500
C	5.83234400	-3.32941500	1.24957100
C	5.87396700	0.29492100	-0.59069500
C	5.66402300	1.34698300	-1.49337900
C	6.83532500	0.47760900	0.40768700
C	6.37639000	2.53629900	-1.39982900
H	4.91990900	1.24086400	-2.28215700
C	7.55315400	1.66532200	0.50833300
H	7.01658200	-0.32199900	1.12243200
C	7.32420900	2.69846200	-0.39377100
H	6.19685000	3.33669500	-2.11225600
H	8.29362300	1.78661400	1.29372600
H	7.88498500	3.62535300	-0.31633300
C	6.28821300	-4.31891700	2.19942300
H	5.45135100	-4.89502400	2.60505400
H	6.98361300	-5.02629300	1.73837100
H	6.80485600	-3.85233300	3.04318700
C	2.09950900	-3.02685700	-0.94820500
H	1.62638400	-3.22672400	-1.91625400
H	3.13604000	-3.38052600	-0.97510600
H	1.56095200	-3.65377700	-0.22790600
C	2.79548900	2.60043000	1.28551800
C	1.34328700	2.27286600	0.95364600
C	-2.31004000	-4.12293100	0.19475000
C	-1.77495900	-4.42133800	-1.20549600
H	3.19425300	3.40852700	0.65905500
H	2.94492100	2.87151800	2.33308200
H	0.78542400	3.10284500	0.51106900
H	0.78519200	1.89919700	1.82159600
H	-2.20188600	-4.96179500	0.88782200
H	-3.36458500	-3.81878600	0.17725700
H	-1.06650000	-5.25986000	-1.21075800
H	-2.56501600	-4.63589800	-1.93111900

93

(*S*)-TSF1O1

imaginary frequencies -122.59

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.896721

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.842919

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.991586

E(M06L/def2TZVP)=-2800.35475387

P	-2.08024800	0.04963600	-0.21330200
Pt	-0.09063000	-0.97313100	-0.70781200
C	-2.53590800	1.37841800	-1.37790200
C	-3.83210200	1.61090800	-1.85053200
C	-1.50333300	2.20947600	-1.82159400
C	-4.08962800	2.65035500	-2.72801100
C	-1.75047400	3.26005300	-2.69646300
C	-3.05159700	3.48410500	-3.15366400
C	-3.54500200	-1.02104700	-0.08927100
C	-3.54294200	-2.23440000	-0.79081800
C	-4.66481100	-0.69239900	0.67388000
C	-4.63547000	-3.07909100	-0.74726500
C	-5.76918200	-1.53646500	0.73211500
C	-5.75731000	-2.73490000	0.01435900
O	-3.40464500	4.47271300	-4.01381900
C	-1.97585600	0.92276700	1.38751300
C	-1.13750300	0.39952400	2.38518700
C	-2.65748100	2.11199800	1.64569400
C	-1.00278700	1.04277500	3.60060200
C	-2.52109500	2.77375100	2.86316000
C	-1.68903000	2.23687500	3.84768800
O	-6.77531900	-3.63120000	0.00330100
O	-1.47014400	2.80235000	5.06233400
C	-7.92116000	-3.32463300	0.77106800
C	-2.37871700	5.32239100	-4.48552400
C	-2.13648700	4.01578600	5.34362500
B	0.59944200	-2.51301700	0.41439400
B	2.16720000	0.51774600	0.27460100
H	-4.64751400	0.96622000	-1.53408400
H	-0.48297000	2.03080600	-1.48187300
H	-5.08913700	2.83711800	-3.10555200
H	-0.92813700	3.88469300	-3.02370800
H	-2.65628300	-2.51362600	-1.35576100
H	-4.67610600	0.23161200	1.24685800
H	-4.64333800	-4.02219900	-1.28248500
H	-6.62163800	-1.25904000	1.34014300
H	-0.55838400	-0.50010900	2.18880900
H	-3.29092200	2.55000900	0.87780000

