Supporting Information for

Mechanistic Studies of Copper-Catalyzed Asymmetric Hydroboration of Alkenes

Yumeng Xi and John F. Hartwig*

Division of Chemical Sciences, Lawrence Berkeley National Laboratory,

and Department of Chemistry, University of California, Berkeley, CA 94720, United States

Email: jhartwig@berkeley.edu

Table of Contents

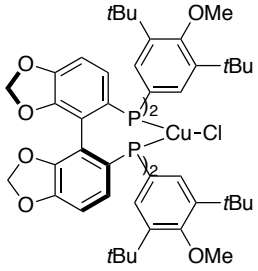
I. General Methods and Materials

All air-sensitive manipulations were performed in an argon-filled glovebox or using standard Schlenk techniques. Glassware was dried at 130 °C for at least 4 hours before use. Pentane, hexanes, THF, DCM, and toluene were collected from a solvent purification system containing a 0.33 m column of activated alumina under nitrogen. Anhydrous cyclohexane was purchased from Aldrich and used as received. CuCl, KO*t*Bu and pinacolborane (HBpin) were purchased from Aldrich. (*S*)-SEGPHOS was purchased from Strem Chemicals and (*S*)-DTBM-SEGPHOS was generously donated by Takasago. All other reagents purchased from commercial suppliers were stored in the glovebox and used as received. Deuterated solvents were purchased from Cambridge Isotope Laboratories and Aldrich and used as received.

^{1}H NMR spectra were recorded on Bruker AVQ-400, AV-500, AV-600, and AV-700 instruments with 400, 500, 600, and 700 MHz frequencies, and ^{13}C NMR spectra were recorded on a Bruker AV-600 instrument with a ^{13}C operating frequency of 150 MHz. ^{19}F NMR spectra were recorded on a Bruker AV-600 spectrometer with a ^{19}F operating frequency of 564 MHz. ^{11}B NMR spectra were recorded on a Bruker AV-600 spectrometer with a ^{11}B operating frequency of 192 MHz. Chemical shifts (δ) are reported in ppm relative to the residual solvent signal ($CDCl_3$ δ = 7.26 for ^{1}H NMR and δ = 77.0 for ^{13}C NMR; benzene-d_6 = 7.16 ppm for ^{1}H NMR; toluene-d_8 = 2.09 ppm for ^{1}H NMR; cyclohexane-d_{12} = 2.12 ppm for ^{1}H NMR). Quantitative analysis by GC was performed with dodecane as an internal standard. Chiral HPLC analysis was conducted on a Waters chromatography system. Elemental analyses were conducted at the Micro Analytical Facility operated by the College of Chemistry, University of California, Berkeley.

II. Synthesis and Characterization of Copper Complexes

(*S*)-DTBM-SEGPHOSCuCl (6)



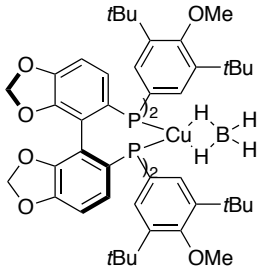
Into a 20 mL vial was placed CuCl (30.0 mg, 0.303 mmol, 1.01 equiv) and (*S*)-DTBM-SEGPHOS (354.0 mg, 0.3000 mmol, 1 equiv) were added, followed by 6 mL of toluene and 2 mL of DCM. The vial was capped and allowed to stir at ambient temperature for 2 hours. The resulting solution was filtered through a pad of Celite and concentrated *in vacuo*. The resulting crude material was recrystallized with 15 drops of DCM and 6 mL of pentane at -40 °C. Crystals formed by the process were suitable for x-ray crystallography. The crystals were washed with cold pentane and dried under vacuum to give complex **6** (359.8 mg, 94%) as an off-white solid.

^{1}H NMR (600 MHz, Toluene-d_8) δ 8.52 (br s, 4H), 7.80 (br s, 4H), 6.76 (dt, J = 8.0, 4.8 Hz, 2H), 6.18 (d, J = 8.1 Hz, 2H), 5.29 (d, J = 1.4 Hz, 2H), 5.13 (d, J = 1.3 Hz, 2H), 3.32 (s, 6H), 3.22 (s, 6H), 1.58 (s, 36H), 1.31 (s, 36H).

^{31}P NMR (243 MHz, Toluene-d_8) δ -4.8.

Anal. Calcd (%) for $C_{74}H_{100}ClCuO_8P_2$: C, 69.52; H, 7.88. Found: C, 69.73; H, 7.61.

(*S*)-DTBM-SEGPHOSCuBH$_4$ (16)



To a 20 mL vial containing (*S*)-DTBM-SEGPHOSCuCl (**6**, 76.7 mg, 0.600 mmol, 1 equiv), was added 2 mL of toluene. Sodium borohydride (56.7 mg, 1.50 mmol, 25 equiv) was then added in one portion. The vial was capped and allowed to stir at ambient temperature overnight. An aliquot was removed and analyzed by ^{31}P NMR spectroscopy to ensure full conversion. The aliquot was combined with the rest of the solution, and the combined material was filtered through a pad of Celite and concentrated *in vacuo*. The resulting solid was treated with 3 mL of pentane and dried under vacuum to give an analytically pure sample of **16** (60.4 mg, 80%) as a white solid. Crystals suitable for x-ray crystallography were obtained by recrystallizing the crude material in hexanes at rt.

^{1}H NMR (600 MHz, Toluene-d_8) δ 8.40 (br s, 4H), 7.85 (br s, 4H), 6.68 (dt, J = 8.0, 4.9 Hz, 2H), 6.15 (d, J = 8.1 Hz, 2H), 5.35 (s, 2H), 5.11 (s, 2H), 3.33 (s, 6H), 3.19 (s, 6H), 1.57 (s, 36H), 1.33 (s, 36H).

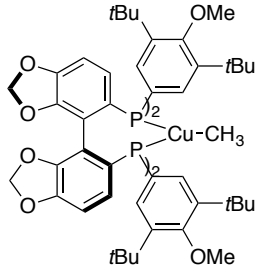
^{31}P NMR (243 MHz, Toluene-d_8) δ 0.5.

^{11}B{^{1}H} NMR (192 MHz, Toluene-d_8) δ -28.0.

FT-IR (cm^{-1}): 2391 (ν(B-H$_t$)), 2360 (ν(B-H$_t$)), 1974 (ν(B-H$_b$)), 1914 (ν(B-H$_b$)).

Anal. Calcd (%) for $C_{74}H_{104}BCuO_8P_2$: C, 70.66; H, 8.33. Found: C, 70.55; H, 8.20.

(*S*)-DTBM-SEGPHOSCuCH$_3$ (7)



To a 20 mL vial containing a suspension of (*S*)-DTBM-SEGPHOSCuCl (**6**, 76.7 mg, 0.600 mmol, 1 equiv) in pentane pre-chilled to -35°C, was added a pre-chilled solution of MeLi (600 μL, 0.10 M in THF) dropwise. The vial was capped and allowed to warm to room temperature. After 45 minutes, the resulting yellow solution was passed through a syringe filter and concentrated *in vacuo*. The residue was re-dissolved in pentane and concentrated *in vacuo*. This material was recrystallized by dissolving in a mixture of 20 drops of THF and 1 mL pentane and layering the resulting solution with 2 mL hexamethyldisiloxane at -40 °C. The crystals were washed with cold hexamethyldisiloxane and dried under vacuum to give complex **7** (64.7 mg, 86%) as a bright yellow solid. Note: 8% (*S*)-DTBM-SEGPHOS is present as an impurity, which we were unable to remove by multiple recrystallization.

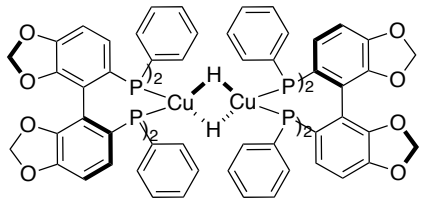
Crystals suitable for x-ray crystallography was obtained by layering a hexane solution of the crude material with hexamethyldisiloxane.

^{1}H NMR (600 MHz, Toluene-d_8) δ 8.44 (s, 4H), 7.82 (s, 4H), 6.71 (s, 2H), 6.19 (d, J = 8.1 Hz, 2H), 5.38 (s, 2H), 5.17 (d, J = 1.4 Hz, 2H), 3.36 (s, 6H), 3.25 (s, 6H), 1.57 (s, 36H), 1.36 (s, 36H), 0.62 (br s, 3H, Cu-C$\underline{H}_3$).

^{31}P NMR (243 MHz, Toluene-d_8) δ -7.9.

Anal. Calcd (%) for $C_{75}H_{103}CuO_8P_2$: C, 71.60; H, 8.25. Found: C, 71.25; H, 7.96.

(*S*)-SEGPHOSCuH dimer (27)



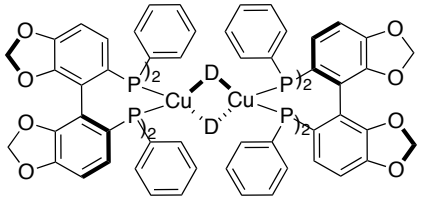
To a 20 mL vial containing a solution of [(*S*)-SEGPHOSCuCl]$_2$ (71.0 mg, 0.0500 mmol) in 1.5 mL of THF was added a solution of NaBHEt$_3$ (100 μL, 1.0 M in THF) dropwise. The vial was capped and allowed to stir at room temperature for 10 minutes. The resulting solution was passed through a syringe filter. The filtrate was layered with pentane at -40 °C. Yellow solids formed overnight were collected by filtration, washed by 4 mL of pentane and dried under vacuum to give complex **27** (42.0 mg, 62%) as a yellow solid. Yellow crystals suitable for x-ray crystallography were obtained by layering a dilute THF solution of **27** with hexanes.

^{1}H NMR (600 MHz, Benzene-d_6) δ 8.42 (br s, 8H), 8.32 (br s, 8H), 6.99 (t, J = 7.4 Hz, 4H), 6.91 (t, J = 7.5 Hz, 8H), 6.61 (t, J = 7.6 Hz, 8H), 6.54 (t, J = 7.3 Hz, 4H), 6.52 – 6.49 (m, 4H), 6.17 (d, J = 8.1 Hz, 4H), 5.41 (d, J = 1.7 Hz, 4H), 5.19 (d, J = 1.8 Hz, 4H), 2.60 (s, 2H).

^{31}P NMR (243 MHz, Benzene-d_6) δ 1.9.

We were unable to obtain a satisfactory elemental analysis.

(*S*)-SEGPHOSCuD dimer (27-d)

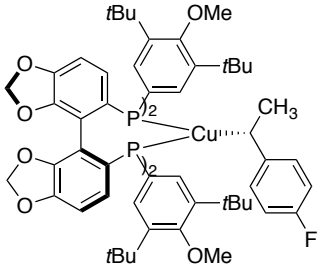


The deuteride dimer was synthesized by a procedure that is analogous to that used to prepare **27**, except LiDBEt$_3$ was used instead of NaHBEt$_3$ as the hydride source.

^{2}H NMR (600 MHz, Benzene) δ 2.60 (br s).

^{31}P NMR (243 MHz, Benzene) δ 1.9.

Characterization of (*S*)-DTBM-SEGPHOSCu[CH(4-F-C$_6$H$_4$)CH$_3$] (5) generated *in situ*



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) and 4-fluorostyrene (2.4 μL, 0.020 mmol) were dissolved in cyclohexane-d_{12} (400 μL). A cyclohexane-d_{12} solution of HBpin (50.0 μL, 0.0202 mmol, 0.401 M) was added in one portion. The tube was capped, shaken and inserted into an NMR instrument, and ^{1}H, ^{31}P, and ^{19}F NMR spectra were obtained.

The combined yield of complex **5** and its diastereomer **5'** (78%, 19:1) was determined by ^{19}F NMR spectroscopy on a sample generated in cyclohexane with 1,3-difluorobenzene as an internal standard, following the same procedure but with cyclohexane as the solvent.

^{1}H NMR (600 MHz, Cyclohexane-d_{12}) δ 7.50 (br s, 4H), 7.31 (t, J = 5.4 Hz, 4H), 6.63 (dt, J = 8.1, 4.1 Hz, 2H), 6.52 (dd, J = 8.6, 5.6 Hz, 2H), 6.35 (d, J = 8.1 Hz, 2H), 6.26 (t, J = 8.8 Hz, 2H), 5.50 (br s, 2H), 5.42 (d, J = 1.7 Hz, 2H), 3.77 (s, 6H), 3.65 (s, 6H), 2.85 (q, J = 7.2 Hz, 1H), 1.73 (d, J = 7.2 Hz, 3H), 1.49 (s, 36H), 1.37 (s, 36H).

^{31}P NMR (243 MHz, cyclohexane-d_{12}) δ -7.7.

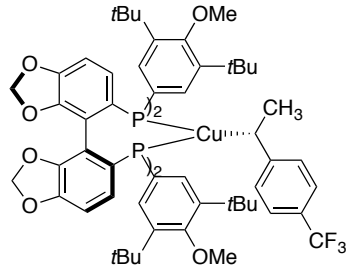
^{19}F NMR (564 MHz, cyclohexane-d_{12}) δ -130.0.

Minor diastereomer **5'**:

^{31}P NMR (192 MHz, cyclohexane-d_{12}) δ -6.2.

^{19}F NMR (564 MHz, cyclohexane-d_{12}) δ -130.4.

Characterization of (*S*)-DTBM-SEGPHOSCu[CH(4-CF_3-C_6H_4)CH_3] (9) *in situ*



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH_3 (**7**) (25.2 mg, 0.0203 mmol) and 4-trifluoromethylstyrene (3.0 μL, 0.020 mmol) were dissolved in cyclohexane-d_{12} (400 μL). A cyclohexane-d_{12} solution of HBpin (50.0 μL, 0.0202 mmol, 0.401 M) was added in one portion. The tube was capped, shaken and inserted into an NMR instrument, and ^{1}H, ^{31}P, and ^{19}F NMR spectra were obtained.

The combined yield of complex **9** and its diastereomer **9'** (90%, 42:1) was determined by ^{19}F NMR spectroscopy on a sample generated in cyclohexane with 4-bromobenzotrifluoride as an internal standard, following the same procedure but with cyclohexane as the solvent.

^{1}H NMR (600 MHz, Cyclohexane-d_{12}) δ 7.53 – 7.42 (m, 4H), 7.26 (t, J = 5.5 Hz, 4H), 6.78 (d, J = 8.2 Hz, 2H), 6.67 (dt, J = 8.2, 4.1 Hz, 2H), 6.51 (d, J = 8.2 Hz, 2H), 6.37 (d, J = 8.1 Hz, 2H), 5.48 (br s, 2H), 5.42 (d, J = 1.7 Hz, 2H), 3.79 (s, 6H), 3.64 (s, 6H), 3.06 (q, J = 6.8 Hz, 1H), 1.79 (d, J = 6.8 Hz, 3H), 1.50 (s, 36H), 1.36 (s, 36H).

^{31}P NMR (243 MHz, cyclohexane-d_{12}) δ -6.6.

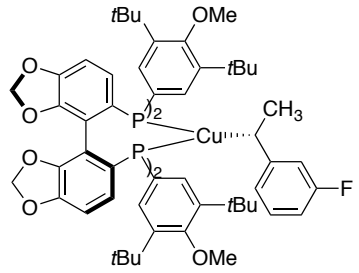
^{19}F NMR (564 MHz, cyclohexane-d_{12}) δ -62.2.

Minor diastereomer **9'**:

^{31}P NMR (192 MHz, cyclohexane-d_{12}) δ -5.6.

^{19}F NMR (564 MHz, cyclohexane-d_{12}) δ -62.3.

Characterization of (*S*)-DTBM-SEGPHOSCu[CH(3-F-C_6H_4)CH_3] (10) *in situ*



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) and 3-fluorostyrene (2.4 μL, 0.020 mmol) were dissolved in cyclohexane-d_{12} (400 μL). A cyclohexane-d_{12} solution of HBpin (50.0 μL, 0.0202 mmol, 0.401 M) was added in one portion. The tube was capped, shaken and inserted into an NMR instrument, and ^{1}H, ^{31}P, and ^{19}F NMR spectra were obtained.

The combined yield of complex **10** and its diastereomer **10'** (82%, 15:1) was determined by ^{19}F NMR spectroscopy on a sample generated in cyclohexane with 1,3-difluorobenzene as an internal standard, following the same procedure but with cyclohexane as the solvent.

^{1}H NMR (600 MHz, Cyclohexane-d_{12}) δ 7.48 (br s, 4H), 7.29 (t, *J* = 5.4 Hz, 4H), 6.67 (dt, *J* = 8.2, 4.1 Hz, 2H), 6.49 (dd, *J* = 14.6, 7.5 Hz, 1H), 6.43 (d, *J* = 7.8 Hz, 1H), 6.36 (d, *J* = 8.1 Hz, 2H), 6.13 (d, *J* = 12.6 Hz, 1H), 5.81 – 5.77 (t, *J* = 8.2 Hz, 1H), 5.48 (s, 2H), 5.42 (d, *J* = 1.7 Hz, 2H), 3.78 (s, 6H), 3.65 (s, 6H), 2.95 (q, *J* = 7.0 Hz, 1H), 1.72 (d, *J* = 7.0 Hz, 3H), 1.49 (s, 36H), 1.37 (s, 36H).

^{31}P NMR (243 MHz, cyclohexane-d$_{12}$) δ -7.2.

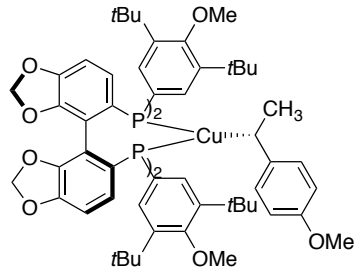
^{19}F NMR (564 MHz, cyclohexane-d$_{12}$) δ -116.9.

Minor diastereomer **10'**:

^{31}P NMR (192 MHz, cyclohexane-d$_{12}$) δ -5.9.

^{19}F NMR (564 MHz, cyclohexane-d$_{12}$) δ -117.2.

Characterization of (*S*)-DTBM-SEGPHOSCu[CH(4-OCH$_3$-C$_6$H$_4$)CH$_3$] (11) *in situ*



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) and 4-vinylanisole (2.7 μL, 0.020 mmol) were dissolved in cyclohexane-d_{12} (400 μL). A cyclohexane-d_{12} solution of HBpin (50.0 μL, 0.0202 mmol, 0.401 M) was added in one portion. The tube was capped, shaken and inserted into an NMR instrument, and ^{1}H and ^{31}P NMR spectra were obtained.

The combined yield of complex **11** and its diastereomer **11'** (68%, 18:1) was determined by ^{1}H NMR spectroscopy on a sample generated with *p*-xylene as an internal standard.

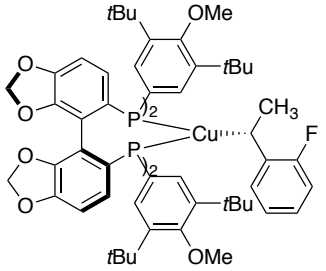
^{1}H NMR (600 MHz, Cyclohexane-d_{12}) δ 7.54 (br s, 4H), 7.32 (t, J = 5.4 Hz, 4H), 6.62 (td, J = 8.0, 4.0 Hz, 2H), 6.55 (d, J = 8.4 Hz, 2H), 6.33 (d, J = 8.2 Hz, 2H), 6.23 (d, J = 8.4 Hz, 2H), 5.51 (s, 2H), 5.42 (d, J = 1.6 Hz, 2H), 3.75 (s, 6H), 3.64 (s, 6H), 3.48 (s, 3H), 2.80 (q, J = 7.5 Hz, 1H), 1.74 (d, J = 7.3 Hz, 3H), 1.49 (s, 36H), 1.36 (s, 36H).

^{31}P NMR (243 MHz, cyclohexane-d_{12}) δ -7.9.

Minor diastereomer **11'**:

^{31}P NMR (192 MHz, cyclohexane-d_{12}) δ -6.3.

Characterization of (*S*)-DTBM-SEGPHOSCu[CH(2-F-C$_6$H$_4$)CH$_3$] (12) *in situ*



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) and 2-fluorostyrene (2.4 μL, 0.020 mmol) were dissolved in cyclohexane-d_{12} (400 μL). A cyclohexane-d_{12} solution of HBpin (50.0 μL, 0.0202 mmol, 0.401 M) was added in one portion. The tube was capped, shaken and inserted into an NMR instrument, and ^{1}H, ^{31}P, and ^{19}F NMR spectra were obtained.

The combined yield of complex **12** and its diastereomer **12'** (88%, 62:1) was determined by ^{1}H NMR spectroscopy on a sample generated with *p*-xylene as an internal standard.

^{1}H NMR (600 MHz, Cyclohexane-d_{12}) δ 7.44 (br s, 4H), 7.35 (br t, J = 5.3 Hz, 4H), 6.61 (dt, J = 8.1, 4.1 Hz, 2H), 6.42 – 6.25 (m, 5H), 6.03 (q, J = 6.7 Hz, 1H), 5.46 (s, 2H), 5.40 (s, 2H), 3.76 (s, 6H), 3.65 (s, 6H), 2.90 (q, J = 7.0 Hz, 1H), 1.74 (d, J = 7.0 Hz, 3H), 1.47 (s, 36H), 1.39 (s, 36H).

^{31}P NMR (243 MHz, cyclohexane-d_{12}) δ -8.4.

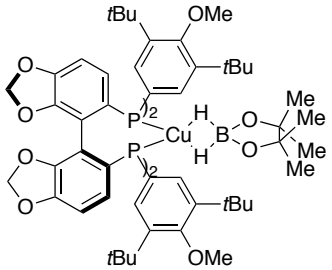
^{19}F NMR (564 MHz, cyclohexane-d_{12}) δ -118.5.

Minor diastereomer **12'**:

^{31}P NMR (192 MHz, cyclohexane-d_{12}) δ -6.6.

^{19}F NMR (564 MHz, cyclohexane-d_{12}) δ -118.5.

Characterization of complex 15 generated *in situ*



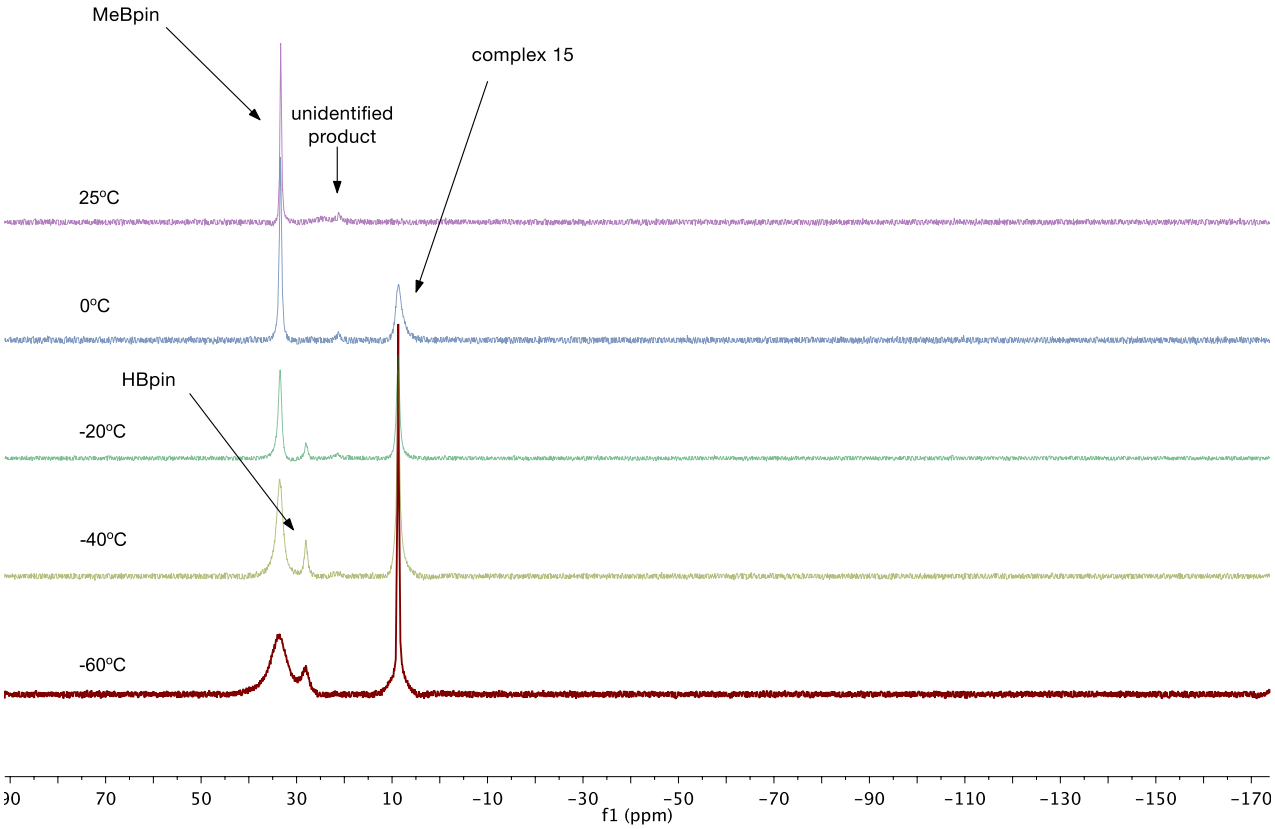
In a screw-capped NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) was dissolved in toluene-d_8 (400 μL). The NMR tube was capped, removed from the glovebox and placed in a dry ice/acetone bath. A toluene-d_8 solution of HBpin (100 μL, 0.0400 mmol, 0.400 M) was added in one portion. The tube was shaken to ensure proper mixing and then inserted into an NMR instrument pre-cooled at the designated temperature. The yield of complex **15** (79%) was determined by ^{1}H NMR spectroscopy with *p*-xylene as an internal standard at 0 °C.