H	-0.34891800	0.65052100	4.37239900
H	-3.05587600	3.70169900	3.02712600
H	-8.39985600	-2.39874000	0.43106900
H	-7.68058600	-3.23168700	1.83660100
H	-8.61008400	-4.15577600	0.63108500
H	-1.61510400	4.76503700	-5.04044700
H	-1.89684200	5.86905700	-3.66643600
H	-2.85968500	6.03305000	-5.15540700
H	-3.22594700	3.89573900	5.31420600
H	-1.84717800	4.80805200	4.64287300
H	-1.83523900	4.30073600	6.35013300
O	2.28782000	0.57906900	1.64028600
O	1.76161300	1.72805400	-0.27777700
O	0.37866200	-3.84286900	0.09336700
O	1.00895800	-2.35608100	1.72760800
Si	4.45680500	-0.37829600	-1.22438000
C	4.47405800	0.14989800	-3.02393100
H	3.83544000	1.02640000	-3.16805700
H	5.48357300	0.40510400	-3.35730300
H	4.09179800	-0.64021000	-3.67465900
C	2.69076700	-0.64178600	-0.62106100
C	1.87016000	-1.65151300	-1.00881000
C	5.46471900	-1.88465000	-0.99345000
C	6.10069100	-2.90568300	-0.81607500
C	5.18691300	0.99869200	-0.16288800
C	4.92113500	2.34337700	-0.46117500
C	5.92798100	0.72379100	0.99383800
C	5.37529900	3.37041800	0.35984600
H	4.33847600	2.59564000	-1.34401300
C	6.38342300	1.74550900	1.81973100
H	6.14862700	-0.30957800	1.25071300
C	6.10819300	3.07254300	1.50422100
H	5.16011700	4.40433500	0.10487500
H	6.95614300	1.50755600	2.71118400
H	6.46582300	3.87176100	2.14674500
C	6.85704200	-4.12052800	-0.61522700
H	6.22677500	-5.00620200	-0.73903600
H	7.68183400	-4.20037100	-1.32921900
H	7.28685200	-4.15995100	0.38985800
C	2.28699700	-2.78521100	-1.90103000
H	1.44332600	-3.17606600	-2.47380500
H	3.07785200	-2.48658100	-2.59806800
H	2.68096300	-3.62347400	-1.31535800
C	2.12115600	1.94402100	2.02419700

C	1.47470900	2.61115900	0.81087700
C	0.91852800	-3.63114900	2.35959000
C	0.81119700	-4.62654700	1.20434700
H	3.11049400	2.36396800	2.24763400
H	1.50267900	2.00047200	2.92391500
H	1.88982700	3.59975700	0.59162700
H	0.38488700	2.70112000	0.91937600
H	1.79938200	-3.78918300	2.98756800
H	0.03031400	-3.64992800	3.00423300
H	1.78025100	-5.08371600	0.96197000
H	0.09261100	-5.42968600	1.38823900

93

(*S*)-G1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.930918

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-2799.877998

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-2800.020884

E(M06L/def2TZVP)=-2800.3876417

P	-1.58193400	0.27048900	-0.34640400
Pt	0.59380500	-0.26024700	-0.10855100
C	-1.87584400	2.02012900	-0.76941500
C	-2.76282400	2.46683200	-1.75439400
C	-1.10789700	2.96711500	-0.08492000
C	-2.88078400	3.81659900	-2.04294500
C	-1.22738300	4.32368000	-0.35434600
C	-2.11541900	4.75438500	-1.34459000
C	-2.51522400	-0.72869400	-1.54803000
C	-1.81196600	-1.52180800	-2.46587400
C	-3.90975700	-0.77577600	-1.55612400
C	-2.48613300	-2.32368300	-3.36794600
C	-4.60009000	-1.57370600	-2.46103700
C	-3.88442800	-2.35375500	-3.37402400
O	-2.29324300	6.05055400	-1.70526500
C	-2.48999600	0.04810100	1.22318900
C	-2.08527100	-0.98382000	2.08456900
C	-3.58132100	0.83384600	1.58950200
C	-2.78110200	-1.24172600	3.25069900
C	-4.27876000	0.59463900	2.77074300
C	-3.88630600	-0.45745600	3.60049800
O	-4.45288000	-3.17484200	-4.29060500
O	-4.49911100	-0.78686100	4.76530600
C	-5.86433600	-3.23949900	-4.32477300
C	-1.50102100	7.02093600	-1.05055700

C	-5.61921800	-0.01706400	5.15137600
B	1.15048000	-2.66324000	0.04133600
B	1.70692900	-0.36049900	2.12703800
H	-3.35718800	1.75103300	-2.31530400
H	-0.38099200	2.63298400	0.65531700
H	-3.55697100	4.17263600	-2.81259100
H	-0.61186000	5.02893000	0.19148000
H	-0.72405300	-1.52472600	-2.44026800
H	-4.47502600	-0.19203400	-0.83330800
H	-1.95125100	-2.94828600	-4.07547100
H	-5.68305800	-1.59153500	-2.44017400
H	-1.19486600	-1.56362700	1.84298000
H	-3.89026600	1.65907600	0.95178700
H	-2.48238300	-2.04248600	3.91941600
H	-5.11764600	1.22872000	3.03127700
H	-6.30780600	-2.26461500	-4.55875400
H	-6.27590800	-3.60116800	-3.37538800
H	-6.11472600	-3.94498900	-5.11500000
H	-0.43096700	6.84443900	-1.21338700
H	-1.69751800	7.04468900	0.02768200
H	-1.77611000	7.97994300	-1.48600800
H	-6.42372200	-0.07416200	4.40880000
H	-5.35279300	1.03492400	5.30800200
H	-5.96852000	-0.44096800	6.09109300
O	1.28383800	-1.29916100	3.04474700
O	1.46525900	0.94325600	2.58084400
O	0.74758900	-3.31736500	-1.12817400
O	0.54525500	-3.21741200	1.15922300
Si	3.83830500	0.78964700	0.48456800
C	4.32567600	1.72385500	2.03181600
H	4.68547800	1.02893600	2.79751200
H	5.14322400	2.41315100	1.80359900
H	3.49112300	2.28314900	2.45295500
C	2.56945400	-0.58215500	0.84333400
C	2.33235500	-1.63500600	-0.07274700
C	3.05591700	1.90471200	-0.73810900
C	2.36724900	2.50970500	-1.53900900
C	5.43434100	0.09510700	-0.23577400
C	5.98392300	0.57945900	-1.42805500
C	6.11794100	-0.93001000	0.43171300
C	7.16887400	0.05930400	-1.93827900
H	5.46578900	1.36764800	-1.97032100
C	7.30022300	-1.45791400	-0.07538400
H	5.71203000	-1.33623200	1.35726200