^{1}H NMR (600 MHz, Toluene-d_8, 0 °C) δ 9.20-7.40 (br m, 8H), 6.57 (dt, J = 9.6, 5.1 Hz, 2H), 6.11 (d, J = 8.1 Hz, 2H), 5.38 (s, 2H), 5.07 (s, 2H), 4.19 (br m, 2H), 3.36 (s, 6H), 3.20 (s, 6H), 1.93 – 1.20 (br m, 84H).

^{31}P NMR (243 MHz, Toluene-d_8, 0 °C) δ 9.0.

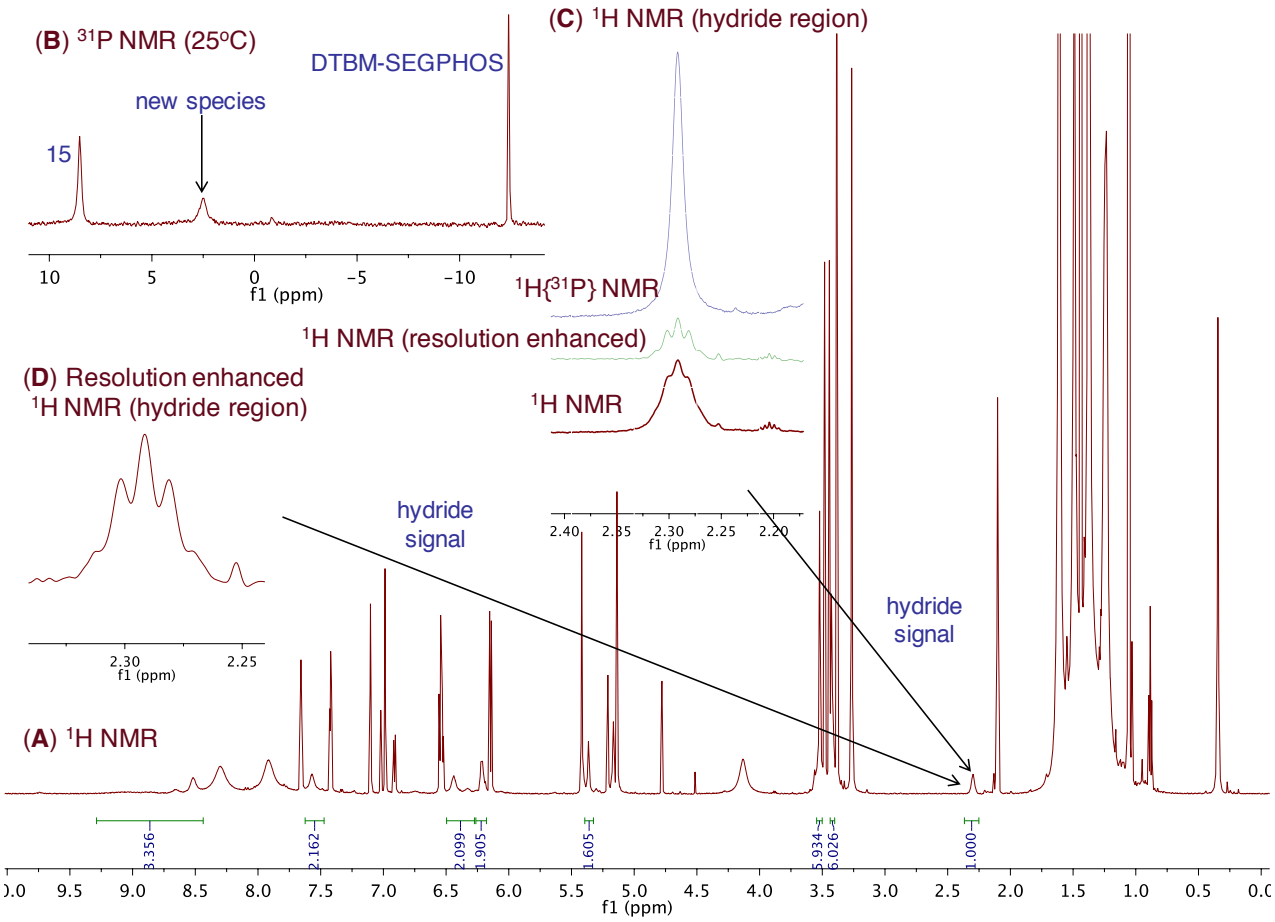
^{11}B NMR (192 MHz, Toluene-d_8, -60 °C) δ 8.8 (t, J = 72 Hz).

Figure S1. VT ^{11}B{^{1}H} NMR spectra of **15**



Note: Multiple baseline corrections were performed to remove the uneven baseline that results from boron in the borosilicate glass NMR tubes.

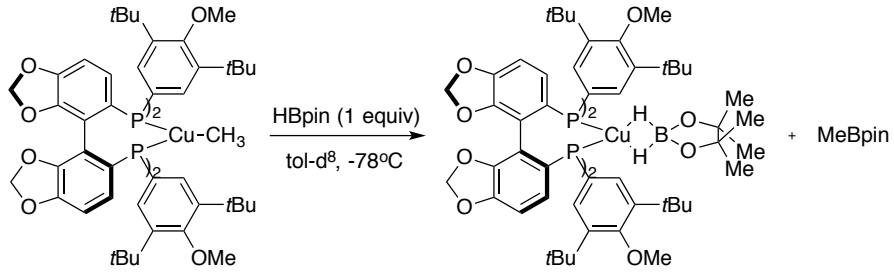
Figure S2. ^{1}H, $^{1}H\{^{31}P\}$, $^{31}P\{^{1}H\}$ NMR spectra of **15** at 25°C



After warming the sample to 25 °C from -60 °C, decomposition products (2.4 ppm and -12.7 ppm) were observed by ^{31}P NMR spectroscopy. We observed a distinct resonance at 2.29 ppm in the ^{1}H NMR spectrum that appears as a quintet.($J_{P\text{-}H}$ = 5.1 Hz) after resolution enhancement (Figure S2D). This quintet was observed as a sharp singlet when the spectrum was acquired with ^{31}P decoupling, indicating that the proton is coupled to four equivalent phosphorus nuclei. These results imply that the decomposition product is likely a dimeric DTBM-SEGPHOS-ligated copper hydride.

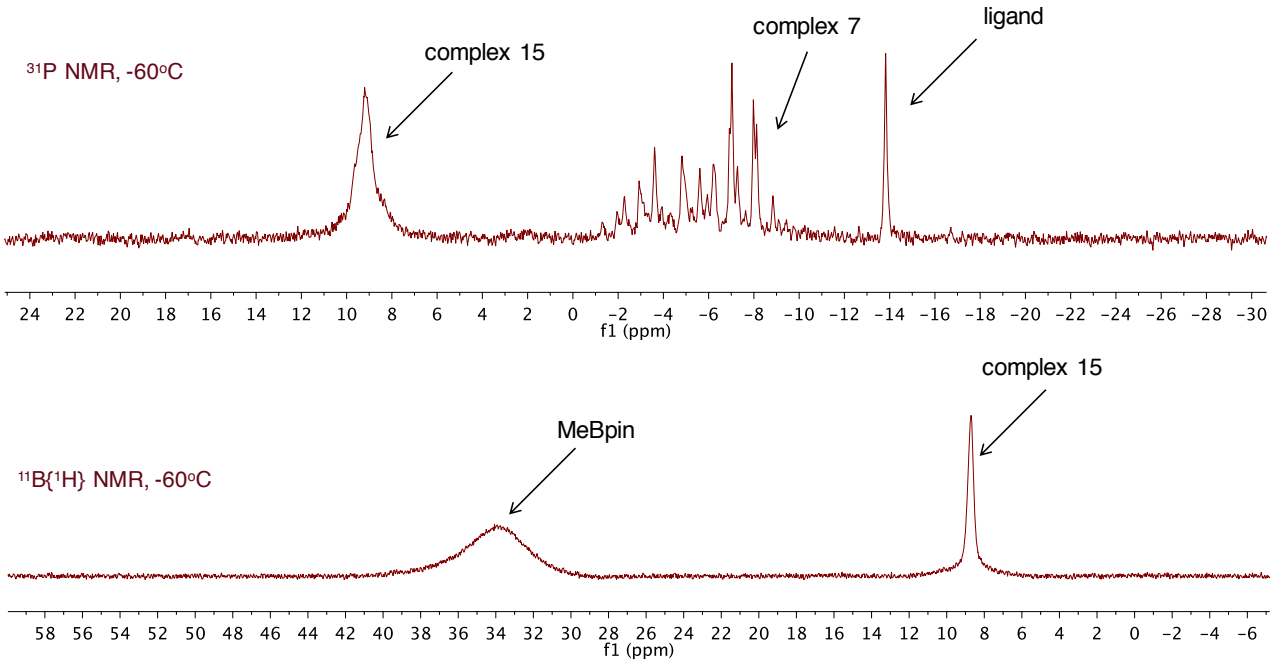
III. Stoichiometric Reactions

Reaction of (*S*)-DTBM-SEGPHOSCuCH$_3$ (7) and HBpin



In a screw-capped NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) was dissolved in toluene-d_8 (400 μL). The solution was cooled to -78 °C, and a toluene-d_8 solution of HBpin (50.0 μL, 0.0200 mmol, 0.400 M) was added in one portion. The tube was shaken to ensure proper mixing and inserted into an NMR instrument pre-cooled at a designated temperature.

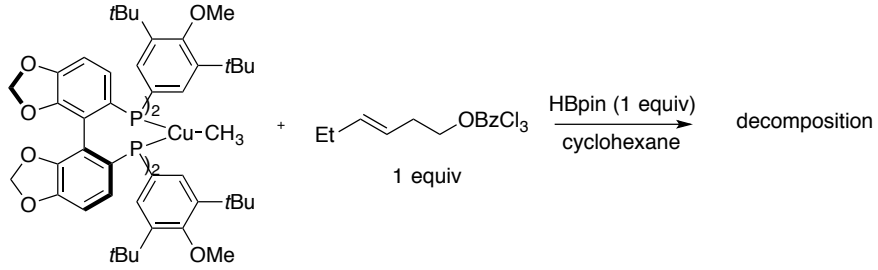
Figure S3. $^{31}P\{^1H\}$ and $^{11}B\{^1H\}$ NMR spectra of the reaction of **7** and HBpin at -60 °C



Note: The ^{31}P NMR spectrum of **7** consists of multiple signals that correspond to each rotamer at low temperature, presumably due to restricted rotation of methoxy groups of DTBM-SEGPHOS. Such multiple peaks were not observed with an analogous complex DTB-SEGPHOSCuCl, which has otherwise an identical structure to complex **7**, except for the absence of the methoxy groups (DTB: 3,5-di-*tert*-butylphenyl).

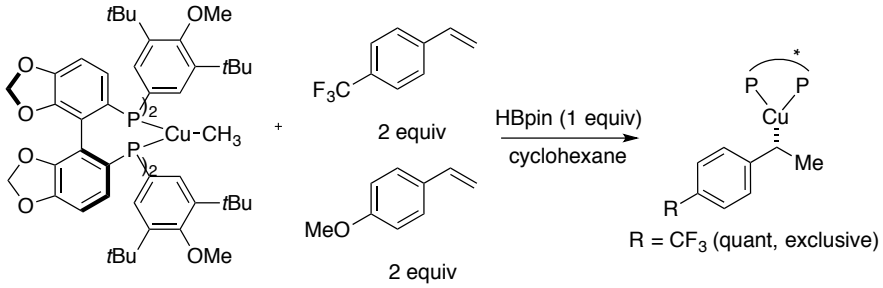
The reaction of methyl complex **7** and 1 equivalent of HBpin at -60 °C afforded **15** as the only product. The ^{31}P NMR spectrum acquired at -60 °C indicated the presence of **15** and unreacted **7**. This result suggests that the reaction of **15** and **7** is slow at -60 °C. After warming the sample to room temperature, complete decomposition to free ligand was observed.

Reaction of (*S*)-DTBM-SEGPHOSCuCH$_3$ (7), 2 and HBpin



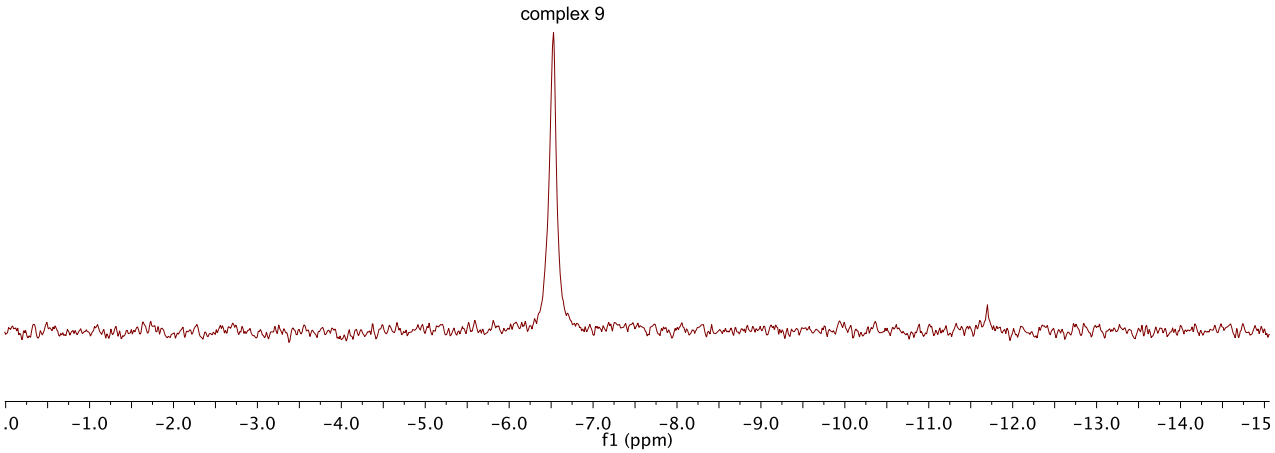
In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (12.6 mg, 0.0101 mmol) was dissolved in cyclohexane (350 μL). Solutions of **1** (25.0 μL, 0.400 M in cyclohexane) and HBpin (25.0 μL, 0.400 M in cyclohexane) were added. The NMR tube was capped and shaken. The sample was analyzed by ^{31}P NMR spectroscopy.

Competition experiment of 4-trifluoromethylstyrene and 4-vinylanisole for insertion



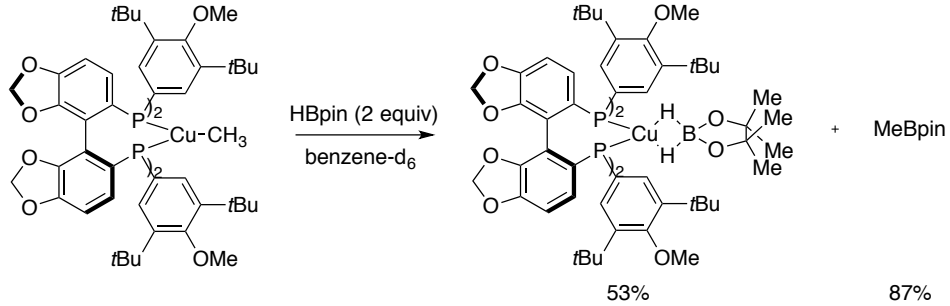
In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (12.6 mg, 0.0101 mmol) was dissolved in cyclohexane (225 μL). Solutions of 4-vinylanisole (50.0 μL, 0.400 M in cyclohexane), 4-trifluoromethylstyrene (50.0 μL, 0.400 M in cyclohexane), and 1,3-difluorobenzene (50 μL in cyclohexane) were added successively. A solution of HBpin in cyclohexane (25.0 μL, 0.400 M) was added. The NMR tube was capped and shaken. The sample was analyzed by ^{31}P and ^{19}F NMR spectroscopy.

Figure S4. $^{31}P\{^{1}H\}$ spectrum of the reaction mixture of methyl complex **7**, HBpin, 4-trifluoromethylstyrene, and 4-vinylanisole



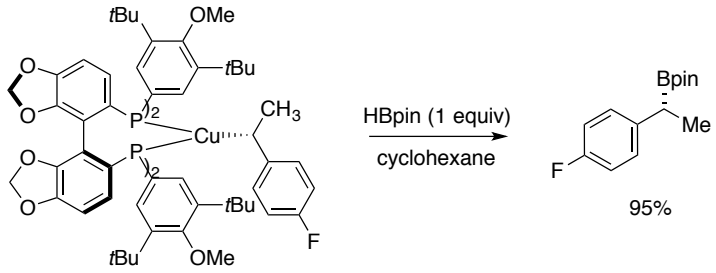
^{31}P NMR spectrum shows that complex **9** was formed exclusively.

Reaction of (*S*)-DTBM-SEGPHOSCuCH$_3$ with HBpin



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (12.6 mg, 0.0101 mmol) was dissolved in benzene-d_6 (300 μL). A benzene-d_6 solution of *p*-xylene (50.0 μL, 0.100 M) was added, followed by a benzene-d_6 solution of HBpin (20.0 μL, 0.0200 mmol, 1.00 M), each in one portion. The NMR tube was capped and shaken. The yields were determined by ^{1}H NMR spectroscopy.

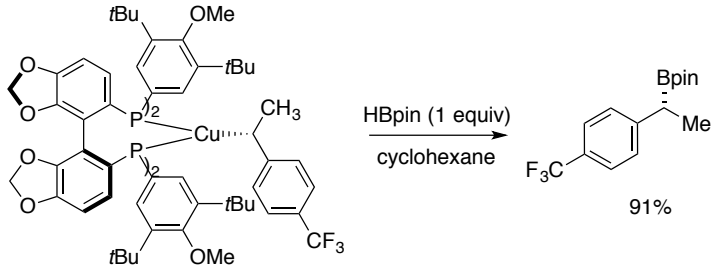
Reaction of (*S*)-DTBM-SEGPHOSCuCHMe(4-F-C$_6$H$_4$) with HBpin



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) was dissolved in cyclohexane (200 μL). Solutions of 4-fluorostyrene (50.0 μL, 0.400 M in cyclohexane), 1,3-difluorobenzene (50.0 μL in cyclohexane), and HBpin (50.0 μL, 0.400 M in cyclohexane) were added subsequently. After the yield of **5** was determined by ^{19}F NMR spectroscopy, a solution of HBpin (50.0 μL, 0.400 M in cyclohexane) was added. The sample was monitored by ^{31}P and ^{19}F NMR spectroscopy periodically.

After the reaction was complete, the solution was diluted with 2 mL of ethyl acetate and filtered through Celite. The volatile materials were removed by rotary evaporation, and the residue was dissolved in 1 mL THF. At 0 °C, a premixed solution of NaOH (2 M, aq)/30% H_2O_2 (2:1, 1.5 mL) was added. The reaction was warmed to room temperature and allowed to stir for 2.5 hours before adding water (2 mL) and ethyl acetate (5 mL). The phases were separated, and the organic phases were combined, dried over Na_2SO_4, and concentrated *in vacuo*. The crude sample was analyzed by HPLC with a chiral stationary phase.

Reaction of (*S*)-DTBM-SEGPHOSCuCHMe(4-CF$_3$-C$_6$H$_4$) with HBpin



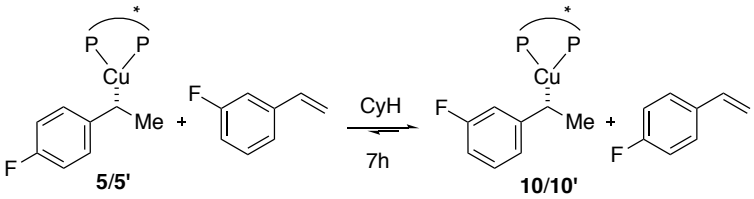
In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) was dissolved in cyclohexane (200 μL). Solutions of 4-trifluoromethylstyrene (50.0 μL, 0.400 M in cyclohexane), 4-bromobenzotrifluoride (50 μL in cyclohexane) as a ^{19}F NMR internal standard, and HBpin (50.0 μL, 0.400 M in cyclohexane) were added subsequently. After the yield was determined by ^{19}F NMR spectroscopy, a solution of HBpin (50.0 μL, 0.400 M in cyclohexane) was added. The sample was monitored by ^{31}P and ^{19}F NMR spectroscopy periodically.

Exchange experiments

The reaction of 4-fluorophenethylcopper complex **5** (formed in situ) and 1 equivalent of 3-fluorostyrene was monitored periodically by ^{19}F and ^{31}P NMR spectroscopy. After 10 minutes, 3-fluorophenethylcopper complex **10** was detected by ^{19}F NMR spectroscopy. Complex **10** became the major copper species after 7 hours. The decrease in the concentration of **5** and 3-fluorostyrene corresponded to the increase in the concentration of **10** and 4-fluorostyrene. This result demonstrates that **5** reacts with 3-fluorostyrene to afford **10** and 4-fluorostyrene. The product (**10**) is likely formed from β-hydrogen elimination, dissociation of 4-fluorostyrene, coordination of 3-flurostyrene, and migratory insertion. Analogous experiments were conducted with **10** (made in situ) and 4-fluorostyrene. Again, after 7 hours we observed both **5** and 3-fluorostyrene. However, **10** remained the major phenethylcopper species, suggesting that **10** is thermodynamically more stable than **5**. Because the

decomposition of the phenethylcopper complexes occurs before the time required to reach the equilibrium, determination of the equilibrium constant was not possible.

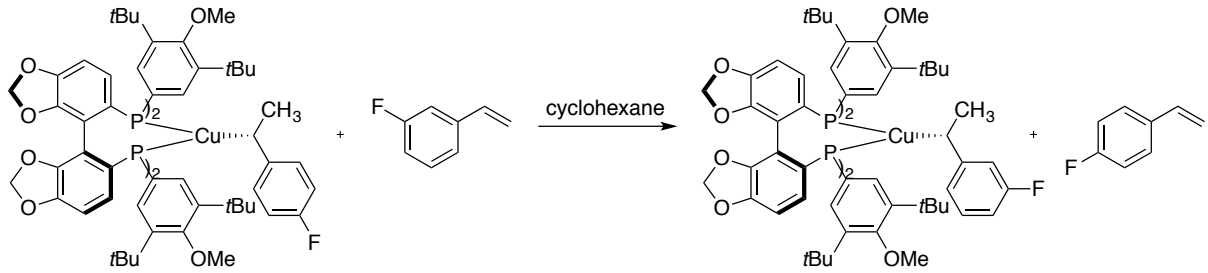
Scheme S1. Exchange experiments



reaction direction	**[5/5']**	[4-F-styrene]	**[10/10']**	[3-F-styrene]
left to right	0.0040 M	0.0248 M	0.0204 M	0.0172 M
right to left	0.0036 M	0.0332 M	0.0244 M	0.0054 M

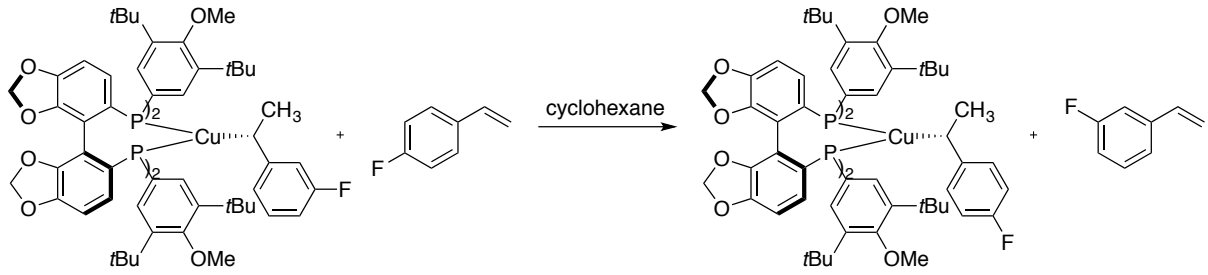
Similar observations were made about the reactions of 4-fluorophenethylcopper **5** and other styrenes, such as 2-fluorostyrene and 4-trifluoromethylstyrene. In all cases, the experiments indicated that phenethylcopper complex containing electron-deficient phenethyl groups are more thermodynamically stable than phenethylcopper complexes containing electron-rich phenethyl groups.

Procedures: reaction of (*S*)-DTBM-SEGPHOSCuCHMe(4-F-C_6H_4) with 3-fluorostyrene



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) was dissolved in cyclohexane (300 μL). Solutions of 4-fluorostyrene (50.0 μL, 0.400 M in cyclohexane), 1,3-difluorobenzene (50.0 μL in cyclohexane), and HBpin (50.0 μL, 0.400 M in cyclohexane) were added subsequently. After the yield of **5** was determined by ^{19}F NMR spectroscopy, a solution of 3-fluorostyrene (50.0 μL, 0.400 M in cyclohexane) was added. The sample was monitored by ^{31}P and ^{19}F NMR spectroscopy periodically.

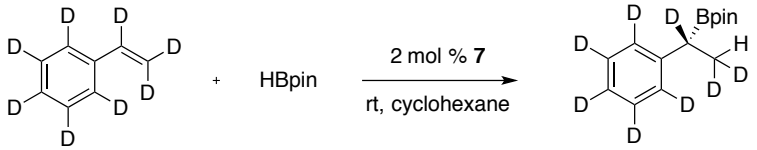
Procedures: reaction of (*S*)-DTBM-SEGPHOSCuCHMe(3-F-C_6H_4) with 4-fluorostyrene



In a J-Young NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (25.2 mg, 0.0203 mmol) was dissolved in cyclohexane (300 μL). Solutions of 3-fluorostyrene (50.0 μL, 0.400 M in cyclohexane), 1,3-difluorobenzene (50 μL in cyclohexane), and HBpin (50.0 μL, 0.400 M in cyclohexane) were added subsequently. After the yield of **10** was determined by ^{19}F NMR spectroscopy, a solution of 4-fluorostyrene (50.0 μL, 0.400 M in cyclohexane) was added. The sample was monitored by ^{31}P and ^{19}F NMR spectroscopy periodically.

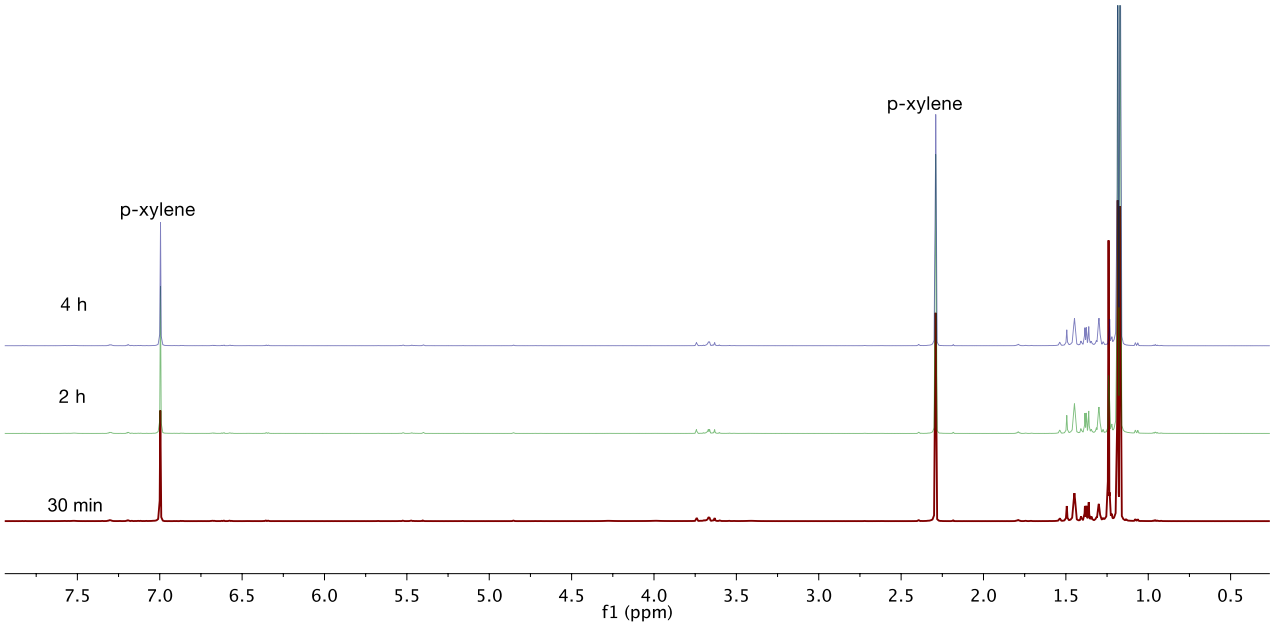
IV. Stereochemistry of Hydroboration

Hydroboration of styrene-d_8 catalyzed by (*S*)-DTBM-SEGPHOSCuCH$_3$ (7)



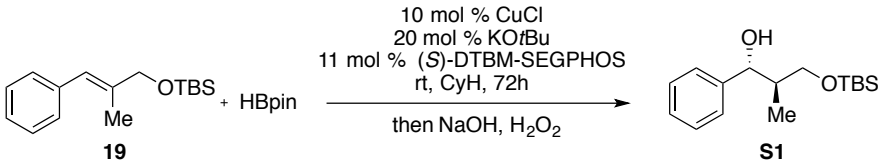
Into a J-Young NMR tube, were added (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (2.5 mg, 0.0020 mmol, 2 mol %), styrene-d_8 (11.5 μL, 0.100 mmol), and *p*-xylene (5 μL), followed by cyclohexane-d_{12} (370 μL). HBpin (14.5 μL, 0.100 mmol) was then added, and the reaction was monitored by ^{1}H NMR spectroscopy periodically. Another reaction with cyclohexane as the solvent and THF-d_8 as an internal standard was monitored by ^{1}H and ^{2}H NMR spectroscopy periodically. The experiment was also repeated with 8 equivalent of styrene-d_8.

Figure S5. ^{1}H spectra of hydroboration of styrene-d$_8$



The ^{1}H NMR spectra show that the incorporation of hydrogen atoms into styrene-d_8 did not occur.

Hydroboration of trisubstituted alkene 19



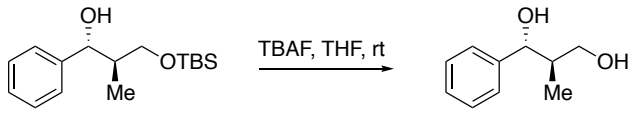
A 1-dram vial was charged with CuCl (4.0 mg, 10 mol %), KO*t*Bu (8.8 mg, 20 mol %), (*S*)-DTBM-SEGPHOS (52.8 mg, 11 mol %) and cyclohexane (400 μL). The mixture was allowed to stir at ambient temperature for 3

minutes before the addition of pinacolborane (71 μL, 0.48 mmol). To the solution was added **19** (105 mg, 0.400 mmol), which was pre-weighed in another vial. The second vial was then washed four times with 100 μL cyclohexane each time. After 72 h of stirring at rt, the reaction vial was diluted with 2 mL of ethyl acetate, and the resulting solution was filtered through Celite. The crude material was concentrated *in vacuo* and purified by flash column chromatography (CombiFlash, 5% ethyl actetate in hexanes) to afford an inseparable mixture that consisted of **19** and the product.

In a 20-mL scintillation vial the above mixture was dissolved in 2 mL of THF. The vial was cooled in an ice bath and a premixed solution of NaOH (2 M, aq.)/30% H_2O_2 (2:1, 3 mL) was added. The reaction was warmed to rt and allowed to stir for 3 hours before the addition of water (5 mL) and ethyl acetate (5 mL). The phases were separated, and the aqueous layer was extracted twice with 5 mL of ethyl acetate. The organic phases were combined, dried over Na_2SO_4, and concentrated *in vacuo*. Alcohol **S1** was purified by preparative TLC (10% ethyl acetate in hexanes) and obtained as a colorless liquid in 45% yield (50.5 mg, 0.180 mmol).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 – 7.31 (m, 4H), 7.31 – 7.21 (m, 1H), 4.58 (d, *J* = 7.4 Hz, 1H), 4.45 (br s, 1H), 3.79 (dd, *J* = 10.0, 3.8 Hz, 1H), 3.63 (dd, *J* = 10.1, 7.3 Hz, 1H), 2.03 – 1.95 (m, 1H), 0.95 (s, 10H), 0.75 (d, *J* = 7.0 Hz, 3H), 0.12 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.62, 128.06, 127.21, 126.60, 79.89, 68.09, 41.30, 25.80, 18.10, 13.89, -5.60, -5.68.



S1 **19-OH**

A 1-dram vial was charged with **S1** (9.8 mg, 0.035 mmol) and THF (300 μL). To the mixture was added TBAF (100 μL, 1.0 M in THF), and the resulting solution was allowed to stir at ambient temperature for 4 hours. Water (5 mL) and ethyl acetate (5 mL) were added. The phases were separated, and the aqueous layer was extracted twice with 5 mL of ethyl acetate. The organic phases were combined, dried over Na_2SO_4, and concentrated *in vacuo*. The pure diol was purified by preparative TLC (50% ethyl acetate in hexanes) and obtained as a colorless liquid in 72% yield (4.2 mg, 0.025 mmol).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.35 (m, 4H), 7.34 – 7.30 (m, 1H), 4.56 (d, *J* = 8.4 Hz, 1H), 3.85 – 3.64 (m, 2H), 3.02 (br s, 1H), 2.99 (br s, 1H), 2.08 (dtd, *J* = 8.2, 7.0, 3.5 Hz, 1H), 0.72 (d, *J* = 7.0 Hz, 3H).

$[\alpha]_D^{23}$= +49.5 (c = 0.42, $CHCl_3$).

The relative configuration of the stereogenic centers was established by comparing the ^{1}H NMR spectra with NMR data in the literature.[1,2] All chemical shifts matched those reported. The characteristic coupling constant (8.4 Hz) for the proton resonance at 4.56 ppm (the benzylic methine) indicates an *anti* configuration; the coupling constant for the ^{1}H NMR signal at 4.94 ppm for the benzylic methine of the *syn* isomer is 3.9 Hz.[3]

The absolute configuration was confirmed by comparing the optical rotation to the value reported previously for (2*R*,3*R*)-2-Methyl-1-phenylpropane-1,3-diol.

$[\alpha]_D^{24}$ = +35.17 (c = 0.34, $CHCl_3$)[1]

$[\alpha]_D^{20}$ = +50 (c = 0.5, $CHCl_3$)[2]

V. Kinetic Studies

Procedure for kinetic studies of the hydroboration of vinylarene 1

In an argon-filled glove box, a 4 mL vial was charged with alkene **1** (0.0500-0.200 mmol) as a solution in cyclohexane (2.00 M), dodecane (10.0 μL, 0.0440 mmol), complex **7** (0.400-1.60 μmol) as a solution in cyclohexane (0.0400 M), and cyclohexane (enough to bring total volume to 500 μL). HBpin (0.0500-0.300 mmol) as a solution in cyclohexane (2.00 M) was added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.

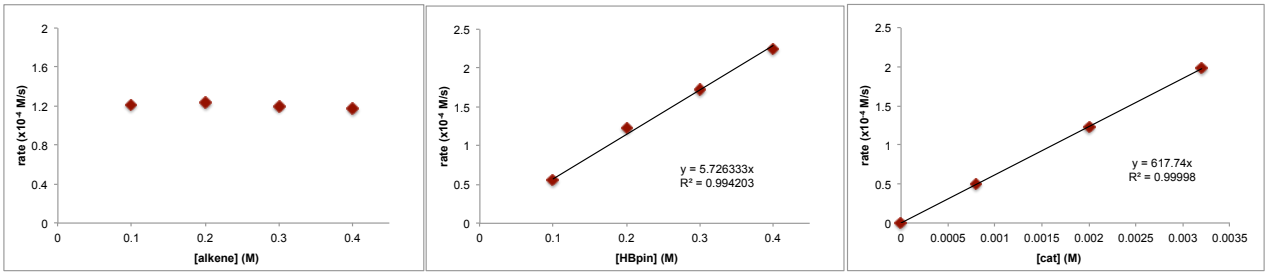
From the chromatograms, the initial rate of the formation of **3** was calculated. The initial rates of formation of **3** for reactions conducted with various concentrations of **1**, complex **7**, and HBpin are tabulated in Table S1.

Table S1. Initial rates for hydroboration of **1**

entry	[**1**]/M	[HBpin]/M	[**7**]/M	initial rate (M/s)
1	0.200	0.200	0.00200	1.2×10^{-4}
2	0.100	0.200	0.00200	1.2×10^{-4}
3	0.300	0.200	0.00200	1.2×10^{-4}
4	0.400	0.200	0.00200	1.2×10^{-4}
5	0.200	0.100	0.00200	5.6×10^{-5}
6	0.200	0.300	0.00200	1.7×10^{-4}
7	0.200	0.400	0.00200	2.3×10^{-4}
8	0.200	0.200	0.00080	5.0×10^{-5}
9	0.200	0.200	0.00320	2.0×10^{-4}

The kinetic dependence of the initial rates on the concentrations of **1**, complex **7**, and HBpin are summarized in Figure S6.

Figure S6. Kinetic dependence of the rates of hydroboration on [**1**], [HBpin], and [**7**]



Procedure for kinetic studies on the hydroboration of internal alkene 2

In an argon-filled glove box, a 4 mL vial was charged with alkene **2** (0.0250-0.300 mmol) as a solution in cyclohexane (2.00 M), dodecane (10.0 μL, 0.0440 mmol), complex **7** (0.050-0.200 mmol) as a solution in

cyclohexane (0.100 M), and cyclohexane (enough to bring total volume to 250 μL). HBpin (0.0500-0.300 mmol) as a solution in cyclohexane (2.00 M) was added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.

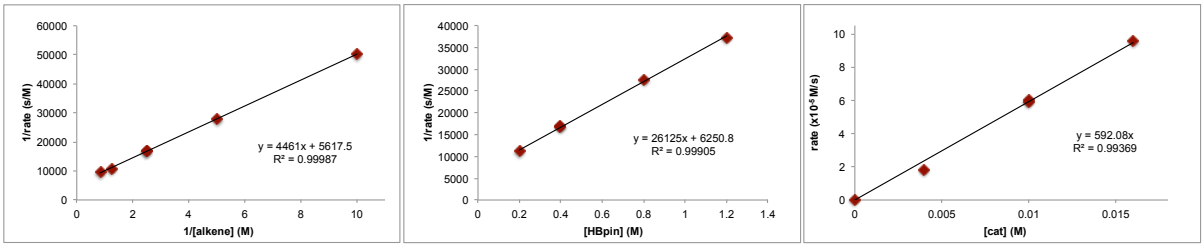
From the chromatograms, the initial rate of formation of **4** was calculated. The initial rates of formation of **4** for reactions conducted with various concentrations of **2**, complex **7**, and HBpin are tabulated in Table S2.

Table S2. Initial rates for hydroboration of **2**

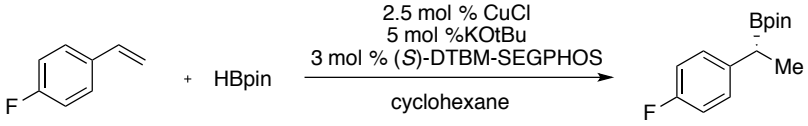
entry	[**1**]/M	[HBpin]/M	[7]/M	initial rate (M/s)
1	0.400	0.400	0.0100	6.0×10^{-5}
2	0.400	0.400	0.0100	5.9×10^{-5}
3	0.200	0.400	0.0100	3.6×10^{-5}
4	0.100	0.400	0.0100	2.0×10^{-5}
5	0.800	0.400	0.0100	9.2×10^{-5}
6	1.20	0.400	0.0100	1.1×10^{-4}
7	0.400	0.800	0.0100	3.6×10^{-5}
8	0.400	1.20	0.0100	2.7×10^{-5}
9	0.400	0.200	0.0100	9.0×10^{-5}
10	0.400	0.400	0.00400	1.8×10^{-5}
11	0.400	0.400	0.0160	9.6×10^{-5}

Kinetic dependence of the initial rates on the concentrations of **2**, complex **7**, and HBpin are summarized in Figure S7.

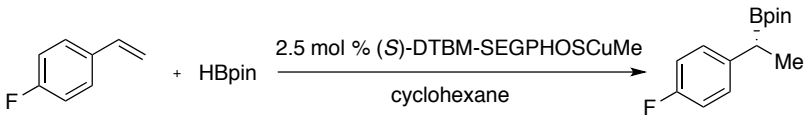
Figure S7. Kinetic dependence of the rates of hydroboration on [**2**], [HBpin], and [**7**]



Monitoring hydroboration of 1 with HBpin catalyzed by Cu/(*S*)-DTBM-SEGPHOS

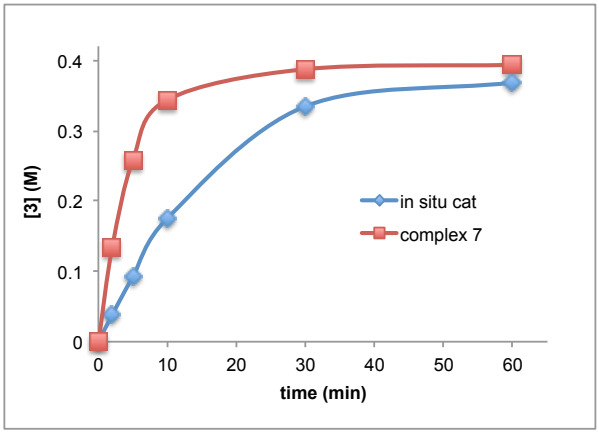


In an argon-filled glove box, a 4 mL vial was charged with CuCl (1.0 mg, 2.5 mol %), KO*t*Bu (2.2 mg, 5 mol %), (*S*)-DTBM-SEGPHOS (14.2 mg, 3 mol %), dodecane (40.0 μL, 0.176 mmol), and cyclohexane (400 μL). The mixture was allowed to stir at rt for 3 minutes before the addition of HBpin (61.0 μL, 0.420 mmol). Alkene **1** (48.0 μL, 0.402 mmol) and cyclohexane (451 μL) was added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.

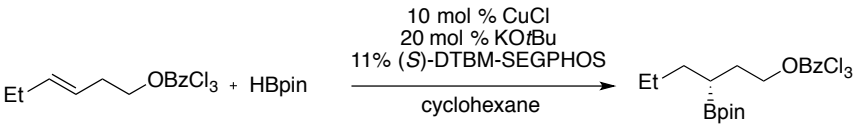


In an argon-filled glove box, a 4 mL vial was charged with complex **7** (12.6 mg, 10 mol %), dodecane (10.0 μL, 0.0440 mmol), alkene **1** (48.0 μL, 0.402 mmol) and cyclohexane (851 μL). HBpin (61.0 μL, 0.420 mmol) was added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography. The yield was 98%, and the ee was 98%.

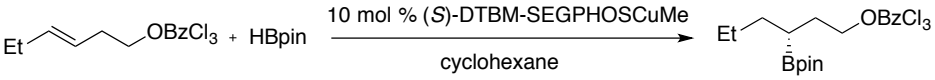
Figure S8. Profile of hydroboration of **1** catalyzed by the catalyst generated *in situ* and by **7**



Monitoring hydroboration of 2 with HBpin catalyzed by Cu/(*S*)-DTBM-SEGPHOS

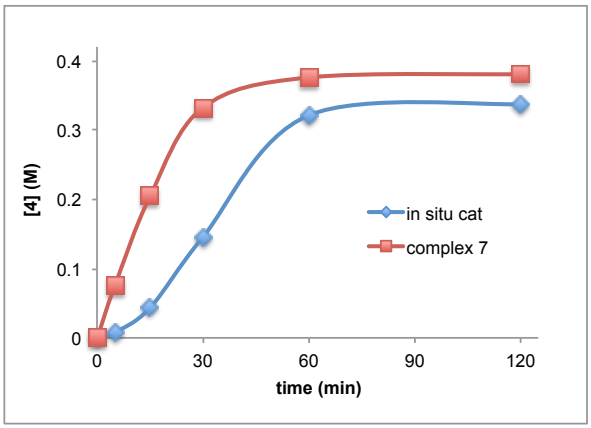


In an argon-filled glove box, a 4 mL vial was charged with CuCl (1.0 mg, 10 mol %), KO*t*Bu (2.2 mg, 20 mol %), (*S*)-DTBM-SEGPHOS (13.2 mg, 11 mol %), dodecane (10.0 μL, 0.0440 mmol), and cyclohexane (130 μL). The mixture was allowed to stir at rt for 3 minutes before addition of HBpin (60.0 μL, 0.120 mmol) as a solution in cyclohexane (2.00 M). Alkene **2** (50.0 μL, 0.100 mmol) as a solution in cyclohexane (2.00 M) and cyclohexane (130 μL) were added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.



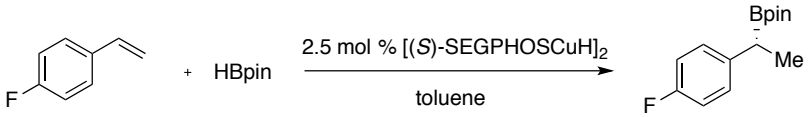
In an argon-filled glove box, a 4 mL vial was charged with complex **7** (12.6 mg, 10 mol %), dodecane (10.0 μL, 0.0440 mmol), alkene **2** (50.0 μL, 0.100 mmol) as a solution in cyclohexane (2.00 M) and cyclohexane (130 μL). HBpin (60.0 μL, 0.120 mmol) as a solution in cyclohexane (2.00 M) was added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography. The yield was 96%, and the ee was 95%.

Figure S9. Profile of hydroboration of **2** catalyzed by the catalyst generated *in situ* and by pure **7**



Monitoring hydroboration of 1 with HBpin catalyzed by Cu/(*S*)-SEGPHOS

In an argon-filled glove box, a 4 mL vial was charged with CuCl (2.0 mg, 5 mol %), KO*t*Bu (4.4 mg, 10 mol %), (*S*)- SEGPHOS (13.3 mg, 11 mol %), dodecane (10.0 μL, 0.0440 mmol), and toluene (400 μL). The mixture was allowed to stir for 5 min before the addition of HBpin (64.0 μL, 0.441 mmol, 1.1 equiv) and alkene **1** (48 μL, 0.40 mmol). At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.



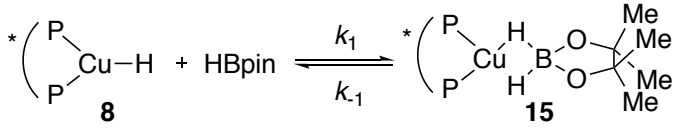
In an argon-filled glove box, a 4 mL vial was charged with SEGPHOS-ligated complex **27** (13.5 mg, 2.5 mol %, 5 mol % per Cu), dodecane (10.0 μL, 0.0440 mmol), HBpin (64.0 μL, 0.441 mmol, 1.1 equiv) and alkene **1** (48.0 μL, 0.402 mmol) and toluene (400 μL). At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.

The profiles of these reactions are shown in Scheme 20 of the main paper.

VI. 2D ^{11}B-EXSY Study of the Equilibrium of Dihydridoborate 15 and HBpin

2D ^{11}B-EXSY[4] spectra were collected on an Bruker AV-600 spectrometer. The temperature was maintained at -10 °C throughout the experiment. To determine the exchanges rates, EXSY experiments were conducted with a mixing time of 3 ms. The reference spectra were obtained with a mixing time of 0 ms. The experiment was repeated at different [HBpin].

The areas of the peaks were determined by integration. From these numbers, the exchange rate matrices and the magnetization exchange rate constants (k_1' and k_{-1}') were calculated by EXSY CALC program.[5] The magnetization exchange rate constants were converted to the chemical exchange rate constants (k_1 and k_{-1}) by the following equations.



(1)

$$k_1 = k_1'/[\text{HBpin}] \quad (2)$$

$$k_{-1} = k_{-1}' \quad (3)$$

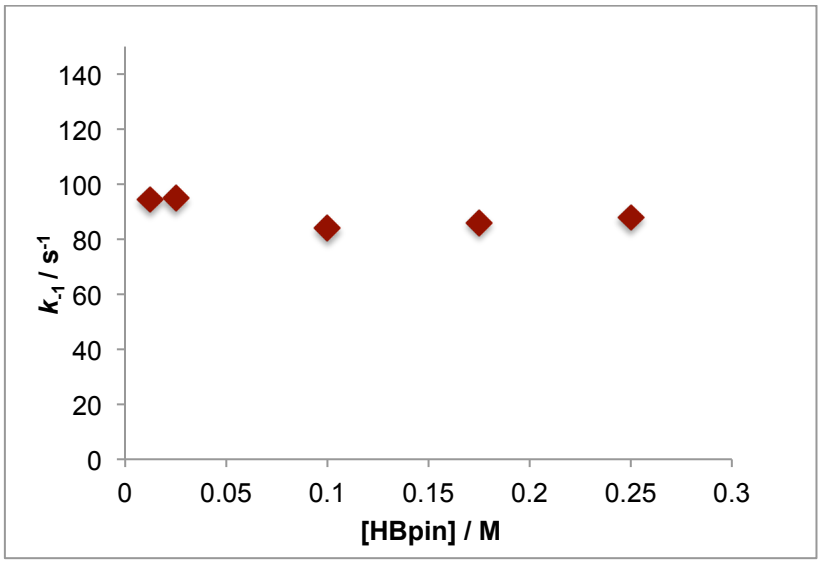
The magnetization exchange rate constants are tabulated in Table S3.