C	7.82770800	-0.96339700	-1.26438000
H	7.57702300	0.44777900	-2.86675600
H	7.80940700	-2.25759100	0.45413000
H	8.74944300	-1.37506100	-1.66406500
C	1.53707000	3.19998600	-2.49893100
H	1.34340300	4.23413200	-2.19760000
H	2.00458200	3.22209000	-3.48770000
H	0.56661700	2.70107800	-2.59709000
C	3.11948600	-1.74014200	-1.35782700
H	2.54623700	-2.27634000	-2.11497800
H	3.40124000	-0.76647100	-1.76639600
H	4.04736700	-2.30223600	-1.19332100
C	0.75367900	-0.60715400	4.16942400
C	0.59621700	0.83902500	3.70172400
C	-0.50571400	-4.05595400	0.69530000
C	-0.17033600	-4.33960600	-0.76905200
H	1.45610900	-0.70074500	5.00795000
H	-0.19504400	-1.06319900	4.46825000
H	0.88174500	1.57577700	4.45846200
H	-0.43449600	1.05274200	3.38213100
H	-0.55359400	-4.95551600	1.31524400
H	-1.46428000	-3.52475000	0.79291900
H	0.30939600	-5.31736200	-0.90734700
H	-1.04777400	-4.29405700	-1.42255800

46

(*S*)-P1

imaginary frequencies no

E(M06L/LanL2DZ(Pd),6-311G(d,p))=-1301.056742

H(M06L/LanL2DZ(Pd),6-311G(d,p))=-1301.030081

G(M06L/LanL2DZ(Pd),6-311G(d,p))=-1301.11478

E(M06L/def2TZVP)=-1301.15382266

B	2.19850000	-1.32595900	0.91790700
B	1.52714000	1.05465300	-0.67851000
O	1.68906800	0.87595500	-2.03304000
O	2.28897100	2.08089200	-0.17606300
O	2.62972300	-2.34459000	1.72758700
O	3.20541300	-0.79631400	0.14401700
Si	-1.29882800	0.96772700	-0.07662400
C	-1.21912700	2.40064700	-1.28171700
H	-0.86637300	2.05497500	-2.25802000
H	-2.19925700	2.86209700	-1.41981500
H	-0.52896400	3.17408400	-0.93050700
C	0.45027400	0.29170700	0.13567900

C	0.73839600	-0.81115300	0.87191700
C	-2.42073200	-0.38764800	-0.74345700
C	-3.63804000	-0.70549200	-0.13075300
C	-2.04007700	-1.12591300	-1.87345300
C	-4.45035600	-1.71933800	-0.62657900
H	-3.94732700	-0.15300800	0.75361700
C	-2.84856200	-2.14069300	-2.37265200
H	-1.09120000	-0.91021700	-2.36349300
C	-4.05670500	-2.43907700	-1.74913300
H	-5.39093700	-1.95131000	-0.13540300
H	-2.53558000	-2.70285100	-3.24744500
H	-4.68727600	-3.23333300	-2.13729800
C	-0.28751800	-1.59357500	1.64269000
H	0.12227000	-1.95370300	2.59050800
H	-1.19310000	-1.02073800	1.85667200
H	-0.59110800	-2.48723100	1.08296300
C	2.59307100	1.88249800	-2.48931500
C	3.19114300	2.47251200	-1.20938900
C	4.43073600	-1.41047900	0.53910800
C	4.00823500	-2.57988800	1.43970900
H	2.03049700	2.62620000	-3.06802900
H	3.34072000	1.43174300	-3.14727400
H	3.27368000	3.56223700	-1.23003300
H	4.18121400	2.05469100	-0.98723700
H	4.97942200	-1.73090500	-0.35046200
H	5.04190200	-0.67140200	1.06978200
H	4.10282800	-3.54996900	0.93945600
H	4.57071200	-2.62489500	2.37578700
C	-1.99507400	1.53463700	1.51535800
C	-2.46014200	1.88937700	2.58107800
C	-3.00938400	2.31194600	3.84892900
H	-2.34500700	3.02005400	4.35207400
H	-3.97856200	2.80220500	3.72048700
H	-3.15537600	1.46167100	4.52129100