Table S3. Magnetization exchange rate constants at different [HBpin] calculated by EXSY CALC

[HBpin]	k_1' (s^{-1})	k_{-1}' (s^{-1})
0.0125	61.6	94.4
0.0250	57.1	94.8
0.100	16.2	84.0
0.175	10.7	86.1
0.250	5.8	87.8

A zero order dependence of the exchange rate constant (k_{-1}) on the concentrations of HBpin was established by plotting k_{-1} against [HBpin], as shown in Figure S10.

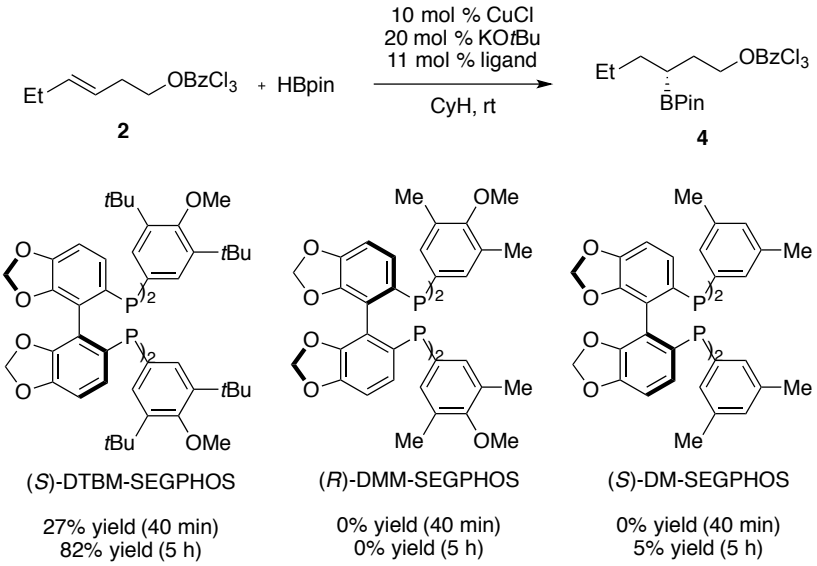
Figure S10. Dependence of exchange rate constant k_{-1} on the concentration of HBpin



Representative procedure for sample preparation:

In a screw-capped NMR tube, (*S*)-DTBM-SEGPHOSCuCH$_3$ (**7**) (12.6 mg, 0.0101 mmol) was dissolved in toluene-d_8 (enough to make a total volume of 400 μL). The NMR tube was capped, removed from the glovebox and placed in a dry ice/acetone bath. A toluene-d_8 solution of HBpin (100 μL, 0.0400 mmol, 0.400 M) was added in one portion. The tube was shaken to ensure proper mixing and then inserted into an NMR instrument pre-cooled at -10 °C.

VII. Effect of Ligand Steric Properties on the Hydroboration of Internal Alkene 2



Experimental procedure:

In an argon-filled glove box, a 4 mL vial was charged with CuCl (2.0 mg, 10 mol %), KO*t*Bu (4.4 mg, 10 mol %), ligand (11 mol %), dodecane (20.0 μL, 0.0880 mmol), and cyclohexane (160 μL). The mixture was allowed to stir at rt for 3 minutes before addition of HBpin (120 μL, 0.240 mmol) as a solution in cyclohexane (2.00 M). Alkene **2** (100 μL, 0.200 mmol) as a solution in cyclohexane (2.00 M) was added to the vial to initiate the reaction. At various time points, aliquots were removed from the mixture and analyzed by gas chromatography.

VIII. Computational Details

General Remarks

DFT calculations were conducted at the Molecular Graphics and Computation Facility at the University of California, Berkeley. Unless otherwise noted, geometry optimizations were performed with the B3LYP functional with Gaussian 09 revision D01 package. SDD and 6-31G(d) basis sets were used for Cu and all other atoms, respectively. Single-point energies were calculated with the M06 functional. SDD and 6-311+G(d,p) basis sets were used for Cu and all other atoms, respectively. The SMD model was used for solvent corrections. Frequency calculations were also conducted with the optimized geometries to confirm that the stationary points were minima (zero imaginary frequencies) or transition states (one imaginary frequency). IRC calculations were conducted for important transition states to ensure that those are linked to proper starting materials and products. The structures were generated using CYLView.

Summary of electronic energies of all computed structures

Electronic energies of all computed structures are summarized in Table S4 and Table S5, which include zero-point energies, enthalpies, free energies, thermal corrections to enthalpies, and free energies, and single-point energies corrected with the SMD model. Imaginary frequencies are also included for all the transition states.

Table S4. Summary of electronic energies of calculated structures with DTBM-SEGPHOS as the ligand[a]

	E	H	G	H_{corr}	G_{corr}	E(SMD)	imaginary frequency
8	-4360.796451	-4360.701812	-4360.931044	1.698341	1.469109	-4360.917267	-
13-TS	-4670.281882	-4670.180113	-4670.422261	1.841272	1.599123	-4670.399011	-799.27
13'-TS	-4670.278835	-4670.177491	-4670.419211	1.841579	1.599858	-4670.394369	-750.35
13-l-TS	-4670.275714	-4670.173983	-4670.418862	1.840728	1.59585	-4670.388258	-818.52
14	-4670.324731	-4670.222436	-4670.468488	1.846479	1.600427	-4670.439344	-
14'	-4670.326699	-4670.224496	-4670.469802	1.846591	1.601285	-4670.443523	-
14-l	-4670.321417	-4670.219067	-4670.467989	1.846312	1.59739	-4670.429488	-
20-TS	-5081.961915	-5081.850075	-5082.110248	2.049762	1.789589	-5082.15288	-190.50
20'-TS	-5081.960773	-5081.848873	-5082.109191	2.049765	1.789447	-5082.158224	-180.48
20-l-TS	-5081.981417	-5081.86902	-5082.134474	2.048864	1.783409	-5082.157628	-208.06
21	-721.231672	-721.213494	-721.277035	0.34824	0.2847	-721.2403754	-
22	-721.232787	-721.214646	-721.279728	0.348148	0.283066	-721.2410909	-
15	-4772.479959	-4772.375084	-4772.623574	1.903874	1.655384	-4772.661129	-
23-TS	-4517.876509	-4517.776304	-4518.014518	1.814634	1.576419	-4518.041636	-831.92
24	-4517.919045	-4517.818422	-4518.060841	1.819978	1.577559	-4518.078461	-
25-TS	-4929.570483	-4929.459973	-4929.717952	2.023146	1.765167	-4929.803601	-172.13
26	-568.831615	-568.815135	-568.874067	0.321916	0.262984	-568.8934795	-
styrene	-309.514545	-309.50683	-309.546034	0.141426	0.102221	-309.4764362	-
HBpin	-411.679090	-411.668611	-411.712239	0.201943	0.158315	-411.7145532	-

***trans*-2-butene**	-157.118418	-157.112008	-157.145812	0.114902	0.081098	-157.1334841	-
23-TS-l-propene	-4478.594876	-4478.496221	-4478.731915	1.784950	1.549256	-4478.749606	-813.05
23-TS-b-propene	-4478.589200	-4478.490448	-4478.725601	1.784931	1.549778	-4478.743765	-875.81
propene	-117.827483	-117.822462	-117.852487	0.085096	0.055071	-117.8370391	-

[a]Single-point energies were corrected with a SMD solvation model in cyclohexane. Unit for electronic energies is Hartree and unit for imaginary frequencies is cm^{-1}.

Table S5. Summary of electronic energies of calculated structures with SEGPHOS as the ligand[a]

	E	H	G	H_{corr}	G_{corr}	E(SMD)	imaginary frequency
27	-5291.684149	-5291.603489	-5291.810347	1.217493	1.010634	-5291.378189	-
28	-2645.823365	-2645.782873	-2645.900886	0.607512	0.489498	-2645.654729	-
S5	-2955.325625	-2955.277612	-2955.409939	0.751232	0.618905	-2955.14507	-
S5'	-2955.326595	-2955.278241	-2955.414257	0.750873	0.614858	-2955.144292	-
S5-l	-2955.326679	-2955.278583	-2955.412423	0.751204	0.617363	-2955.143919	-
S6-TS	-2955.312904	-2955.265501	-2955.3966	0.75001	0.618912	-2955.130816	-787.93
S6'-TS	-2955.30677	-2955.259436	-2955.39123	0.749753	0.617959	-2955.123711	-815.54
S6-l-TS	-2955.313142	-2955.26571	-2955.396762	0.749987	0.618935	-2955.132772	-798.63
S7	-2955.35829	-2955.310042	-2955.445584	0.755394	0.619852	-2955.179482	-
S7'	-2955.359419	-2955.311239	-2955.446427	0.7554	0.620212	-2955.180165	-
S7-l	-2955.352659	-2955.304389	-2955.443072	0.755283	0.6166	-2955.168173	-
S8	-3153.342198	-3153.291497	-3153.434603	0.76621	0.623104	-3153.198648	-
S9-TS	-3367.002312	-3366.944357	-3367.096598	0.958639	0.806398	-3366.886016	-164.79
S9'-TS	-3367.006751	-3366.948726	-3367.101042	0.958534	0.806218	-3366.891109	-158.35
S9-l-TS	-3367.011039	-3366.952817	-3367.109113	0.957969	0.801674	-3366.886668	-201.55
21	-721.231672	-721.213494	-721.277035	0.34824	0.2847	-721.2422951	-
22	-721.232787	-721.214646	-721.279728	0.348148	0.283066	-721.2431329	-
styrene	-309.514545	-309.50683	-309.546034	0.141426	0.102221	-309.4772266	-
HBpin	-411.67909	-411.668611	-411.712239	0.201943	0.158315	-411.7113404	-
SEGPHOS	-2447.894759	-2447.85676	-2447.970325	0.597463	0.483898	-2447.646735	-

[a]Single-point energies were corrected with a SMD solvation model in toluene. Unit for electronic energies is Hartree and unit for imaginary frequencies is cm^{-1}.

DFT Study on the Structure of Complex 27

Various DFT functionals were examined to reproduce the structure of complex **27** determined by single-crystal X-ray diffraction. The calculations were performed with Gaussian 09 revision D01 package. In all cases, SDD and 6-31G(d) basis sets were used for Cu and all other atoms, respectively. The results are summarized in Table S6. Calculations with PBE and BP86 as the functionals provided the most consistent results for the Cu-Cu bond

length and averaged P-Cu-P bond angle, but the calculated dihedral angle of the ligand deviated from that determined by the x-ray study. A small difference was observed between the Cu-Cu bond length and P-Cu-P bond angles determined by x-ray and those calculated with B3LYP-D3 and M06 functionals, but good agreement between the dihedral angle of the ligand from X-ray and calculations with B3LYP-D3 and M06 functionals. Calculations with all the functionals showed that the copper center adopts a tetrahedral geometry with a Cu-H bond length of 1.73(1) Å.

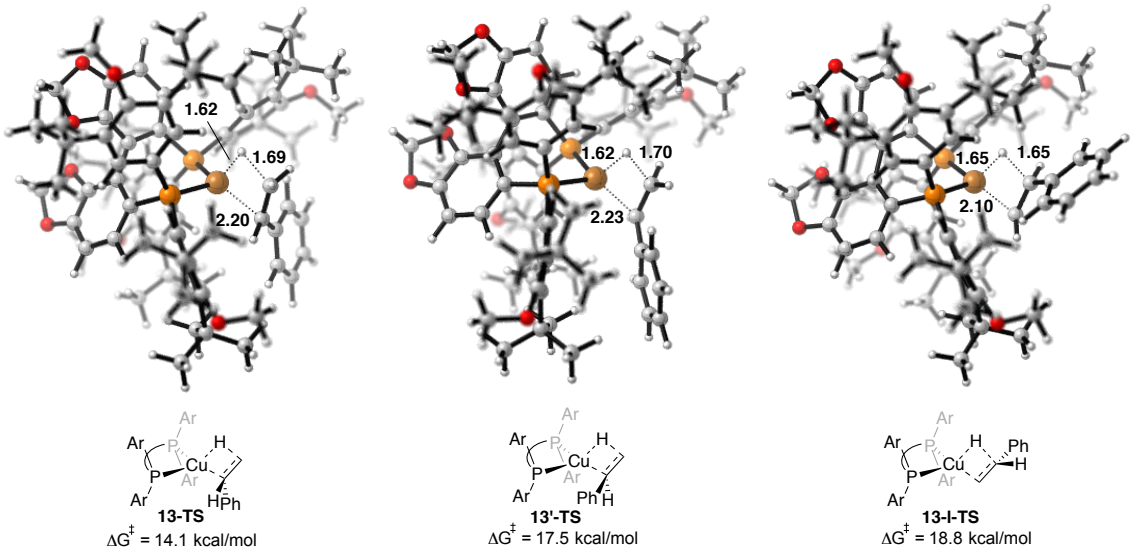
Table S6. DFT calculation results for complex **27**

DFT functional	Cu-Cu (Å)	averaged P-Cu-P (°)	averaged ligand dihedral angle (°)	Averaged Cu-H (Å)	Geometry at copper center
x-ray structure	2.374	101.4	80.0	-	-
B3LYP-D3	2.324	102.6	79.4	1.73	tetrahedral
M06	2.343	102.4	79.9	1.74	tetrahedral
PBE	2.387	101.3	77.0	1.73	tetrahedral
BP86	2.390	100.9	76.6	1.73	tetrahedral

Structures of key transition states and intermediates for the hydroboration with (*S*)-DTBM-SEGPHOS

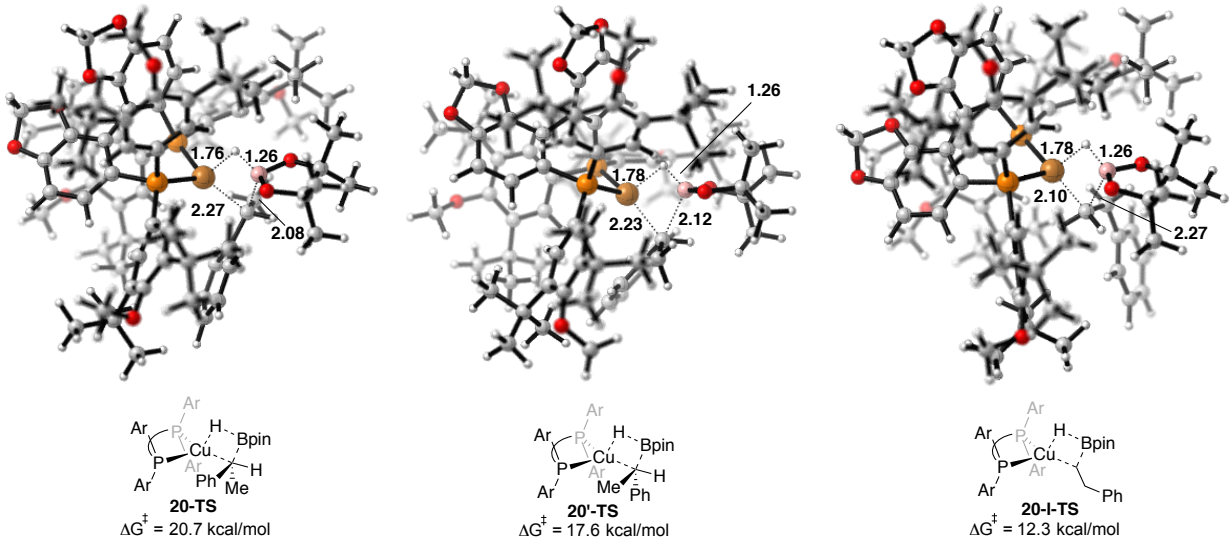
The structures of transition states **13-TS**, **13'-TS**, and **13-l-TS** for alkene insertion into the copper hydride **8** computed at the M06/6-311+g(d,p)/SDD//B3LYP/6-31g(d)/SDD level of theory are shown in Figure S11.

Figure S11. Computed structures of **13-TS**, **13'-TS**, **13-l-TS**



The structures of transition states for the borylation of **20-TS**, **20'-TS**, and **20-l-TS** computed at the M06/6-311+g(d,p)/SDD//B3LYP/6-31g(d)/SDD level of theory are shown in Figure S12.

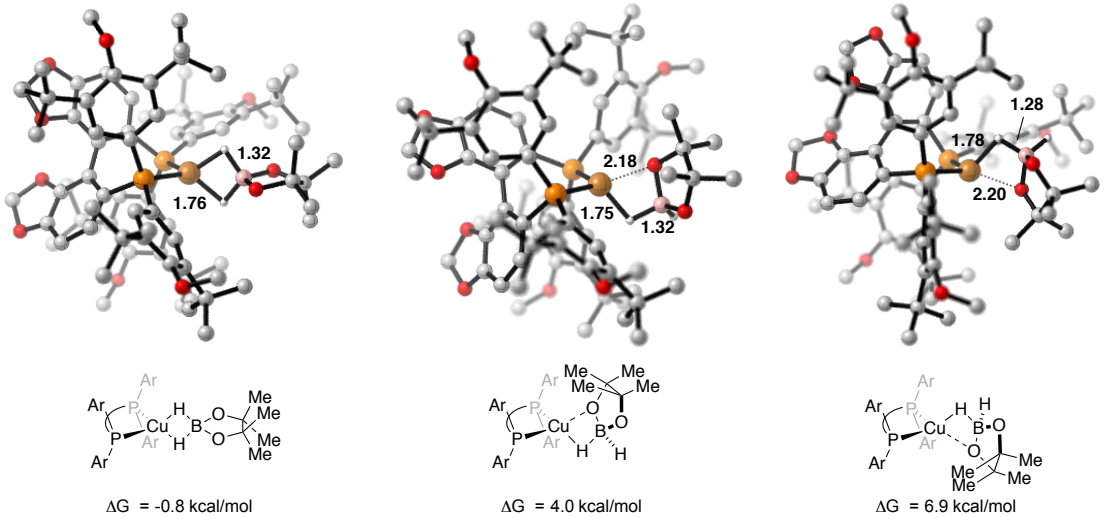
Figure S12. Computed structures of **20a-TS**, **20b-TS**, **20c-TS**



Evaluation of possible structures of 15

We computed several different structures of dihydridoborate **15**. The structures of a κ^2-dihydridoborate with two bridging hydrides, and the structures of two κ^2-dihydridoborates with only one bridging hydride were calculated. As illustrated in Figure S13, the structure with two bridging hydrides is clearly more stable than the structures with only one bridging hydride.

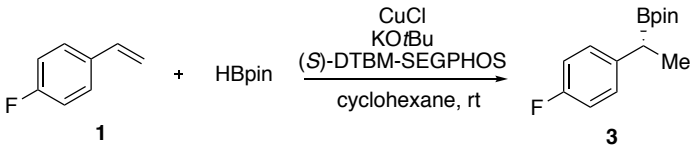
Figure S13. Evaluation of possible structures of **15**[a]



[a]Single-point energies were corrected with a SMD solvation model in cyclohexane and relative to sum of **8** and HBpin.

IX. Hydroboration of Vinylarene 1

Procedure for the hydroboration of 1 catalyzed by Cu/DTBM-SEGPHOS



1 **3**

In an argon-filled dry box, a 1-dram vial was charged with CuCl (2.0 mg, 2 mol %), KO*t*Bu (4.4 mg, 4 mol %), (*S*)-DTBM-SEGPHOS (26.4 mg, 2.2 mol %) and cyclohexane (200 μL). The mixture was allowed to stir at ambient temperature for 3 minutes before the addition of pinacolborane (152 μL, 1.05 mmol, 1.05 equiv). After brief stirring (30 – 60 seconds), the solution was added the alkene (119 μL, 1.00 mmol, 1 equiv) and cyclohexane (800 μL). The vial was then capped, sealed with electrical tape, and removed from the drybox. After 4 h of stirring at rt, the reaction vial was diluted with 2 mL of ethyl acetate, and the resulting solution was filtered through Celite. The crude material was concentrated *in vacuo* and purified by flash column chromatography (CombiFlash, 5% ethyl acetate in hexanes) to afford the product in 83% yield (208.0 mg, 0.832 mmol).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.21 – 7.11 (m, 2H), 7.01 – 6.86 (m, 2H), 2.41 (q, J = 7.5 Hz, 1H), 1.31 (d, J = 7.5 Hz, 3H), 1.21 (s, 6H), 1.20 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 160.82 (d, $J_{C\text{-}F}$ = 242.6 Hz), 140.48 (d, $J_{C\text{-}F}$ = 2.9 Hz) 128.96 (d, $J_{C\text{-}F}$ = 7.6 Hz) 114.91 (d, $J_{C\text{-}F}$ = 21.0 Hz), 83.30, 24.56, 24.52, 17.19 (the benzylic carbon was not detected because of the rapid relaxation of the bound boron atom).

^{19}F NMR (192 MHz, $CDCl_3$) δ 33.5.

^{11}B NMR (564 MHz, $CDCl_3$) δ -120.0.

The compound was reported previously. Our data are a corrected version of the published data. Our data include ^{13}C-^{19}F coupling.[6]

Procedures for the hydroboration of 1 reported in Scheme 2

The reactions were conducted following the above procedure, but with a slight alteration outlined by the following conditions.

Condition A in Scheme 2: **1** (48.0 μL, 0.400 mmol), HBPin (64.0 μL, 0.440 mmol, 1.1 equiv), CuCl (2.0 mg, 5 mol %), KO*t*Bu (4.4 mg, 10 mol %), and (*S*)-DTBM-SEGPHOS (26.4 mg, 5.5 mol %), cyclohexane (400 μL), 54 h.

Condition B in Scheme 2: **1** (60.0 μL, 0.500 mmol), HBPin (76.0 μL, 0.525 mmol, 1.05 equiv), CuCl (1.0 mg, 2 mol %), KO*t*Bu (2.2 mg, 4 mol %), and (*S*)-DTBM-SEGPHOS (13.2 mg, 4.4 mol %), cyclohexane (500 μL), 4 h.

Yields were determined by GC using dodecane as an internal standard.

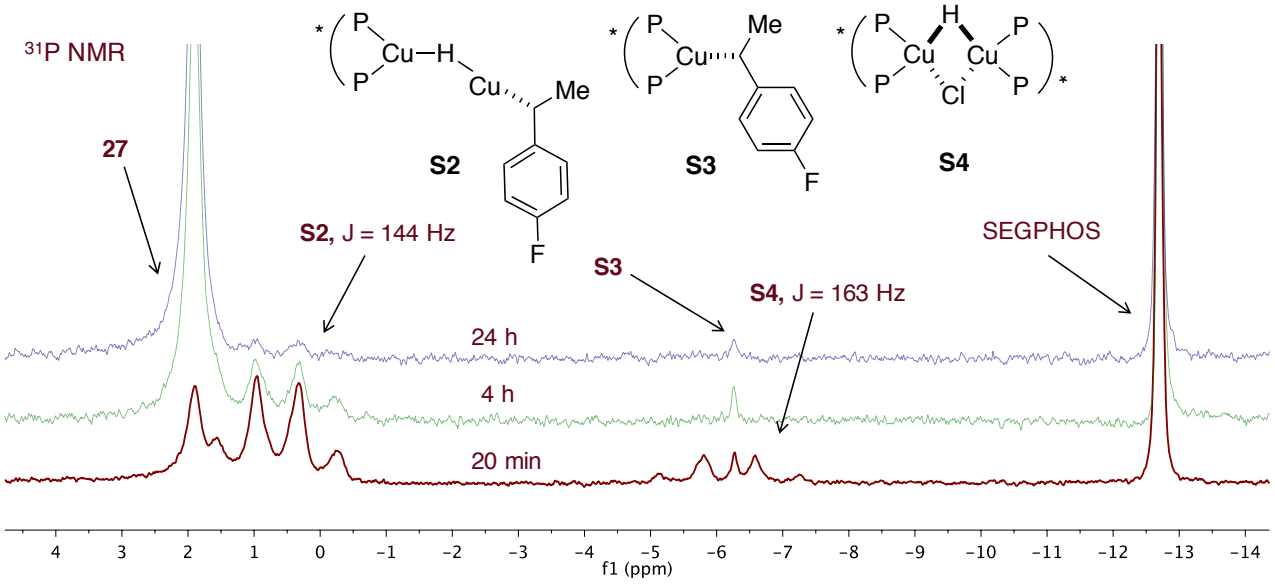
Enantioselectivity was determined by HPLC analysis after oxidation of the boronate by H_2O_2/NaOH.

HPLC conditions: OB-H, 5% IPA/hexanes, 0.5 mL/min, 210 nm; t_R (major) = 18.8 min, t_R (minor) = 17.0 min.

X. Study of the Hydroboration of Vinylarene 1 Catalyzed by Cu/(*S*)-SEGPHOS

Experimental studies. Monitoring a hydroboration reaction of **1** with HBpin in toluene at rt by ^{31}P NMR spectroscopy revealed five species at the early stage of the reaction. Based on the ^{31}P NMR chemical shift, a sharp singlet at -12.7 ppm was assigned to the free ligand (*S*)-SEGPHOS. Two sets of AB-quartets were observed (1.2 ppm and 0.1 ppm for **S2**; -5.6 ppm and -6.8 ppm for **S4**), respectively, due to ^{31}P-^{31}P coupling ($J_{P\text{-}P}$ = 144.3, 163.0 Hz, respectively) from two inequivalent phosphorus nuclei. Additionally, a sharp singlet and a broad singlet were observed at -6.3 ppm (**S3**) and 1.9 ppm (**27**), respectively. As the reaction progressed, the two AB-quartets decayed, and the broad signal at 1.9 ppm accumulated. Monitoring of the reaction by ^{19}F NMR spectroscopy revealed multiple resonances with distinct upfield chemical shifts (relative to those of **1** and **3**), which likely belong to phenethylcopper species.

Figure S14. Representative ^{31}P NMR spectra of the reaction of **1** with HBpin catalyzed by a combination of CuCl, KO*t*Bu, and (*S*)-SEGPHOS



Compound **S4** was generated independently by treating [(*S*)-SEGPHOSCuCl]$_2$ with one equivalent of sodium triethylborohydride (Figure S15). The chemical shifts of its NMR spectra match those observed during the reactions. We assigned a quintet at 2.93 ppm with a coupling constant of 10 Hz in the ^{1}H NMR spectrum as a hydride resonance. With ^{31}P decoupling, the quintet converted into a singlet, suggesting that the proton has ^{1}H-^{31}P coupling to four phosphorus nuclei. We proposed that complex **S4** is a dinuclear copper complex with one bridging hydrideand one bridging chloride.

Figure S15. Synthesis and NMR spectra of **S4**

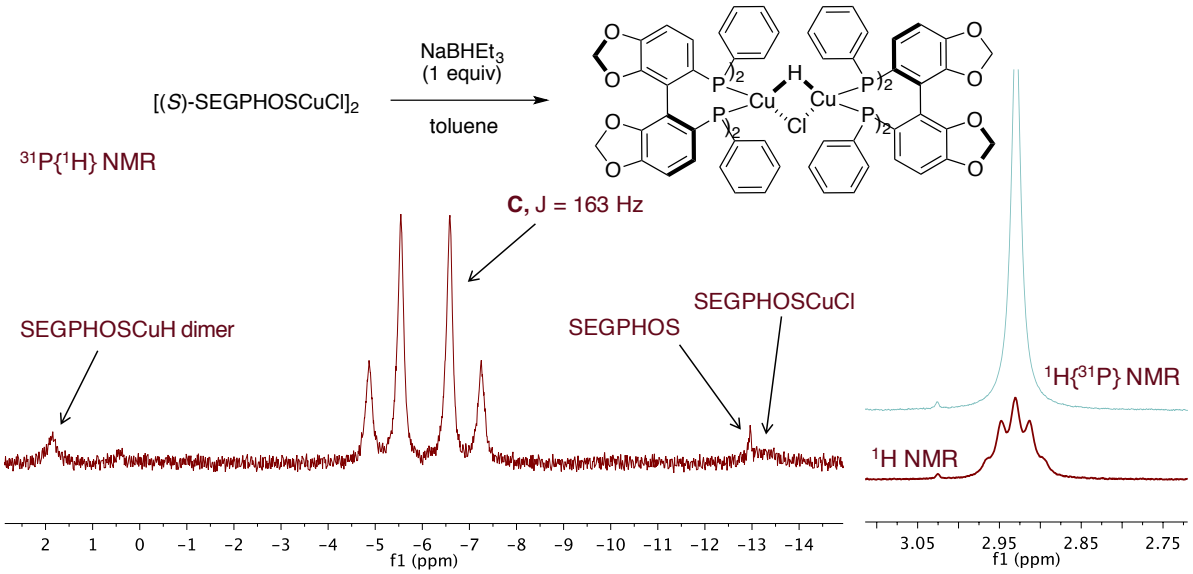
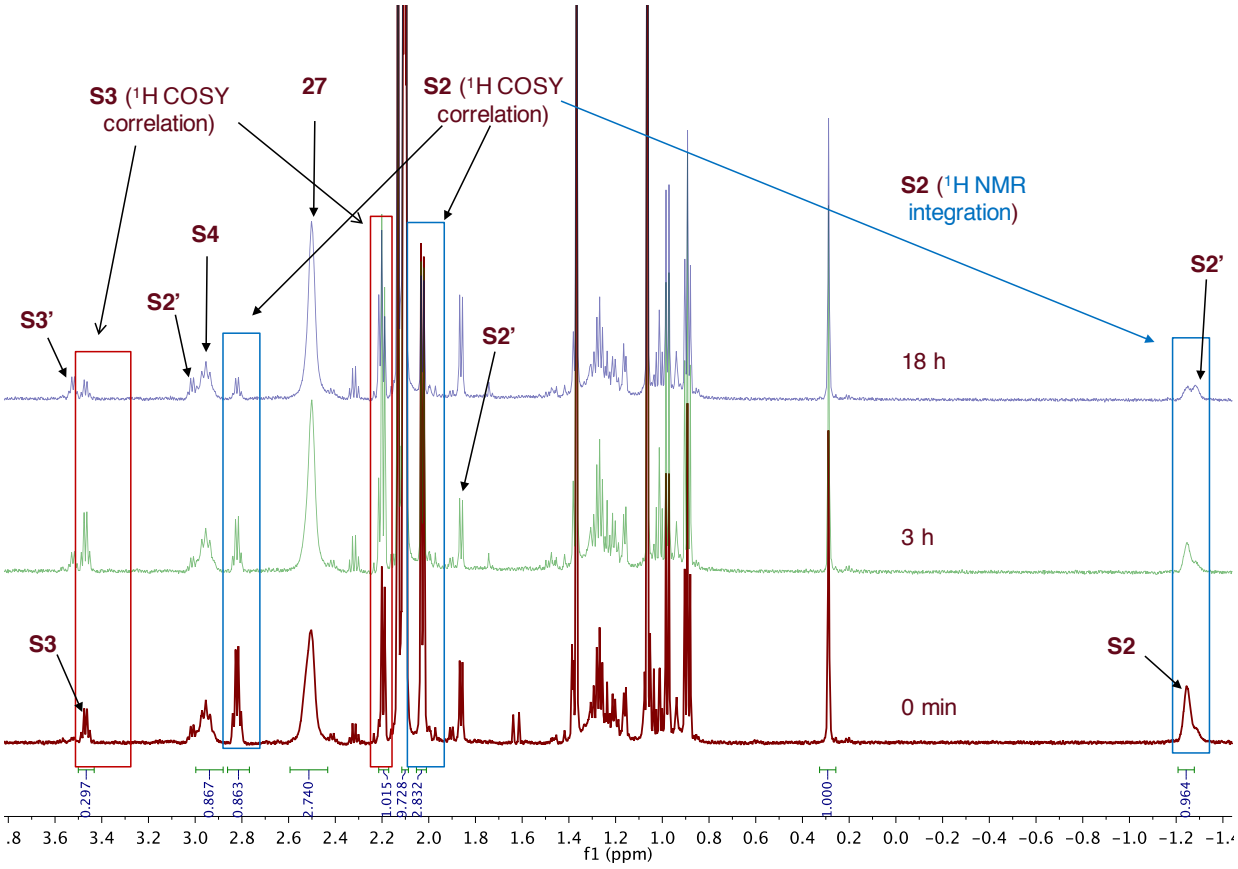


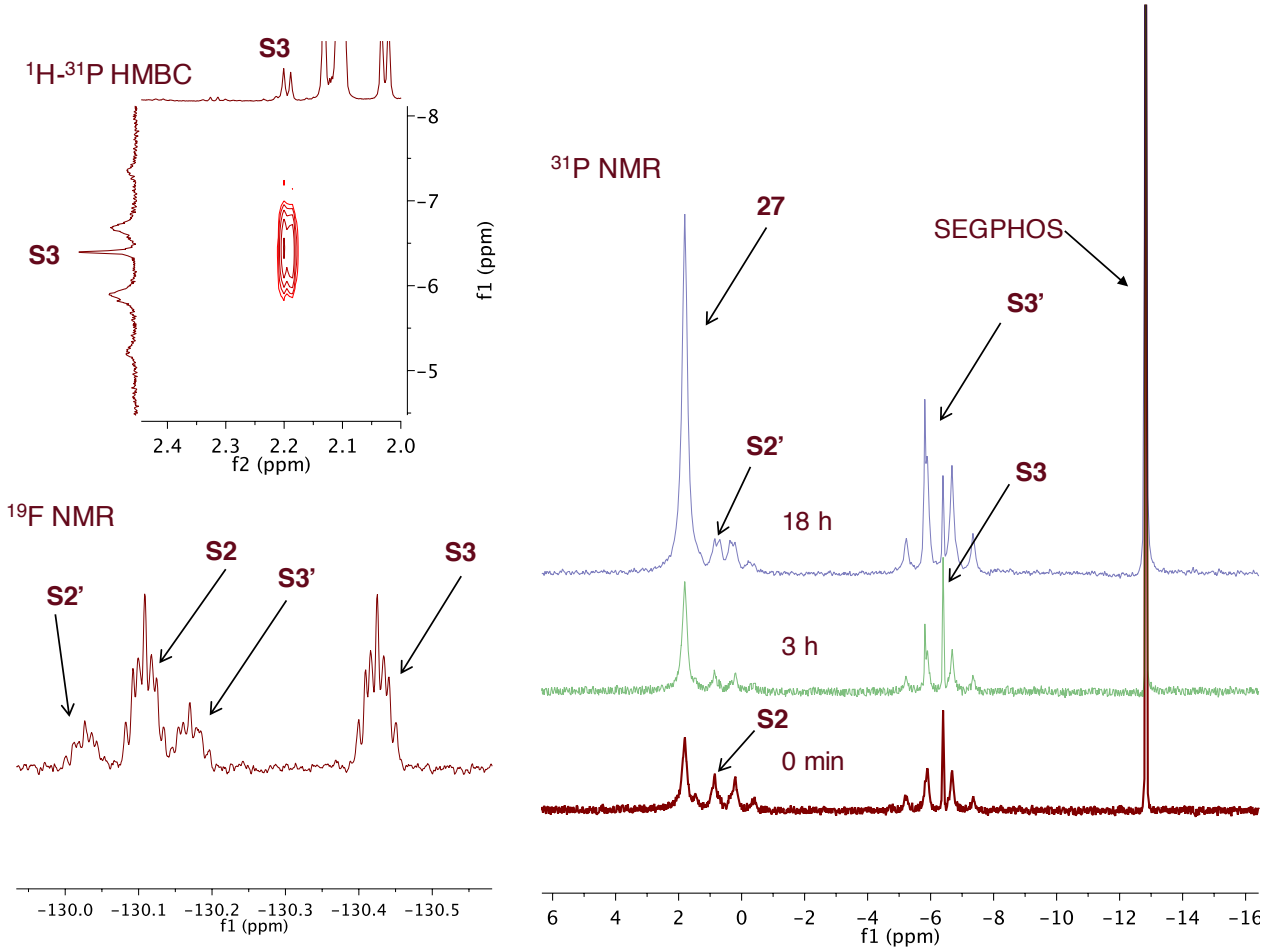
Figure S16. NMR spectra of the crude reaction mixture taken at different time points



Compounds **S2/S2'** and **S3/S3'** were characterized from a reaction mixture obtained after removing the reactants and the products by vacuum and trituration (Figures S16 and S17).

The ^{1}H COSY NMR spectrum of this mixture contained crosspeaks between a quartet at 3.47 ppm and a doublet at 2.20 ppm, which is characteristic of a $CHCH_3$ moiety. An ^{1}H-^{31}P HMBC NMR experiment confirmed a correlation between the doublet at 2.20 ppm in the proton NMR spectrum and a singlet at -6.3 ppm in the ^{31}P NMR spectrum (**S3**). The ^{31}P NMR chemical shift of **24** is close to the singlet resonance due to **5**. We were able to assign an ^{19}F signal at -130.4 ppm to **S3**. Thus, compound **S3** is likely a mononuclear phenethylcopper complex. In addition, the ^{31}P NMR signal at -6.3 ppm was converted to a singlet at -5.7 ppm slowly over 18 hours. ^{1}H NMR spectrum showed concomitant conversion of the quartet at 3.47 ppm and the doublet at 2.20 ppm to a new quartet at 3.52 ppm and a new doublet at 2.21 ppm. This conversion is presumably due to isomerization of **S3** to its diastereomer **S3'**.

Figure S17. NMR spectra of a crude reaction mixture taken at different time points



The identity of **S2/S2'** was challenging to determine. In the ^{1}H NMR spectrum, we found a characteristic resonance at -1.25 ppm, which likely belonged to a bridging hydride moiety.[7,8] Over time, this hydride

resonance was converted to the hydride signal of **27**. We also observed a concomitant decrease in the intensity of a quartet at 2.82 ppm and a doublet at 2.03 ppm during this time. The decrease in ^{1}H NMR integration of the hydride resonance at -1.25 ppm matched that of the quartet at 2.82 ppm and the doublet at 2.03 ppm. Although a ^{1}H COSY NMR spectrum of the mixture did not show any crosspeak for the hydride signal at -1.25 ppm and the quartet or the doublet, it did show that the quartet and the doublet were coupled to each other, indicating the presence of a $CHCH_3$ moiety. We assigned an ^{19}F signal at -130.1 ppm to **S2** based on how the peak intensity changed over time. Taken together, these observations lead us to propose that **S2** contains a hydride and a phenethyl moiety. DFT calculation of the minimum structure of a dinuclear copper complex starting with a bridging hydride and a bridging phenethyl moiety yielded a structure shown in Figure S14, which contains two copper atoms but only one SEGPHOS ligand. Although the structure obtained from DFT calculation was unusual, it did match the NMR spectral data. The ^{31}P NMR spectrum contained an AB-quartet of chemical shifts at 1.2 ppm and 0.1 ppm, which are close to those of **27**, consistent with the proposal that **S2** contains a fragment of SEGPHOSCuH.[9]

Despite the absence of definitive structural assignments of **S2/S2'** and **S3/S3'**, the observation of discrete ^{19}F NMR signals upfield to those of **1** and **3** suggests that phenethylcopper complexes were present at early stages of the reaction.

Procedure for characterization of crude reaction mixture

In an argon-filled glove box, a 4 mL vial was charged with CuCl (8.0 mg, 20 mol %), KO*t*Bu (17.6 mg, 40 mol %), (*S*)-SEGPHOS (48.8 mg, 22 mol %), and toluene (500 μL). The mixture was allowed to stir for 5 minutes before addition of HBpin (61.0 μL, 0.420 mmol). Alkene **1** (48.0 μL, 0.400 mmol) was then added. After 5 minutes, the mixture was passed through a syringe filter and concentrated. The non-volatile materials were triturated three times with pentane. The resulting yellow solids were dried under vacuum. A toluene-d_8 solution was analyzed by NMR spectroscopy at different time points.

DFT Computational Studies. Because of the presence of multiple copper species in different forms, we investigated the hydroboration further by DFT computations. The full free energy surface was depicted in Scheme S2, which is similar to that calculated with DTBM-SEGPHOS as the ligand. The red pathway represents the reaction coordinate for formation of (*R*)-**21**, which is the major product of the reaction. The turnover-limiting step is predicted to be the borylation, which is consistent with the observation of several phenethylcopper complexes at the early stage of the reaction.

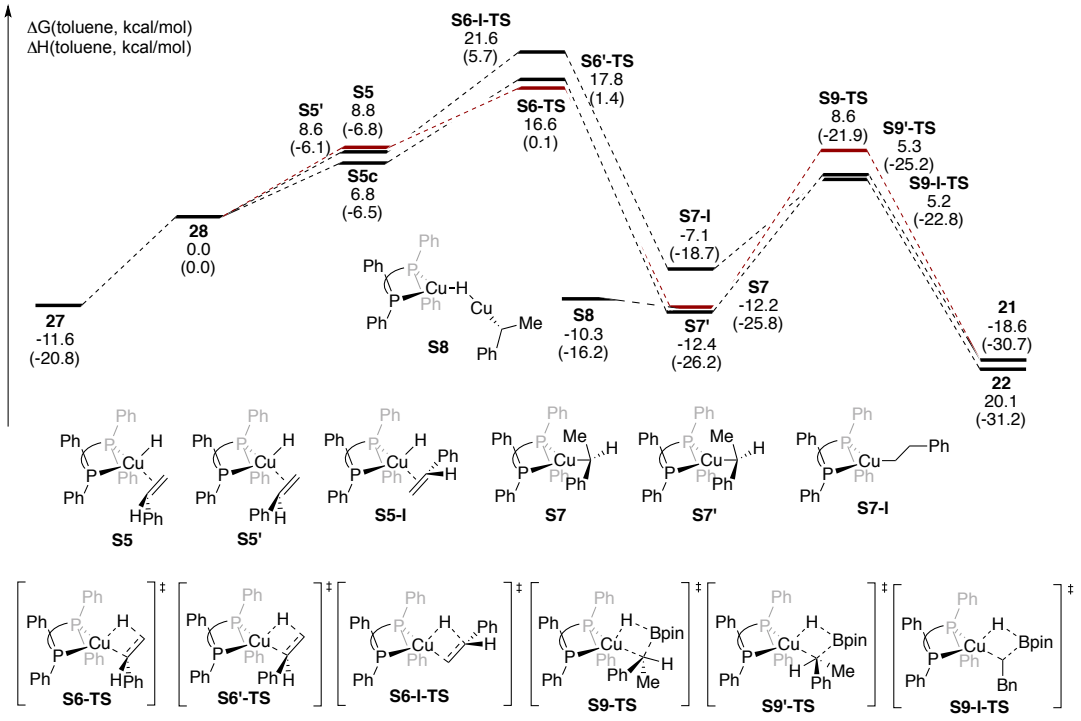
We evaluated a series of on-cycle and off-cycle intermediates and transition states, and their energy was assessed. From our results, the formation of the dimeric copper hydride **27** from its monomeric form **28** is exergonic by 11.6 kcal/mol in toluene and is also exothermic (20.8 kcal/mol). These computations suggests that the equilibrium lies far towards the dimeric form, and a monomeric copper hydride does not exist in an appreciable amount in solution.

Insertion of styrene by **28** gives rise to phenethylcopper intermediate **S7**, which requires an activation free

energy of 16.6 kcal/mol. This activation barrier is lower than that for the borylation (20.8 kcal/mol) step, and these relative rates are consistent with the observation of several phenethylcopper complexes at the early stage of the reaction.

In addition, the energy of the proposed heterodinuclear copper species **S8**, an analog of **S2**, was assessed. Formation of **S8** from **28** is favored by -10.3 kcal/mol. This value is close to but slightly less negative than that for the formation of **S7**. Because **S2** was observed as a major copper species at the early stage of the reaction, it is likely that the formation of **S8a** is kinetically more favorable than the direct insertion of styrene by **28** to form **S7**. However, the pathway that leads to the formation of **3** remains elusive. One possibility involves dissociation of one molecule of SEGPHOS from **27**, followed by rapid insertion of styrene by a transient LCuHCuH[9] species.

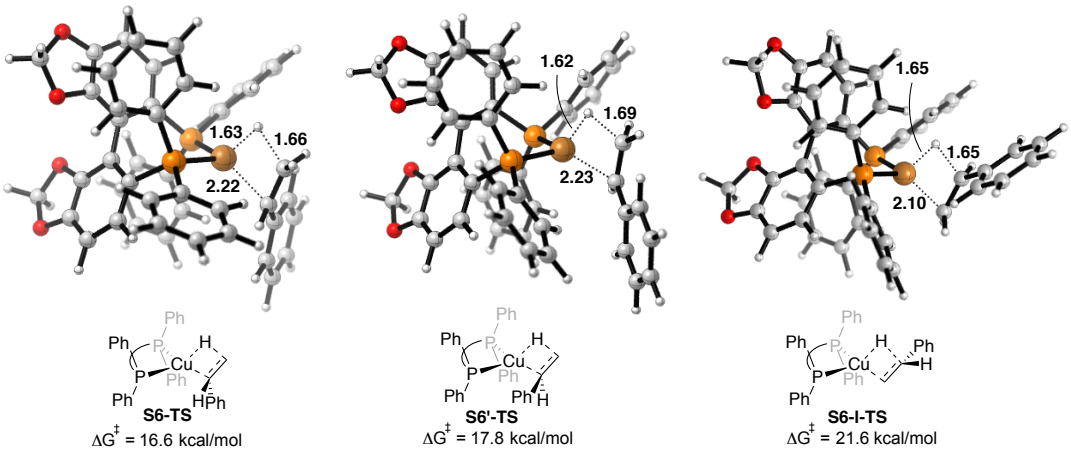
Scheme S2. Computed energy surface for hydroboration of styrene with (*S*)-SEGPHOS as the ligand



Analysis of key transition states and intermediates for the hydroboration of 1 with (*S*)-SEGPHOS

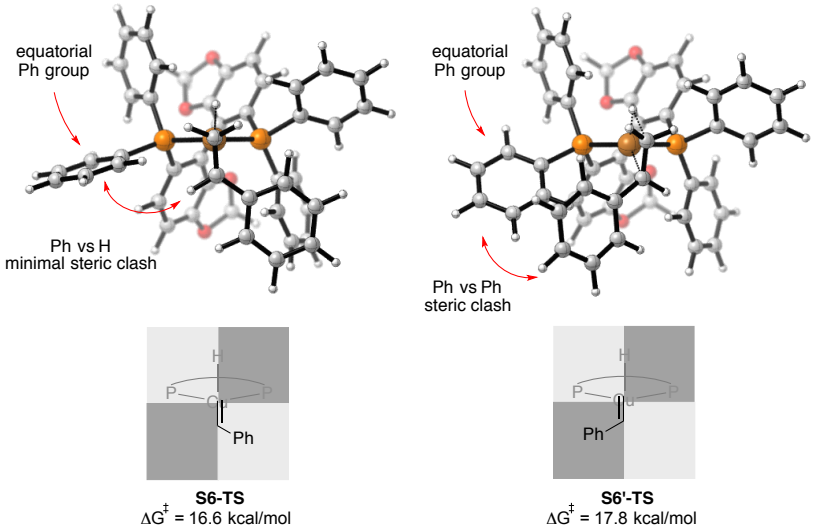
The alkene insertion occurs through a co-planar transition state, wherein the Cu-H bond is lengthened and the hydride moves closer to the terminal carbon at which the C-H bond is forming. The alkene moiety of the styrene is significantly elongated, and the four substituents on the alkene are distorted out of the plane. **S6-TS**, which leads to the major product ((*R*)-**21**), is 1.2 kcal/mol more stable than **S6'-TS**, which leads to the minor product ((*S*)-**21**). This calculated energy difference (predicted 77% ee) matches well with the ee value measured experimentally (78% ee). **S6-I-TS**, which leads to the linear product **22**, is less stable than **S6-TS** and **S6'-TS** by several kcal/mol. This result is also consistent with the fact that **22** was not detected in the reaction.

Figure S18. Structures of transition states for alkene insertion **S6-TS**, **S6'-TS**, and **S6-l-TS**



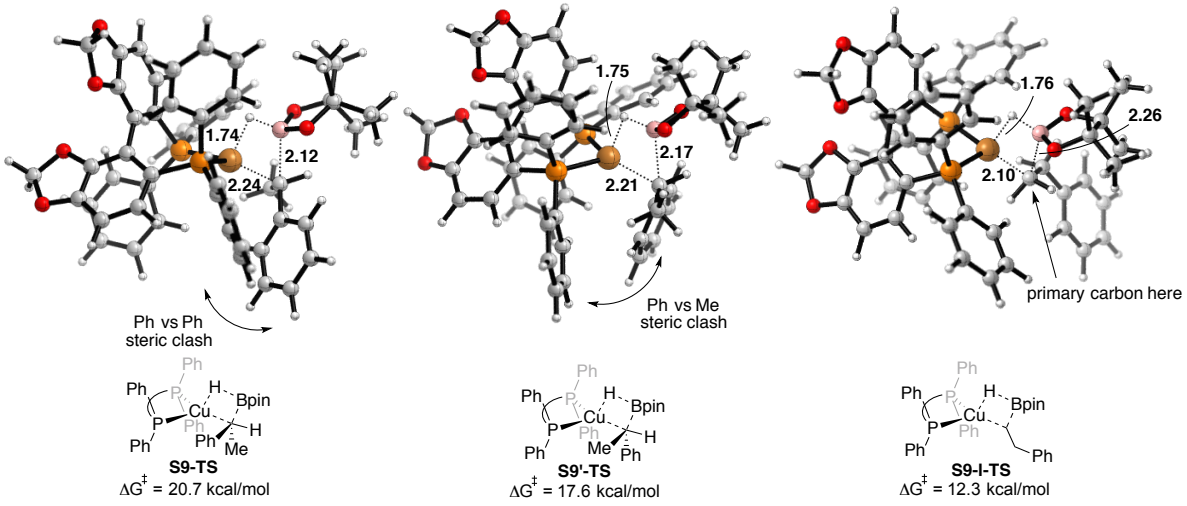
Similar to the interactions in **13-TS** and **13'-TS**, the interactions in transition states **S6-TS** and **S6'-TS** could be analyzed by quadrant diagrams. The different steric environments of the four-membered insertion transition states lead to the energy difference, and therefore the observed enantioselectivity.

Figure S19. Origin of enantioselectivity explained by structural analysis of **S6-TS** and **S6'-TS**



Structures of the borylation transition states **S9-TS**, **S9'-TS**, and **S9-l-TS** are shown in Figure S20. The activation barrier for **S8** to **S9-TS** is 3.1 kcal/mol higher than that for **S8'** to **S9'-TS**. This is due to steric interaction between the equatorial phenyl group of the ligand and the phenyl group of the phenethyl fragment in **S9-TS**. This interaction is lower in **S9'-TS** because the methyl group of the phenethyl fragment is close to the equatorial phenyl group in **S9'-TS**. The computed barrier for borylation of a primary alkyl copper species is much lower than that for borylation of phenethylcopper complexes.

Figure S20. Structures and analysis of transition states for alkene insertion **S9-TS**, **S9'-TS**, and **S9-l-TS**



The mechanism of the borylation step was investigated by DFT calculations. The borylation could occur by two possible mechanisms: a one-step σ-bond metathesis, which was proposed by Yun, or a two-step pathway involving oxidative addition of the H-B bond of HBpin and C-B bond-forming reductive elimination. Both mechanisms were probed by DFT calculations. The activation free energy we computed for the σ-bond metathesis mechanism is approximately 20 kcal/mol for **S8**. In contrast, we were unable to locate stationary points for a hydridoborylcopper(III) intermediate that would result from oxidative addition of the borane, suggesting that the hydridoborylcopper(III) intermediate likely lies far uphill on the free energy surface. Thus, the borylation step occurs by a σ-bond metathesis mechanism.

DFT calculations provide insights into why the activity of the catalyst ligated by (*S*)-SEGPHOS is low. The formation of dimeric copper hydride (**27**) from the active monomeric copper hydride is thermodynamically favored. With **27** as the starting point of the reaction, the activation barrier for the alkene insertion, as well as the overall reaction, was computed to be 28.2 kcal/mol. This high barrier is consistent with the slow rate of reactions initiated with **27** as catalyst and concomitant sharp reduction in the rate of reactions catalyzed by the species generated in situ and observation of **27** as the dominant copper species at the late stage of the reaction. These results imply that catalysts ligated by bulky ligands are likely to be more reactive than catalysts ligated by small ligands because of the absence of dinuclear hydride complexes in reactions catalyzed by complexes with bulky ligands.

XI. Crystallographic Information

Complex 6

A colorless prism 0.060 x 0.050 x 0.030 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K. The crystal-to-detector distance was 40 mm, and the exposure time was 60 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 25.000° in θ. A total of 54649 reflections were collected, covering the indices, -16<=*h*<=16, -27<=*k*<=27, -35<=*l*<=35. 17071 reflections were found to be symmetry independent, with an R_{int} of 0.0630. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be $P2_12_12_1$ (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

Table S7. Crystal data and structure refinement for **6**.

Empirical formula	$C_{74}H_{100}ClCuO_8P_2$	
Formula weight	1278.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 13.8472(11) Å	α = 90°
	b = 23.0453(15) Å	β = 90°
	c = 29.284(2) Å	γ = 90°
Volume	9344.8(12) $Å^3$	
Z	4	
Density (calculated)	0.909 Mg/m^3	
Absorption coefficient	0.336 mm^{-1}	
F(000)	2736	
Crystal size	0.060 x 0.050 x 0.030 mm^3	
Theta range for data collection	1.391 to 25.381°.	
Index ranges	-16<=h<=16, -27<=k<=27, -35<=l<=35	
Reflections collected	54649	
Independent reflections	17071 [R(int) = 0.0630]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.928 and 0.844	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17071 / 0 / 803
Goodness-of-fit on F2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0718, wR2 = 0.1748
R indices (all data)	R1 = 0.0971, wR2 = 0.1850
Absolute structure parameter	0.048(7)
Extinction coefficient	n/a
Largest diff. peak and hole	0.537 and -0.387 e.$Å^{-3}$

Complex 7•$C_6H_{18}OSi_2$

A yellow prism 0.100 x 0.080 x 0.060 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K. Crystal-to-detector distance was 40 mm and exposure time was 60 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 25.000° in θ. A total of 147781 reflections were collected covering the indices, -23<=*h*<=23, -31<=*k*<=28, -41<=*l*<=42. 33109 reflections were found to be symmetry independent, with an R_{int} of 0.0576. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be $P2_12_12_1$ (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

Table S8. Crystal data and structure refinement for **7•$C_6H_{18}OSi_2$**.

Empirical formula	$C_{81}H_{121}CuO_9P_2Si_2$	
Formula weight	1420.43	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 19.7038(15) Å	α = 90°
	b = 26.008(2) Å	β = 90°
	c = 35.273(3) Å	γ = 90°
Volume	18076(3) $Å^3$	
Z	8	
Density (calculated)	1.044 Mg/m^3	
Absorption coefficient	0.350 mm^{-1}	
F(000)	6128	

Crystal size	0.100 x 0.080 x 0.060 mm^3
Theta range for data collection	1.155 to 25.364°.
Index ranges	-23<=h<=23, -31<=k<=28, -41<=l<=42
Reflections collected	147781
Independent reflections	33109 [R(int) = 0.0576]
Completeness to theta = 25.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928 and 0.867
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	33109 / 0 / 1710
Goodness-of-fit on F2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0678, wR2 = 0.1711
R indices (all data)	R1 = 0.0969, wR2 = 0.1908
Absolute structure parameter	0.005(3)
Extinction coefficient	n/a
Largest diff. peak and hole	1.005 and -0.707 e.$Å^{-3}$

Complex 12'•2C_7H_8•$C_6H_{18}OSi_2$

A yellow plate 0.160 x 0.120 x 0.040 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K. Crystal-to-detector distance was 60 mm and exposure time was 20 seconds per frame using a scan width of 2.0°. Data collection was 99.8% complete to 67.000° in θ. A total of 306878 reflections were collected covering the indices, -16<=*h*<=16, -24<=*k*<=27, -34<=*l*<=34. 17588 reflections were found to be symmetry independent, with an R_{int} of 0.0963. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be $P2_12_12_1$ (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2016). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2016. Absolute stereochemistry was unambiguously determined to be *S* at C1.

Table S9. Crystal data and structure refinement for **12'•2C_7H_8•$C_6H_{18}OSi_2$**.

Empirical formula	$C_{102}H_{142}CuFO_9P_2Si_2$
Formula weight	1712.81
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic

Space group	$P2_12_12_1$	
Unit cell dimensions	a = 14.0112(9) Å	α = 90°
	b = 23.8266(17) Å	β = 90°
	c = 28.7899(19) Å	γ = 90°
Volume	9611.2(11) $Å^3$	
Z	4	
Density (calculated)	1.184 Mg/m^3	
Absorption coefficient	1.318 mm^{-1}	
F(000)	3688	
Crystal size	0.160 x 0.120 x 0.040 mm^3	
Theta range for data collection	2.407 to 68.497°.	
Index ranges	-16<=h<=16, -24<=k<=27, -34<=l<=34	
Reflections collected	306878	
Independent reflections	17588 [R(int) = 0.0963]	
Completeness to theta = 67.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.749 and 0.607	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17588 / 3 / 1006	
Goodness-of-fit on F2	1.090	
Final R indices [I>2sigma(I)]	R1 = 0.1031, wR2 = 0.2649	
R indices (all data)	R1 = 0.1089, wR2 = 0.2704	
Absolute structure parameter	0.006(17)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.081 and -0.839 e.$Å^{-3}$	

Complex 16

A colorless prism 0.050 x 0.040 x 0.030 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 2.0°. Data collection was 99.6% complete to 67.000° in θ. A total of 232804 reflections were collected covering the indices, -23<=*h*<=18, -31<=*k*<=31, -42<=*l*<=42. 32838 reflections were found to be symmetry independent, with an R_{int} of 0.0717. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be $P2_12_12_1$ (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their

parent atom using the appropriate HFIX command in SHELXL-2014.

Table S10. Crystal data and structure refinement for **16**.

Empirical formula	$C_{74}H_{104}BCuO_8P_2$	
Formula weight	1257.86	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 19.5026(11) Å	α= 90°
	b = 26.0918(16) Å	β= 90°
	c = 35.420(2) Å	γ = 90°
Volume	18023.9(19) $Å^3$	
Z	8	
Density (calculated)	0.927 Mg/m^3	
Absorption coefficient	0.995 mm^{-1}	
F(000)	5408	
Crystal size	0.050 x 0.040 x 0.030 mm^3	
Theta range for data collection	2.103 to 68.488°.	
Index ranges	-23<=h<=18, -31<=k<=31, -42<=l<=42	
Reflections collected	232804	
Independent reflections	32838 [R(int) = 0.0717]	
Completeness to theta = 67.000°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.737	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	32838 / 0 / 1605	
Goodness-of-fit on F2	1.065	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1175	
R indices (all data)	R1 = 0.0547, wR2 = 0.1229	
Absolute structure parameter	0.010(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.428 and -0.283 e.$Å^{-3}$	

Complex 27

A yellow prism 0.100 x 0.080 x 0.050 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 200(2) K. Crystal-to-detector distance was 60 mm and exposure time was 20 seconds per frame using a scan width of 2.0°. Data collection was 100.0% complete to 67.000° in θ. A total of 178733 reflections were collected covering the indices, -26<=*h*<=26, -26<=*k*<=25, -21<=*l*<=21. 15250 reflections were found to be symmetry independent, with an R_{int} of 0.0510. Indexing and unit cell refinement indicated a primitive, tetragonal lattice. The space group was found to be P4 (No. 75). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by iterative methods (SHELXT-2014) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014.

Table S11. Crystal data and structure refinement for **27**.

Empirical formula	$C_{76}H_{58}Cu_2O_8P_4$	
Formula weight	1350.18	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	P4	
Unit cell dimensions	a = 21.5938(4) Å	α = 90°
	b = 21.5938(4) Å	β = 90°
	c = 17.8485(4) Å	γ = 90°
Volume	8322.6(4) $Å^3$	
Z	4	
Density (calculated)	1.078 Mg/m^3	
Absorption coefficient	1.719 mm^{-1}	
F(000)	2784	
Crystal size	0.100 x 0.080 x 0.050 mm^3	
Theta range for data collection	2.046 to 68.402°.	
Index ranges	-26<=h<=26, -26<=k<=25, -21<=l<=21	
Reflections collected	178733	
Independent reflections	15250 [R(int) = 0.0510]	
Completeness to theta = 67.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.929 and 0.817	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	15250 / 1 / 814
Goodness-of-fit on F2	1.066
Final R indices [I>2sigma(I)]	R1 = 0.0799, wR2 = 0.2013
R indices (all data)	R1 = 0.0941, wR2 = 0.2204
Absolute structure parameter	n/a
Extinction coefficient	n/a
Largest diff. peak and hole	1.858 and -0.534 e.Å^{-3}

XII. References

1. Denmark, S. E.; Beutner, G. L. *J. Am. Chem. Soc.* **2003**, *125*, 7800.
2. Pietruszka, J.; Schöne, N. *Eur. J. Org. Chem.* **2004**, 5011.
3. Liu, Z.; Takeuchi, T.; Pluta, R.; Arteaga, F. A.; Kumagai, N.; Shibasaki, M. *Org. Lett.* **2017**, *19*, 710.
4. Derose, E. F.; Castillo, J.; Saulys, D.; Morrison, J. *J. Magn. Reson.* **1991**, *93*, 347.
5. Cobas, J. C.; Martin-Pastor, M. *EXSYCalc Ver 1.0*; Mestrelab Research S.L.: A Coruña, Spain, 2007.
6. Noh, D.; Chea, H.; Ju, J.; Yun, J. *Angew. Chem. Int. Ed.* **2009**, *48*, 6062.
7. Zall, C. M.; Linehan, J. C.; Appel, A. M. *J. Am. Chem. Soc.* **2016**, *138*, 9968.
8. Wyss, C. M.; Tate, B. K.; Bacsa, J.; Gray, T. G.; Sadighi, J. P. *Angew. Chem. Int. Ed.* **2013**, *52*, 12920.
9. Dilts, J. A.; Shriver, D. F. *J. Am. Chem. Soc.* **1969**, *91*, 4088.

XIII. Cartesian Coordinates of Computed Structures

8 [(*S*)-DTBM-SEGPHOSCuH]

Cartesian coordinates:

C	-3.10718300	1.31490200	-0.96603000
C	-2.83431700	2.10339600	-2.08901500
H	-1.82739500	2.08529400	-2.48774100
C	-3.82668100	2.85776300	-2.72488400
C	-5.14519200	2.75491400	-2.20693500
C	-5.43070800	2.09968200	-0.98379100
C	-4.38850800	1.34937500	-0.41714500
H	-4.58507000	0.76905800	0.47718900
C	-3.45543500	3.80363600	-3.89636700
C	-1.92861200	3.83339200	-4.13232400
H	-1.37992400	4.14430400	-3.23592900
H	-1.70610700	4.55996200	-4.92190100
H	-1.53516000	2.86347600	-4.45582800
C	-3.89494000	5.24671800	-3.54374700
H	-4.97346100	5.30974000	-3.38532800
H	-3.62536200	5.92902800	-4.35977000
H	-3.38906300	5.59565000	-2.63547100
C	-4.10728200	3.38044800	-5.23443800
H	-3.90708100	2.32572500	-5.45675900
H	-3.68673700	3.97757200	-6.05291500
H	-5.18569800	3.54279400	-5.23323700
C	-6.93370200	2.41596200	-3.70757200
H	-6.29593200	1.84611400	-4.39251300
H	-7.64717700	3.01115500	-4.28341900
H	-7.48199300	1.71170800	-3.07227600
C	-6.76596700	2.16288000	-0.18716100
C	-7.75960000	3.25912200	-0.63770000
H	-8.56012600	3.32639200	0.10919700
H	-8.23290700	3.05058400	-1.59719400
H	-7.27888400	4.23914000	-0.70560500
C	-7.47479100	0.78792200	-0.23277300
H	-8.39206100	0.81260300	0.36876400
H	-6.83400000	-0.00838700	0.16200700
H	-7.75326100	0.51007100	-1.25539200

C	-6.43606600	2.49542400	1.29481600
H	-5.91949700	3.45895600	1.37273800
H	-5.80997400	1.73937400	1.77631500
H	-7.36567900	2.56289200	1.87189800
C	-2.59361300	-1.27230100	0.19973200
C	-2.69841400	-2.25175900	-0.78811400
H	-2.25050000	-2.04958400	-1.75598500
C	-3.36943000	-3.46750000	-0.58006200
C	-3.84304700	-3.70650700	0.73060600
C	-3.86195800	-2.69450500	1.72967000
C	-3.21490800	-1.48900600	1.43462600
H	-3.17489200	-0.70419900	2.17876600
C	-3.55355000	-4.38955700	-1.81921200
C	-4.06860000	-3.52125700	-3.00141400
H	-4.23337600	-4.15915300	-3.87758100
H	-3.36570300	-2.73885100	-3.29860300
H	-5.02104300	-3.04209900	-2.74751800
C	-2.19434000	-5.00731600	-2.22669000
H	-2.31269000	-5.62160800	-3.12793300
H	-1.78586400	-5.64775400	-1.43684200
H	-1.45111900	-4.23244300	-2.44394400
C	-4.59723900	-5.51886800	-1.65511200
H	-5.55272600	-5.13669000	-1.28422200
H	-4.27462500	-6.31925700	-0.98899400
H	-4.77354000	-5.96971700	-2.63925000
C	-3.32722300	-5.92434600	1.35176600
H	-2.72648000	-6.14795500	0.46385000
H	-3.84822800	-6.83097300	1.67063600
H	-2.65817100	-5.58655900	2.15131100
C	-4.64266000	-2.86034700	3.05926800
C	-4.08874800	-4.00934400	3.93771200
H	-2.99805600	-3.95166400	4.02944800
H	-4.34803000	-4.98850600	3.53456200
H	-4.51823900	-3.94538200	4.94547000
C	-4.58862300	-1.57286500	3.91136000
H	-3.56717100	-1.32063000	4.21611600
H	-5.18445000	-1.72072900	4.81915400

H	-5.01082500	-0.71068600	3.38272300
C	-6.13250800	-3.13928600	2.73890400
H	-6.70235600	-3.25238300	3.67006700
H	-6.24890600	-4.05277000	2.15193400
H	-6.57165400	-2.30661900	2.17648700
C	-1.24616300	1.13484100	1.28541200
C	-1.73712900	2.42626900	1.53402700
H	-2.45603300	2.85360700	0.84580600
C	-1.35747500	3.19546100	2.64690300
H	-1.75774500	4.18921900	2.81573800
C	-0.46931300	2.60928500	3.52018800
C	0.66423500	1.98499200	5.31963300
H	-0.03588500	1.57663500	6.06409500
H	1.60972400	2.27941000	5.77589200
C	0.03659000	1.33317800	3.28811100
C	-0.28751000	0.55872000	2.18245500
C	0.30961800	-0.81428300	2.12369700
C	-0.02140100	-1.68262900	3.15526200
C	-0.65831500	-2.50903600	5.11900800
H	0.03989300	-2.16808000	5.89845300
H	-1.60570400	-2.84022200	5.54504400
C	0.48165500	-2.97513400	3.27672900
C	1.37359600	-3.48383000	2.35973200
H	1.77082700	-4.48965000	2.44183400
C	1.76051700	-2.62040800	1.32107100
H	2.48158100	-2.98715500	0.60078900
C	1.27338900	-1.31063500	1.18536300
C	3.19065500	-1.26927200	-1.02702500
C	4.44868300	-1.34779500	-0.42438000
H	4.59633600	-0.86299600	0.53406800
C	5.52635100	-2.01056400	-1.02458700
C	5.30203200	-2.56541600	-2.31320500
C	4.01725800	-2.60947200	-2.90643900
C	2.98996700	-1.91942600	-2.24436900
H	2.00746900	-1.84728500	-2.70045800
C	6.85019800	-2.07147500	-0.20908400
C	7.44140200	-0.64558100	-0.08861100

H	8.35425900	-0.66245100	0.51995700
H	6.73677800	0.05065300	0.37918100
H	7.70207500	-0.24049600	-1.07329600
C	6.52686600	-2.60296000	1.21395900
H	7.44584100	-2.64669400	1.81037700
H	6.10804800	-3.61476300	1.16483000
H	5.81602500	-1.97302800	1.75607300
C	7.95156800	-3.00523700	-0.76092600
H	8.40423100	-2.63555100	-1.68205600
H	7.57873500	-4.01514000	-0.94993100
H	8.74971900	-3.07209900	-0.01089300
C	7.02887400	-2.13004600	-3.84722900
H	6.34488900	-1.72635800	-4.60461500
H	7.84724200	-2.65844800	-4.34313500
H	7.43703300	-1.29359300	-3.26466200
C	3.62330200	-3.33987400	-4.22108000
C	4.68478600	-4.29231800	-4.81600500
H	5.05265100	-5.01192500	-4.07959300
H	5.54553500	-3.76801100	-5.23422300
H	4.21831800	-4.85353900	-5.63524600
C	3.24933100	-2.28832500	-5.29476600
H	4.10687400	-1.65014700	-5.53962400
H	2.43201700	-1.63944400	-4.96323400
H	2.93033300	-2.78896000	-6.21759400
C	2.37769800	-4.22219500	-3.93278100
H	2.07837400	-4.74593900	-4.84831700
H	1.51581100	-3.64222500	-3.59246600
H	2.60283000	-4.97715500	-3.17018000
C	2.55585700	1.21448800	0.29152800
C	3.18026300	1.36368800	1.53511700
H	3.17916100	0.52458500	2.21871400
C	3.78079600	2.56898400	1.91617900
C	3.70942500	3.65218800	0.99720900
C	3.23252800	3.49371100	-0.32420800
C	2.61069300	2.26965600	-0.61895400
H	2.16372000	2.12328200	-1.59727500
C	4.57093000	2.66584000	3.24718500

C	6.04440800	3.02709000	2.93315100
H	6.62170300	3.09241600	3.86428600
H	6.11724500	3.98627700	2.41616500
H	6.50823000	2.25751200	2.30463400
C	3.98531400	3.72298100	4.21576500
H	2.89926800	3.61584100	4.31690600
H	4.20069000	4.73890800	3.88408600
H	4.43262000	3.60136800	5.21038200
C	4.57842900	1.31678700	3.99987600
H	5.02860100	0.51468100	3.40412800
H	3.57154400	1.00084700	4.29352600
H	5.17853100	1.42003600	4.91099400
C	3.10517700	5.79010700	1.79099400
H	2.48284200	6.05068600	0.92830000
H	3.58928800	6.69359200	2.17099100
H	2.46300100	5.36374100	2.56998400
C	3.36667900	4.51398500	-1.49069500
C	1.97870200	5.09994600	-1.84480900
H	1.54855800	5.66005600	-1.00689300
H	1.26829000	4.31159600	-2.11716200
H	2.06295600	5.78500800	-2.69750700
C	3.91210900	3.76142500	-2.73682500
H	4.04014300	4.46944700	-3.56386900
H	3.24438000	2.97075200	-3.08844200
H	4.88750400	3.30967600	-2.52344700
C	4.35948500	5.67430500	-1.24616400
H	4.50791400	6.20507500	-2.19438900
H	5.33387000	5.30952900	-0.90870800
H	4.00557100	6.40700200	-0.52058500
O	-6.16876000	3.34257300	-2.93490500
O	-4.33982400	-4.95467400	1.07660200
O	0.06914200	3.11794000	4.68070300
O	0.90704300	1.00570800	4.30859600
O	-0.89639100	-1.44473900	4.19653500
O	-0.06290000	-3.58265300	4.38554800
O	6.37940300	-3.08194600	-3.01050500
O	4.15622900	4.89078700	1.43340400

P	-1.73707300	0.28187200	-0.28823000
P	1.76795000	-0.33552200	-0.31279800
Cu	-0.00154100	-0.07094500	-1.80327600
H	-0.04184100	-0.17562900	-3.35759200

13-TS

Cartesian coordinates:

P	1.66318100	-0.46775800	-0.15609000
P	-1.89024200	0.35746300	-0.10102300
O	0.55335400	-0.72523600	4.50344900
O	-0.13595400	1.19878700	5.56719000
O	-1.54429000	-2.78763900	3.42397600
O	-0.91681400	-4.94175500	2.89705400
O	-5.12216400	-4.69949000	0.30413500
O	-5.31042400	4.77404300	-2.29555100
O	4.29866700	2.71910400	4.21350200
O	5.76448400	-2.22073000	-4.16274500
C	-1.40382000	0.64603100	1.66553400
C	-0.54265000	-0.29279000	2.32229000
C	-0.22302700	0.01614200	3.63759000
C	-0.65050300	1.17052600	4.28996800
C	-1.46354000	2.08926400	3.66654300
C	-1.83784700	1.79204600	2.34472200
C	0.33660700	-0.13341800	5.78493000
C	0.93834700	-1.87517200	0.81996000
C	1.32781200	-3.19205400	0.54274100
C	0.76521800	-4.31149800	1.18042300
C	-0.19769300	-4.05247200	2.12880100
C	-0.58470400	-2.74961000	2.43332600
C	-0.07310700	-1.62239100	1.80433300
C	-1.51336000	-4.12955000	3.91145600
C	-2.97081800	-1.13457800	0.02259100
C	-3.88133800	-1.31530700	1.06557000
C	-4.68433200	-2.46093200	1.17598900
C	-4.47460100	-3.47716200	0.20505200
C	-3.65268000	-3.27754200	-0.93610900
C	-2.89667100	-2.09987900	-0.98295900

C	-3.58690500	-4.28149300	-2.11625900
C	-2.89699700	-5.60268600	-1.70122900
C	-5.01095700	-4.57286700	-2.65138200
C	-2.77491200	-3.70806100	-3.29993200
C	-5.73664300	-2.51180100	2.32194400
C	-7.02418200	-3.27070100	1.92156900
C	-6.19777400	-1.07963600	2.70173800
C	-5.12360400	-3.12650000	3.60380200
C	-4.59319300	-5.65387700	1.22496800
C	-3.05453400	1.72420400	-0.54472000
C	-2.56537000	3.03861400	-0.61923700
C	-4.37294300	1.48906000	-0.92872500
C	-5.20461400	2.49806200	-1.45080600
C	-4.62303500	3.77273200	-1.62589400
C	-3.33678700	4.09499700	-1.10944800
C	-2.82281300	5.55513100	-1.00574200
C	-1.48424100	5.62998900	-0.23806900
C	-2.58620800	6.21035200	-2.38735300
C	-5.23908200	4.67548300	-3.71902000
C	-3.85202900	6.39565900	-0.20844300
C	-6.68099300	2.11025700	-1.75215100
C	-6.74283000	1.21269800	-3.01181600
C	-7.65430500	3.30005200	-1.92511700
C	-7.23875100	1.29613600	-0.55247200
C	2.56321500	0.47901900	1.14802700
C	2.55356000	1.87513500	1.11106100
C	3.16526300	2.64455300	2.10969500
C	3.78426500	1.94801100	3.18234500
C	3.94208600	0.53615600	3.18028700
C	3.27493100	-0.16373800	2.16384200
C	4.81211600	-0.27485200	4.18532200
C	6.08139500	0.49239000	4.62715100
C	3.98235400	-0.70660700	5.41867000
C	5.32526600	-1.58420900	3.53072700
C	4.63685200	4.71256700	2.03508100
C	3.58010900	2.75135700	5.44650200
C	3.17862800	4.19123100	1.99707900

C	2.56795500	4.66661200	0.66146100
C	4.87199600	-1.97960900	-3.12437000
C	5.32827800	-1.30244200	-1.96702800
C	7.51190800	-2.50910400	-1.63202200
C	4.35379000	-0.91067400	-1.03363300
C	2.99859800	-1.20074000	-1.20786100
C	2.62275400	-2.00655800	-2.29103300
C	3.54351200	-2.46601900	-3.24025700
C	5.75939700	-1.19927800	-5.16979600
C	7.58955100	-0.20086300	-2.63794500
C	3.16062300	-3.10470900	-5.73779400
C	3.12163700	-3.56072300	-4.26014200
C	1.68159000	-4.05152900	-3.98669500
C	7.03807000	-0.49563900	-0.24173900
C	2.35065700	4.85273300	3.12476100
C	6.83665700	-1.11428000	-1.64201100
C	4.06276200	-4.77962500	-4.08641800
H	-1.81442300	2.98207800	4.17265500
H	-2.50733000	2.47914600	1.84206200
H	1.27667600	-0.10153600	6.33524300
H	-0.42949100	-0.70786900	6.32773400
H	2.10672200	-3.36465700	-0.18994300
H	1.08524200	-5.32154400	0.94830400
H	-2.53096800	-4.47144500	4.10105600
H	-0.89794400	-4.17327600	4.82307100
H	-3.96507800	-0.53681600	1.81329300
H	-2.20511900	-1.92418100	-1.79844700
H	-1.91436700	-5.40849900	-1.25531700
H	-2.74562400	-6.23549200	-2.58464500
H	-3.49222300	-6.17419600	-0.98885300
H	-5.65223100	-5.00693600	-1.88323000
H	-4.95473900	-5.27281600	-3.49453100
H	-5.48216400	-3.65152300	-3.01459000
H	-3.18553800	-2.75725900	-3.65774300
H	-2.81320800	-4.41921800	-4.13282600
H	-1.71981900	-3.55115300	-3.05094200
H	-7.75636900	-3.19138100	2.73405900

H	-6.85922200	-4.32605000	1.71290200
H	-7.47123900	-2.82624600	1.02479100
H	-7.02687100	-1.14972700	3.41477500
H	-6.55193600	-0.52232400	1.82854900
H	-5.41213500	-0.49267100	3.18717200
H	-4.23185400	-2.56725000	3.90625500
H	-4.83716700	-4.17261300	3.46907700
H	-5.84972800	-3.08662800	4.42564500
H	-3.54229000	-5.45179400	1.45978600
H	-4.67329200	-6.64019500	0.75783400
H	-5.17884000	-5.66631400	2.15120200
H	-1.55067400	3.22836500	-0.29265600
H	-4.76638700	0.48556200	-0.83260000
H	-1.19964600	6.68149900	-0.12116200
H	-0.66693800	5.12957800	-0.76905000
H	-1.55836000	5.19628300	0.76556100
H	-3.52199100	6.40891500	-2.91053000
H	-1.95273000	5.58121900	-3.02390200
H	-2.07367000	7.17117800	-2.25575200
H	-5.76866700	3.79210700	-4.09203000
H	-4.20018500	4.63390100	-4.06504700
H	-5.71919300	5.57458400	-4.11415300
H	-4.82469200	6.41185800	-0.70381500
H	-3.49569500	7.42903200	-0.11288400
H	-3.98352200	5.99220400	0.80275200
H	-6.13145800	0.31171800	-2.88967700
H	-6.38401200	1.73781500	-3.90373300
H	-7.77584900	0.89608000	-3.20283700
H	-8.67871100	2.90850400	-1.94157900
H	-7.50675200	3.85397100	-2.85186100
H	-7.57801000	4.00837500	-1.09492000
H	-7.17725100	1.87424500	0.37661500
H	-6.71468900	0.34953000	-0.39810800
H	-8.29286800	1.05541000	-0.73228100
H	2.04378200	2.35927700	0.28726700
H	3.31303800	-1.24561700	2.15519700
H	5.86727500	1.40406000	5.18174100

H	6.68337700	0.77414600	3.75554200
H	6.69487300	-0.15973900	5.26042000
H	4.59234200	-1.33324800	6.08166900
H	3.10926400	-1.28809900	5.10458000
H	3.62954100	0.14523200	6.00475700
H	6.03142900	-2.07074200	4.21289800
H	5.84999500	-1.38639400	2.59074400
H	4.52665800	-2.30589100	3.33371000
H	4.64213600	5.80631700	1.94680100
H	5.21147000	4.30808000	1.19345900
H	5.14195100	4.43835500	2.96251600
H	4.05975600	2.10652200	6.19146800
H	2.53582100	2.44700800	5.31677500
H	3.60908300	3.78010100	5.81848400
H	1.50356300	4.41945800	0.57893400
H	3.08252100	4.25105100	-0.20987300
H	2.65253400	5.75783200	0.60329400
H	7.05144000	-3.16018200	-0.87969300
H	8.57648400	-2.40944600	-1.38482800
H	7.43021400	-2.99499500	-2.60697000
H	4.65260700	-0.34923400	-0.16009100
H	1.57565400	-2.26018400	-2.39551600
H	6.44201200	-1.53956800	-5.95302800
H	6.10943200	-0.24241600	-4.77288700
H	4.76146300	-1.05501800	-5.59163300
H	8.58084200	0.03947200	-2.23470000
H	7.05919700	0.74575900	-2.79506300
H	7.74350700	-0.68711400	-3.60161100
H	4.18113000	-2.99595500	-6.10697400
H	2.62790700	-2.15712900	-5.88117600
H	2.66875700	-3.85804700	-6.36517500
H	1.45407200	-4.88046500	-4.66617200
H	0.93355300	-3.26949900	-4.16022200
H	1.55812800	-4.42103800	-2.96286100
H	6.57343900	-1.09949400	0.54404000
H	6.63979700	0.52316900	-0.17464900
H	8.11093500	-0.44471000	-0.02559100

H	1.34052600	4.42830500	3.17102000
H	2.25316500	5.92769400	2.92839600
H	2.81744300	4.74143300	4.10315000
H	3.77183600	-5.57922900	-4.77937500
H	3.99983900	-5.17909400	-3.06733500
H	5.10179300	-4.51065500	-4.28871400
Cu	-0.05134400	0.29114200	-1.47099900
H	-0.23566700	-0.79494800	-2.66478000
C	-0.17954800	0.62009000	-3.58176000
C	0.12140900	1.87884300	-2.98160200
H	-0.72426300	2.52852300	-2.76984800
H	0.56653500	0.16552600	-4.22950400
H	-1.19821800	0.45907100	-3.92349600
C	1.41686400	2.54935100	-3.10508400
C	1.49291700	3.95495800	-2.97209600
C	2.62244600	1.87556300	-3.41139200
C	2.69186000	4.64531900	-3.13445700
H	0.58167000	4.51041400	-2.75847400
C	3.81995100	2.56843500	-3.57147300
H	2.62258400	0.79344600	-3.50769300
C	3.87213600	3.95923800	-3.43512800
H	2.70282700	5.72835100	-3.03099800
H	4.72628800	2.01253800	-3.80361800
H	4.80876800	4.49515800	-3.56285600

13'-TS

Cartesian coordinates:

P	1.90968800	-0.40157900	-0.13324000
P	-1.69166800	0.13414900	-0.05189200
O	0.99903900	-0.04553500	4.57614700
O	0.13351800	1.92625600	5.39563500
O	-0.85611900	-2.41948800	3.95778700
O	0.12606500	-4.50410700	3.85281300
O	-4.95861800	-4.84201200	0.69615400
O	-6.40646100	3.76903300	-0.90352400
O	4.94399800	4.06173600	2.48325500
O	6.30842000	-2.47960500	-3.65866200

C	-1.16160600	0.69983200	1.64824600
C	-0.20029300	-0.04673500	2.40651300
C	0.12153700	0.48348800	3.65027300
C	-0.40168100	1.66936800	4.15545500
C	-1.31507700	2.40457700	3.43564800
C	-1.68403500	1.88666700	2.18287100
C	0.76675500	0.70103900	5.77210800
C	1.44225900	-1.66398700	1.14294600
C	2.02591700	-2.93812700	1.10524000
C	1.65393800	-3.98034900	1.97078700
C	0.66973100	-3.69050000	2.88883900
C	0.07942900	-2.43055300	2.94404300
C	0.41316000	-1.38068800	2.09824000
C	-0.62363700	-3.62320700	4.69248700
C	-2.54228900	-1.46866300	0.30619200
C	-2.40245700	-2.53099700	-0.58098600
C	-3.11389100	-3.73589500	-0.43418100
C	-4.06714500	-3.78237800	0.60731300
C	-4.13412300	-2.78307500	1.61914400
C	-3.36331300	-1.63314000	1.43019500
C	-4.96200500	-2.96553400	2.91803000
C	-6.48584700	-2.96537700	2.65115300
C	-4.56307300	-4.29567600	3.60353200
C	-4.67850300	-1.83064600	3.92763200
C	-2.73819200	-4.89429000	-1.40063400
C	-3.25159300	-6.29383100	-0.98997200
C	-1.18876900	-5.01302200	-1.43139800
C	-3.22861900	-4.57203500	-2.83266500
C	-6.05715500	-4.75753600	-0.21119300
C	-3.12411100	1.23474800	-0.48019800
C	-4.40041300	0.71298000	-0.70960400
C	-2.92931600	2.60880300	-0.67858600
C	-3.99915800	3.49507600	-0.87441900
C	-5.29912500	2.92750100	-0.90209700
C	-5.50568200	1.52951500	-0.98775000
C	-6.83029900	0.89561100	-1.49722100
C	-6.67373700	-0.62669600	-1.71291800

C	-8.03829300	1.08743100	-0.55044500
C	-6.93185400	4.01875500	0.40554800
C	-7.16866900	1.52118700	-2.87406100
C	-3.73047600	4.99964000	-1.15586200
C	-2.21680100	5.29053600	-1.24762800
C	-4.29609200	5.93849100	-0.06286900
C	-4.36097600	5.38039900	-2.51832400
C	2.71478300	0.96046700	0.81319500
C	3.45433100	0.75745400	1.98545300
C	4.15820100	1.79703500	2.60199500
C	4.11713500	3.07229800	1.97204500
C	3.24582300	3.35593100	0.89560400
C	2.59085700	2.25575000	0.31521700
C	2.90750600	4.76259500	0.32529000
C	3.30742500	5.95363200	1.22735900
C	3.55336500	4.93973200	-1.07001400
C	1.36587300	4.86719600	0.16122700
C	4.26299900	2.54115900	5.00739800
C	6.12114600	4.29365900	1.70968200
C	4.86539400	1.56716100	3.96336900
C	4.63789700	0.12943700	4.48101300
C	5.34505100	-2.13192100	-2.71862400
C	5.70261200	-1.26112400	-1.66003800
C	7.90536800	-2.30914700	-1.03286800
C	4.65700500	-0.77162700	-0.86220100
C	3.32829100	-1.15996800	-1.05254300
C	3.05540500	-2.15582300	-2.00023400
C	4.05005300	-2.70264100	-2.82189500
C	6.32915300	-1.60872000	-4.79808300
C	7.95811000	-0.15440400	-2.33746600
C	3.86136400	-3.73627600	-5.20413500
C	3.74454800	-3.96318600	-3.67845100
C	2.31366500	-4.48386100	-3.41548300
C	7.26201400	-0.15635800	0.04266800
C	6.39677200	1.77777100	3.89346300
C	7.17806800	-0.96210700	-1.27346900
C	4.72605700	-5.08769900	-3.26152500

H	-1.74310700	3.32425600	3.81935400
H	-2.42757000	2.43406800	1.61991300
H	1.71971300	0.91729600	6.25658000
H	0.09685800	0.13154100	6.43398800
H	2.81128100	-3.13465000	0.38604000
H	2.12960100	-4.95414900	1.92897600
H	-1.57876600	-4.08596000	4.94556200
H	-0.03872000	-3.39285000	5.59580900
H	-1.70310100	-2.41007000	-1.40227600
H	-3.40476300	-0.83418300	2.15869100
H	-6.78865100	-2.07680400	2.08399700
H	-7.02904700	-2.95188700	3.60438800
H	-6.80511800	-3.85396500	2.10540900
H	-4.77893000	-5.15607300	2.96820900
H	-5.11268500	-4.41239700	4.54614400
H	-3.49150900	-4.30041800	3.83307000
H	-3.61234100	-1.75158800	4.16511900
H	-5.21739100	-2.03923200	4.85894200
H	-5.02365500	-0.85561600	3.56468100
H	-2.76795600	-7.03998300	-1.63211900
H	-4.32829500	-6.41782400	-1.10926300
H	-2.99837500	-6.52887000	0.04791100
H	-0.89926000	-5.84612800	-2.08299100
H	-0.79214300	-5.21100700	-0.42914200
H	-0.69981800	-4.11323800	-1.81335000
H	-2.81257800	-3.62498000	-3.19334000
H	-4.32086400	-4.49584800	-2.88173200
H	-2.91772500	-5.36257300	-3.52710000
H	-6.62127000	-3.82792700	-0.06999500
H	-6.70332900	-5.61166200	0.00798600
H	-5.73001300	-4.81202100	-1.25491700
H	-4.53391100	-0.35792100	-0.67743200
H	-1.91782100	2.99396900	-0.65653200
H	-7.59420900	-1.01817700	-2.16049500
H	-6.51124500	-1.16557700	-0.77189000
H	-5.84780900	-0.86534400	-2.39129000
H	-8.39344600	2.11863500	-0.54420700

H	-7.79716700	0.78832400	0.47685700
H	-8.87191200	0.46025400	-0.88966400
H	-6.20104800	4.52591000	1.04201200
H	-7.23951000	3.09315900	0.90016500
H	-7.80298200	4.66477300	0.26716100
H	-7.31979400	2.59978200	-2.79193300
H	-8.08714100	1.07346200	-3.27458300
H	-6.36219100	1.33826500	-3.59336600
H	-1.72122700	4.68817400	-2.01412900
H	-1.70717000	5.13063600	-0.28977900
H	-2.07626900	6.34337500	-1.51765300
H	-3.89396100	6.94846400	-0.20835400
H	-4.00656100	5.61085800	0.94330400
H	-5.38291200	6.01601200	-0.11043300
H	-5.44164300	5.22137200	-2.51392500
H	-3.91800100	4.79116900	-3.32703600
H	-4.17094400	6.44040400	-2.73083800
H	3.47786500	-0.23646400	2.41322400
H	1.95166500	2.40701500	-0.54814500
H	4.38293200	6.12376400	1.27701500
H	2.93962300	5.82672400	2.24982300
H	2.85453100	6.86412100	0.81676900
H	3.26795100	5.90783300	-1.49987900
H	3.22777900	4.15546200	-1.76252000
H	4.64757500	4.90583200	-1.02178200
H	1.10230900	5.87477500	-0.17997900
H	0.85768200	4.68633300	1.11520900
H	0.96412900	4.16556200	-0.57403900
H	4.71020500	2.36031800	5.99335000
H	3.17907600	2.40072100	5.09185900
H	4.44812000	3.58166700	4.73278200
H	5.88499900	4.69729400	0.71932200
H	6.70386900	3.37336300	1.58437200
H	6.71414700	5.02639100	2.26330800
H	5.10663000	-0.62097900	3.83327500
H	3.57519000	-0.11506500	4.57303500
H	5.09468900	0.03216300	5.47256500

H	7.42191800	-2.87500300	-0.22800300
H	8.94634800	-2.12631200	-0.73760000
H	7.90776100	-2.92421500	-1.93537800
H	4.87946600	-0.06954400	-0.07187600
H	2.03405800	-2.50543000	-2.08783400
H	7.10606000	-1.99492800	-5.46315100
H	6.57039400	-0.58084900	-4.51314500
H	5.36863100	-1.60778100	-5.32034400
H	8.91436800	0.17868400	-1.91572200
H	7.40514900	0.73942000	-2.64990500
H	8.18683800	-0.75476800	-3.21860500
H	4.89839400	-3.62746600	-5.52399300
H	3.29535800	-2.85360900	-5.52481800
H	3.44866000	-4.60308900	-5.73442100
H	2.16808000	-5.41687400	-3.97121300
H	1.54395500	-3.77948800	-3.75080100
H	2.13951500	-4.70116400	-2.35630200
H	6.75883100	-0.66473000	0.87208200
H	6.83189800	0.84724300	-0.05578000
H	8.31565000	-0.03717500	0.31883500
H	6.84289300	1.18512300	3.08577000
H	6.85556000	1.45179900	4.83517400
H	6.65989600	2.82535600	3.74730100
H	4.51670300	-5.99905400	-3.83566000
H	4.61455600	-5.32836100	-2.19774100
H	5.76316300	-4.79780000	-3.44395500
Cu	0.05062000	-0.02515300	-1.50959800
H	-0.05853900	-1.32969500	-2.47108800
C	0.54675800	-0.19721400	-3.58673700
H	-0.19883900	-0.53373300	-4.30260300
C	0.60658500	1.19459400	-3.28990100
H	1.58074700	1.58906600	-3.00980400
H	1.48623200	-0.73705600	-3.65522500
C	-0.32211500	2.16657200	-3.86580100
C	0.08998000	3.50650400	-4.05171700
C	-1.60491300	1.82179100	-4.35085500
C	-0.70697500	4.43124900	-4.72211000

H	1.07295100	3.80708600	-3.69282300
C	-2.39958700	2.74770100	-5.02219100
H	-1.97851600	0.81179200	-4.20319100
C	-1.95756000	4.05917300	-5.22530800
H	-0.34417400	5.44721100	-4.86313800
H	-3.37563900	2.44160300	-5.39281600
H	-2.57507600	4.77536600	-5.76033200

13-I-TS

Cartesian coordinates:

P	-1.90483600	0.37932700	0.09986000
P	1.62456800	-0.53292600	0.02175700
O	-1.44701100	-2.73166800	3.80995400
O	-0.70268300	-4.88170800	3.43598900
O	0.55660600	-0.61806900	4.73448100
O	-0.26159100	1.26196800	5.79315500
O	4.94649700	2.87912800	3.69457400
O	5.31320100	-2.74209900	-4.16572000
O	-5.24539700	-4.60854500	-0.23317000
O	-5.36063100	4.82587600	-1.97689300
C	0.93764800	-1.88349500	1.09559200
C	-0.06357000	-1.60885000	2.08575000
C	-0.51035600	-2.71704100	2.79597800
C	-0.06256200	-4.01783300	2.58012400
C	0.88759900	-4.29756400	1.62498200
C	1.37697300	-3.20073000	0.89691300
C	-1.34891600	-4.03382500	4.38853600
C	-1.48507000	0.61268200	1.89100700
C	-1.97845100	1.73907200	2.56451100
C	-1.63015000	2.06146700	3.88665400
C	-0.76440500	1.19663900	4.51584000
C	-0.26901000	0.06775900	3.86778100
C	-0.58023100	-0.27828400	2.55857300
C	0.35273300	-0.01010800	6.01098900
C	2.69287900	0.44553900	1.16644700
C	3.35664500	-0.11283100	2.25950400
C	4.19558500	0.64240300	3.09755800

C	4.27550100	2.03090100	2.82525500
C	3.72025100	2.61162100	1.65295700
C	2.91068400	1.79251900	0.85893700
C	4.04117500	4.06044300	1.20021800
C	3.50308300	5.12835400	2.18257800
C	5.57590400	4.21864200	1.05842100
C	3.41952100	4.37063000	-0.17956100
C	4.97488800	-0.11657000	4.21253200
C	6.23200100	0.61819000	4.73632500
C	5.49750700	-1.46653900	3.65044400
C	4.03360000	-0.44037600	5.39712800
C	4.19552100	3.27285700	4.84252200
C	2.83645800	-1.38207100	-1.09300100
C	2.32481700	-2.15700600	-2.14628100
C	4.21674200	-1.22374500	-0.99915700
C	5.10586700	-1.74162400	-1.96163500
C	4.52866200	-2.38215700	-3.07982100
C	3.14344100	-2.70335400	-3.13663300
C	2.55325300	-3.67021000	-4.19581900
C	1.06582200	-3.97629600	-3.91145500
C	2.62733100	-3.10273700	-5.63349600
C	5.59240100	-1.66258300	-5.05874900
C	3.31778200	-5.01630800	-4.13404700
C	6.62653300	-1.58615300	-1.67303800
C	7.04181700	-0.10201500	-1.81457000
C	7.56351700	-2.45821800	-2.54121500
C	6.89404900	-2.03202900	-0.20970100
C	-2.98968100	-1.11348400	0.06341900
C	-3.04951000	-1.83065000	-1.13692800
C	-3.85573100	-2.96324800	-1.28540800
C	-4.57959300	-3.39486700	-0.14107200
C	-4.66289000	-2.62005700	1.04152500
C	-3.81318500	-1.50190500	1.12025100
C	-5.63677800	-2.87067600	2.23077100
C	-6.84646200	-3.77762300	1.90169800
C	-4.86757600	-3.45777000	3.43750100
C	-6.25310700	-1.51695500	2.67779100

C	-5.49091000	-3.66096300	-3.08174800
C	-4.57476300	-5.69921100	0.39818700
C	-3.99691000	-3.64562800	-2.67121200
C	-3.23392300	-2.86426200	-3.76392700
C	-4.62436400	3.85029900	-1.31308000
C	-5.26536600	2.64392800	-0.93779200
C	-7.39819700	3.62202400	-0.01950200
C	-4.44253200	1.60977900	-0.46151200
C	-3.06127600	1.76588800	-0.31866400
C	-2.50582000	3.03246100	-0.54310900
C	-3.26857000	4.11749300	-0.99171200
C	-5.28943700	4.71625400	-3.40473800
C	-7.48435900	2.53902300	-2.29285200
C	-2.54033800	6.19425100	-2.38420900
C	-2.66036800	5.54770700	-0.98426200
C	-1.24136100	5.54705400	-0.37131400
C	-7.22623500	1.14958900	-0.25578600
C	-3.44399300	-5.09074500	-2.68584200
C	-6.81160900	2.49008600	-0.90066100
C	-3.54714300	6.45124300	-0.09046400
H	1.25243800	-5.30470500	1.45503400
H	2.14314400	-3.38989600	0.15544900
H	-2.34936400	-4.41555100	4.59701900
H	-0.74052200	-3.98202600	5.30415900
H	-2.66773900	2.39577000	2.04796600
H	-2.03174700	2.93625400	4.38646200
H	1.31589500	0.12931200	6.50495300
H	-0.31678400	-0.64158800	6.61437000
H	3.21638900	-1.16791400	2.46279600
H	2.41391700	2.19728100	-0.01482800
H	2.43861400	4.97194700	2.39458700
H	3.60855500	6.12410600	1.73457900
H	4.05178800	5.13568300	3.12472900
H	6.08759100	4.03710800	2.00583300
H	5.81701800	5.23576900	0.72446400
H	5.96940800	3.51996300	0.31043000
H	3.75692000	3.67882700	-0.95799600

H	3.72073900	5.37917300	-0.48461300
H	2.32425500	4.34829100	-0.15802500
H	6.80503000	-0.07519700	5.36400200
H	6.00631100	1.49479300	5.34213700
H	6.87887300	0.93958200	3.91401000
H	6.08023700	-1.97957800	4.42417100
H	6.15328500	-1.30714100	2.78808100
H	4.69847900	-2.14827400	3.34777800
H	3.16064500	-1.00882100	5.06050000
H	3.67131700	0.47051400	5.88627900
H	4.56421900	-1.03454800	6.15202000
H	3.18931300	3.60789900	4.56763900
H	4.74231700	4.10163500	5.30040500
H	4.10980300	2.45949900	5.57141700
H	1.25357900	-2.30530300	-2.19304200
H	4.61726900	-0.66747000	-0.16089300
H	0.71061900	-4.71801000	-4.63550500
H	0.43153800	-3.08855000	-4.01406000
H	0.91433700	-4.39354600	-2.90960600
H	3.65182800	-3.06410300	-6.00471200
H	2.19358000	-2.09719400	-5.68693300
H	2.05616100	-3.74722700	-6.31311000
H	6.23229800	-0.90523000	-4.59217100
H	4.67081600	-1.17941300	-5.40231900
H	6.11731800	-2.09739000	-5.91342700
H	4.37988200	-4.88264400	-4.34876800
H	2.90219700	-5.71636400	-4.86980200
H	3.21850800	-5.47465900	-3.14274700
H	6.45655800	0.54477800	-1.15185900
H	6.90133300	0.26039800	-2.83929500
H	8.10144100	0.02294700	-1.55877700
H	8.57410000	-2.40278100	-2.11830600
H	7.63127100	-2.12815100	-3.57783000
H	7.25574600	-3.50770300	-2.54158900
H	6.59764000	-3.07632500	-0.05871600
H	6.36255800	-1.42246300	0.52450800
H	7.96477600	-1.94854900	0.01042900

H	-2.43271700	-1.48859100	-1.95898800
H	-3.79514000	-0.91330100	2.03031000
H	-6.58327000	-4.82607500	1.76583300
H	-7.36492000	-3.44350900	0.99782700
H	-7.55661500	-3.72499000	2.73599400
H	-5.54296500	-3.58034000	4.29383500
H	-4.04609500	-2.79910500	3.73654700
H	-4.44137800	-4.44031400	3.20549600
H	-6.96445600	-1.69318100	3.49294900
H	-6.79638400	-1.04294900	1.85363300
H	-5.51027800	-0.80585700	3.04878500
H	-5.60216400	-4.12757900	-4.06867100
H	-5.88475500	-2.63975400	-3.14849000
H	-6.09738700	-4.21991100	-2.36657800
H	-4.60671000	-5.61987300	1.49027700
H	-3.52797400	-5.76286500	0.08069800
H	-5.10414100	-6.60546200	0.09187400
H	-2.15088600	-2.86356600	-3.59775300
H	-3.56981300	-1.82418500	-3.83886100
H	-3.41613600	-3.34009900	-4.73398100
H	-6.99912100	3.56850100	1.00018000
H	-8.48951700	3.52337600	0.04081300
H	-7.16489200	4.60625900	-0.43133800
H	-4.88277500	0.65635900	-0.20493600
H	-1.44361500	3.15538100	-0.37146100
H	-5.88622100	5.54048300	-3.80442100
H	-5.69994000	3.76522600	-3.75550700
H	-4.26039500	4.80333400	-3.76382900
H	-8.53287000	2.22952800	-2.20340500
H	-6.99765300	1.85634400	-2.99945400
H	-7.48049100	3.54533100	-2.71294600
H	-3.51180400	6.48441400	-2.78658900
H	-2.04730000	5.52222100	-3.09704800
H	-1.93311400	7.10499500	-2.31532700
H	-0.88390100	6.58067900	-0.30373600
H	-0.52135800	4.98947400	-0.98107100
H	-1.22932400	5.12675800	0.64013500

H	-6.82057800	1.03834800	0.75486400
H	-6.91106900	0.28455000	-0.85077000
H	-8.31866900	1.11440800	-0.17864600
H	-2.41904000	-5.12731400	-2.29782000
H	-3.42214200	-5.46582500	-3.71652500
H	-4.06427700	-5.77292900	-2.10390000
H	-3.12689100	7.46403100	-0.04785100
H	-3.59141500	6.06298100	0.93387100
H	-4.56561100	6.51809600	-0.47953200
Cu	-0.00689500	0.50235900	-1.15706700
H	0.32195800	2.09771200	-1.39390700
C	0.11802600	1.68756500	-2.98049100
C	-0.15923600	0.30235400	-3.24227800
H	0.62443400	-0.31256000	-3.67417700
H	-0.74062500	2.35372100	-3.04717900
C	1.38091500	2.34387300	-3.44453400
C	1.34653800	3.68278000	-3.86213700
C	2.60734000	1.66314200	-3.50605000
C	2.49436700	4.32491100	-4.32926100
H	0.40489000	4.22697300	-3.82260900
C	3.75694400	2.30461200	-3.96689300
H	2.66413300	0.62866000	-3.18203100
C	3.70836700	3.63840000	-4.38255900
H	2.43850600	5.36198800	-4.65121100
H	4.69710500	1.75894900	-3.99888700
H	4.60551400	4.13509700	-4.74279400
H	-1.17187800	0.04424100	-3.53936800

14

Cartesian coordinates:

P	1.66549200	-0.54088400	0.05842400
P	-1.86133700	0.33760200	0.08310100
O	0.59820500	-0.25529900	4.78176800
O	-0.20615700	1.71402100	5.67461500
O	-1.41016900	-2.43500500	4.00327700
O	-0.63897100	-4.60243300	3.82682400
O	-5.51038600	-4.43050200	0.30044400

O	-5.01662800	4.85598500	-2.30317200
O	4.83479700	3.35899500	3.35168300
O	5.46907100	-3.05707200	-3.83551100
C	-1.42034900	0.75063900	1.83553900
C	-0.52251100	-0.08570100	2.57796700
C	-0.21524200	0.36386100	3.85599300
C	-0.70215200	1.54820500	4.40472400
C	-1.55345800	2.36754700	3.69932700
C	-1.90247000	1.93696000	2.40855100
C	0.38741700	0.45544800	6.00318600
C	1.01379000	-1.79613800	1.26539500
C	1.47197600	-3.11985400	1.19266500
C	0.98217500	-4.15555000	2.00588200
C	0.00827500	-3.80764600	2.91305300
C	-0.45635200	-2.49806400	3.00845400
C	-0.00542400	-1.45001100	2.21537900
C	-1.32997200	-3.68921600	4.68295000
C	-3.03605800	-1.07604800	0.20485200
C	-3.83152800	-1.32344700	1.32347500
C	-4.75228200	-2.38517000	1.37307200
C	-4.76910900	-3.25949400	0.25946100
C	-4.07506500	-2.97047200	-0.94711900
C	-3.19803900	-1.88134300	-0.93005900
C	-4.32614400	-3.75374500	-2.26226500
C	-3.88103500	-5.23315100	-2.17281700
C	-5.83491000	-3.68949700	-2.60953900
C	-3.55884000	-3.12832900	-3.44778900
C	-5.68885800	-2.46511300	2.61485500
C	-6.95570100	-3.33243500	2.42419300
C	-6.21545400	-1.04086600	2.94240100
C	-4.90186200	-2.97291800	3.84599000
C	-4.87850000	-5.50267100	1.00037200
C	-2.91947600	1.74897900	-0.47004500
C	-2.29156500	2.97038700	-0.76249200
C	-4.29533900	1.64975600	-0.65558500
C	-5.06455100	2.69939700	-1.19334800
C	-4.36438800	3.85614800	-1.59799800

C	-2.99065500	4.06011600	-1.28602900
C	-2.30757200	5.44735200	-1.41249100
C	-0.86271300	5.41724000	-0.86667000
C	-2.22714400	5.96166000	-2.86979300
C	-5.13935700	4.58297500	-3.70079900
C	-3.10304200	6.46691200	-0.55824700
C	-6.60475300	2.48626000	-1.24189900
C	-6.95073000	1.40483400	-2.29378700
C	-7.45067300	3.74935400	-1.52585100
C	-7.07212600	1.98696900	0.15266800
C	2.68159000	0.60147700	1.08631300
C	2.88237300	1.90732000	0.62149500
C	3.65396800	2.83368500	1.33238200
C	4.20300100	2.40329800	2.57073600
C	4.15898600	1.05231400	2.99358200
C	3.34012300	0.18968100	2.24564100
C	4.97253700	0.43272100	4.16836500
C	6.18345100	1.27436000	4.63610200
C	4.04699100	0.15248100	5.37546300
C	5.57220800	-0.92409900	3.70690500
C	5.48873200	4.40177400	0.59117200
C	4.05535800	3.83371700	4.44922200
C	3.95473000	4.23047300	0.72839200
C	3.35002300	4.37762100	-0.68376700
C	4.64635700	-2.61666800	-2.80599100
C	5.19112100	-1.78302500	-1.79937200
C	7.35681400	-3.00950100	-1.40661100
C	4.28563300	-1.20561400	-0.89365900
C	2.91442200	-1.45963200	-0.95190300
C	2.44953500	-2.41245300	-1.86779500
C	3.29800500	-3.06155400	-2.77206600
C	5.43779800	-2.20603900	-4.99099700
C	7.43664500	-0.87630700	-2.74618800
C	2.78472400	-4.11863200	-5.10069500
C	2.79234200	-4.29996100	-3.56452500
C	1.34959200	-4.67498300	-3.15555000
C	7.02078100	-0.80111900	-0.30386400

C	3.38270300	5.38671600	1.58354800
C	6.72057800	-1.60795400	-1.58628600
C	3.69951400	-5.50468900	-3.20700200
H	-1.94666500	3.28614200	4.12101200
H	-2.58736700	2.55227200	1.83841400
H	1.34602800	0.62167700	6.49700700
H	-0.29923200	-0.11624600	6.64536400
H	2.25443200	-3.36346700	0.48525800
H	1.36317700	-5.16827200	1.93195600
H	-2.33688400	-4.06217700	4.87754000
H	-0.76290400	-3.56343400	5.61736400
H	-3.73630200	-0.66452200	2.17854700
H	-2.61777800	-1.63966200	-1.81244400
H	-2.84629800	-5.31596000	-1.81927000
H	-3.92862200	-5.69127400	-3.16829100
H	-4.52538400	-5.81618400	-1.51446300
H	-6.44635600	-4.13882100	-1.82454500
H	-6.02549100	-4.22776800	-3.54645000
H	-6.15664900	-2.65056200	-2.74983000
H	-3.82056800	-2.07622600	-3.60390700
H	-3.81694300	-3.67049100	-4.36415100
H	-2.47213400	-3.19642200	-3.32396000
H	-7.62528100	-3.15872100	3.27536000
H	-6.75165500	-4.40211400	2.38624800
H	-7.49544400	-3.06214800	1.51166000
H	-6.89885500	-1.09365600	3.79777000
H	-6.77037500	-0.62350000	2.09524500
H	-5.42258500	-0.33674300	3.20753000
H	-4.02936300	-2.34237300	4.04434000
H	-4.54744300	-3.99993400	3.70118700
H	-5.54425700	-2.96482200	4.73563600
H	-3.86636700	-5.68536900	0.62230600
H	-5.49644300	-6.38806700	0.82942100
H	-4.82192900	-5.30861000	2.07694700
H	-1.22856600	3.06105300	-0.57365500
H	-4.78863300	0.72473700	-0.38413900
H	-0.44592200	6.42963600	-0.90963000

H	-0.20796300	4.76855100	-1.45916800
H	-0.82299000	5.09101000	0.17892200
H	-3.20757000	6.23651600	-3.25944300
H	-1.77816500	5.21484400	-3.53452600
H	-1.59613600	6.85815200	-2.90628600
H	-5.75318100	3.69472500	-3.88737400
H	-4.15834600	4.43450200	-4.16575200
H	-5.62487600	5.45643300	-4.14370800
H	-4.13418500	6.55997500	-0.90617900
H	-2.62895700	7.45470300	-0.61768100
H	-3.11734000	6.16507100	0.49594300
H	-6.44328400	0.45753000	-2.08045200
H	-6.65817400	1.71706400	-3.30265600
H	-8.03115000	1.21400700	-2.30192900
H	-8.50492300	3.50218400	-1.35035300
H	-7.37195100	4.10386200	-2.55375800
H	-7.18325400	4.57621800	-0.86227900
H	-6.83957700	2.72482900	0.92907600
H	-6.61303400	1.03890700	0.44287400
H	-8.15793300	1.83552300	0.14438400
H	2.42546000	2.19360800	-0.31836700
H	3.22101000	-0.83818100	2.56776900
H	5.90448800	2.18068300	5.17261700
H	6.81910800	1.56626200	3.79469900
H	6.78732200	0.66379400	5.31848100
H	4.60732800	-0.35060000	6.17370900
H	3.20576300	-0.48646400	5.08848500
H	3.63729400	1.07996700	5.79135400
H	6.17941700	-1.34706800	4.51552100
H	6.22057000	-0.78895700	2.83457300
H	4.81252900	-1.66807600	3.45309500
H	5.71602400	5.38121300	0.15195500
H	5.90580300	3.63437300	-0.07169200
H	5.98949600	4.33466700	1.55920900
H	3.93447900	3.06875300	5.22403600
H	3.06297000	4.16339100	4.12193500
H	4.60059900	4.68298100	4.86943000

H	2.25512300	4.34122800	-0.67562600
H	3.70745400	3.61453500	-1.38167000
H	3.63809000	5.35227800	-1.09310900
H	6.92435500	-3.52618400	-0.54170700
H	8.43634700	-2.91230300	-1.23503200
H	7.20488200	-3.63012900	-2.29241300
H	4.65277400	-0.53115100	-0.13334400
H	1.39356600	-2.65330000	-1.86635300
H	6.09751000	-2.67013000	-5.72887400
H	5.80011200	-1.20113200	-4.75780400
H	4.42856500	-2.12424100	-5.40249400
H	8.45710400	-0.61625900	-2.43931400
H	6.92353300	0.05550900	-3.01149700
H	7.51744200	-1.50210800	-3.63550300
H	3.79282600	-4.11671100	-5.51693500
H	2.27416400	-3.19471800	-5.39519100
H	2.24600900	-4.95504300	-5.56253000
H	1.06610500	-5.60166400	-3.66680200
H	0.62386400	-3.90640400	-3.44443400
H	1.25662500	-4.85196200	-2.07828500
H	6.57870700	-1.26262700	0.58516700
H	6.66420900	0.23334700	-0.36854800
H	8.10522600	-0.76542100	-0.15184500
H	2.31787200	5.23371000	1.79682200
H	3.47672400	6.32992600	1.03169200
H	3.91691900	5.50582000	2.52647400
H	3.35358100	-6.40298600	-3.73381100
H	3.66760100	-5.71300500	-2.13094500
H	4.73711700	-5.31771900	-3.49253600
Cu	-0.04081800	0.17174900	-1.38821600
H	0.91452800	-1.34496900	-4.03230500
C	0.00804700	-0.76268600	-4.23253600
C	-0.08112100	0.51567400	-3.38091200
H	-1.06655400	0.96976400	-3.55798100
H	0.00199800	-0.54773500	-5.31636500
C	0.95406300	1.53724100	-3.70545500
C	2.30086000	1.20882300	-3.98624000

C	0.62419100	2.91170200	-3.76196500
C	3.24555200	2.18608900	-4.29960100
H	2.60943800	0.16716000	-3.95662500
C	1.56716400	3.89032400	-4.07132600
H	-0.40843100	3.20143800	-3.57462600
C	2.89233500	3.53783600	-4.34655300
H	4.26975100	1.88702100	-4.51708200
H	1.26185200	4.93421500	-4.11553800
H	3.62818600	4.29650700	-4.60010500
H	-0.84327700	-1.42570600	-4.03025300

14'

Cartesian coordinates:

P	-1.84164400	0.26534700	0.08727800
P	1.69666100	-0.53200400	-0.02308100
O	-1.33163000	-2.91610100	3.68813000
O	-0.54731900	-5.03783600	3.23761400
O	0.60157600	-0.79800000	4.71557100
O	-0.22237800	1.06133900	5.80234400
O	4.67780600	3.12623700	3.69333700
O	5.58531700	-2.56181100	-4.11145000
O	-5.26399500	-4.66914200	-0.10723700
O	-5.16960200	4.86778900	-1.83916400
C	1.05825300	-1.92503400	1.02635100
C	0.04408500	-1.70669000	2.01857300
C	-0.38771000	-2.84708700	2.68431600
C	0.08399700	-4.13124300	2.42141500
C	1.04299500	-4.35855800	1.46145500
C	1.51851000	-3.22680400	0.77836900
C	-1.22529100	-4.24089100	4.21198100
C	-1.39089000	0.50583100	1.86997700
C	-1.87888800	1.62727200	2.55669600
C	-1.54409400	1.92139500	3.88897700
C	-0.70227000	1.03112900	4.51544200
C	-0.20442100	-0.08755800	3.85050300
C	-0.49393600	-0.39947200	2.52828300
C	0.35810400	-0.22969300	6.00346200

C	2.68244500	0.51871000	1.12604500
C	3.33464300	0.02247300	2.25601700
C	4.10765900	0.84094600	3.09862700
C	4.10530900	2.22652900	2.80736000
C	3.56440300	2.75247500	1.60311100
C	2.84466100	1.86956700	0.79080300
C	3.81920200	4.21190000	1.14356600
C	3.19207100	5.25788500	2.09657300
C	5.34755400	4.45071000	1.05232400
C	3.22894700	4.47454600	-0.25780500
C	4.92759500	0.14633500	4.22622800
C	6.08083500	0.99391400	4.81409000
C	5.61147500	-1.11931300	3.64160400
C	3.99325700	-0.30612400	5.37238700
C	3.85148700	3.45645500	4.80977100
C	2.95951000	-1.32313400	-1.11906100
C	2.49024200	-1.99775200	-2.25684300
C	4.33460900	-1.24591000	-0.91607100
C	5.26418900	-1.74200200	-1.85057200
C	4.73987900	-2.25996200	-3.05520700
C	3.35010900	-2.50740200	-3.23143400
C	2.79395700	-3.35474800	-4.40480900
C	1.27910500	-3.61384000	-4.24440800
C	2.98934900	-2.67173100	-5.77949700
C	5.97360700	-1.41788600	-4.87626000
C	3.49720800	-4.73513400	-4.41058400
C	6.76220200	-1.71339600	-1.43327200
C	7.25423000	-0.24978100	-1.33158500
C	7.73384500	-2.50216900	-2.34138000
C	6.87937000	-2.37987200	-0.03530300
C	-2.95917100	-1.19905600	0.07984500
C	-3.06157400	-1.93048000	-1.11028900
C	-3.87791800	-3.06073400	-1.21818100
C	-4.57983400	-3.46453200	-0.04998700
C	-4.62687400	-2.66907900	1.12094100
C	-3.75775400	-1.56457200	1.16389800
C	-5.58311700	-2.88094800	2.33204800

C	-6.81753600	-3.76573500	2.03638700
C	-4.80733000	-3.46654500	3.53525700
C	-6.16173100	-1.50693300	2.76768800
C	-5.55372100	-3.76693100	-2.97237100
C	-4.60144900	-5.75855000	0.53513000
C	-4.05327100	-3.77190200	-2.58568000
C	-3.29145300	-3.03413200	-3.70868500
C	-4.44776800	3.85453800	-1.22043900
C	-5.12958700	2.68566600	-0.80159300
C	-7.15209200	3.77721100	0.23236000
C	-4.33696300	1.61112700	-0.36600000
C	-2.94421600	1.69437000	-0.30879600
C	-2.33252500	2.92441000	-0.58338900
C	-3.06158200	4.05030600	-0.98503600
C	-5.18143000	4.76102500	-3.27039800
C	-7.42193900	2.69825700	-2.02912100
C	-2.36532300	6.14108200	-2.38422700
C	-2.38926000	5.45175900	-0.99998700
C	-0.92319100	5.37441400	-0.51810700
C	-7.12531200	1.29893800	-0.00360000
C	-3.52900600	-5.22794500	-2.57323400
C	-6.67693800	2.61490000	-0.67593200
C	-3.15859700	6.35889500	-0.00595500
H	1.42364800	-5.35264600	1.25379300
H	2.28959200	-3.37467600	0.03251800
H	-2.22401100	-4.64524200	4.38344000
H	-0.63681300	-4.22063400	5.14153500
H	-2.55931800	2.29722500	2.04550600
H	-1.94213100	2.79160700	4.39944300
H	1.30239900	-0.12593400	6.53949100
H	-0.34882900	-0.86652500	6.55628400
H	3.24408100	-1.03409200	2.48183600
H	2.39407400	2.22758500	-0.12730000
H	2.13154900	5.04505200	2.27751600
H	3.25557500	6.25250700	1.63865300
H	3.71012200	5.30590600	3.05466200
H	5.83516900	4.30709100	2.01890800

H	5.54489800	5.47607500	0.71531400
H	5.80336900	3.76723700	0.32623800
H	3.62245400	3.79524900	-1.01962000
H	3.48668100	5.49375000	-0.56640500
H	2.13592700	4.39928700	-0.27128600
H	6.70199900	0.34392400	5.44247900
H	5.74163100	1.81969000	5.43883200
H	6.71771000	1.40904000	4.02734100
H	6.21093700	-1.60371900	4.42109300
H	6.28377900	-0.85402500	2.81857100
H	4.90068600	-1.86370600	3.27329800
H	3.19467500	-0.95563300	5.00050100
H	3.52429200	0.55136600	5.86830600
H	4.56375600	-0.85765700	6.13041000
H	2.85743800	3.78592700	4.48747500
H	4.35401100	4.27378500	5.33370000
H	3.73598400	2.60983600	5.49532000
H	1.41968500	-2.09619400	-2.38642800
H	4.70056200	-0.77471200	-0.01147300
H	0.94501200	-4.27698600	-5.05009800
H	0.69006600	-2.69224200	-4.31400400
H	1.04292800	-4.10520400	-3.29356900
H	4.03798000	-2.64991900	-6.07785100
H	2.60114200	-1.64663900	-5.77233800
H	2.44096700	-3.22984700	-6.54839600
H	6.55401700	-0.70776100	-4.27676500
H	5.10068000	-0.89764300	-5.28601200
H	6.59449400	-1.79147500	-5.69459100
H	4.57593800	-4.63323800	-4.54492900
H	3.10427900	-5.35097500	-5.22933400
H	3.31265500	-5.27009700	-3.47113100
H	6.65360500	0.33346800	-0.62534900
H	7.20670800	0.25668000	-2.30237600
H	8.29648900	-0.22235800	-0.98999600
H	8.70667500	-2.55348200	-1.83697600
H	7.90133700	-2.03246800	-3.31111200
H	7.39011500	-3.52513900	-2.51590900

H	6.55601100	-3.42649100	-0.07638900
H	6.28320000	-1.87583500	0.72852700
H	7.92422000	-2.36213700	0.29691600
H	-2.48034700	-1.59937300	-1.96210500
H	-3.70629000	-0.96621200	2.06603600
H	-6.57903200	-4.82102400	1.90874300
H	-7.34500000	-3.43148000	1.13776100
H	-7.51131000	-3.68771600	2.88229200
H	-5.46764400	-3.54749800	4.40795900
H	-3.95713100	-2.83124100	3.80313300
H	-4.42151700	-4.46870900	3.31707300
H	-6.86839200	-1.65549300	3.59225100
H	-6.70173100	-1.02980000	1.94319400
H	-5.39792500	-0.80978700	3.12247700
H	-5.68988700	-4.25633400	-3.94491500
H	-5.92788400	-2.74000900	-3.05964800
H	-6.15976300	-4.29531100	-2.23382500
H	-4.62014300	-5.66023400	1.62590200
H	-3.55958000	-5.84271400	0.20658600
H	-5.14723300	-6.66197800	0.25041000
H	-2.20595200	-3.04962000	-3.55728900
H	-3.60886600	-1.99086900	-3.80990600
H	-3.49459400	-3.53304900	-4.66270500
H	-6.69921500	3.70402500	1.22813500
H	-8.24184700	3.73601600	0.35477000
H	-6.89139700	4.74725200	-0.19618700
H	-4.81020800	0.68373900	-0.07424400
H	-1.25685000	2.99913000	-0.47620900
H	-5.75747900	5.61560800	-3.63483500
H	-5.65721900	3.83267000	-3.59842900
H	-4.17032500	4.79842500	-3.68391900
H	-8.47915500	2.44650900	-1.88053300
H	-7.01247500	1.98935300	-2.75838900
H	-7.38624100	3.70220700	-2.45309200
H	-3.35656600	6.47606900	-2.69197100
H	-1.95404300	5.48108100	-3.15636100
H	-1.72355200	7.02905700	-2.33528200

H	-0.51533600	6.38972300	-0.46127400
H	-0.29001600	4.80562200	-1.20822400
H	-0.83927300	4.93190700	0.48089900
H	-6.67184700	1.16735100	0.98418700
H	-6.88914400	0.41815800	-0.61202300
H	-8.21217400	1.32142100	0.13313600
H	-2.50104700	-5.27677200	-2.19450400
H	-3.52456800	-5.62488000	-3.59576400
H	-4.15676000	-5.88527400	-1.97132800
H	-2.69404700	7.35231200	0.03002800
H	-3.13335200	5.93945200	1.00677000
H	-4.20255700	6.47947600	-0.30513000
Cu	-0.04132800	0.28581500	-1.39384000
C	0.02709000	0.70958300	-3.37132600
H	0.52547500	-0.16942700	-3.80474700
C	-1.36163900	0.84812300	-4.01487800
H	-2.00235100	1.57339000	-3.49790600
H	-1.89422500	-0.11062300	-3.98574000
C	0.92430700	1.88178700	-3.57304400
C	0.44113900	3.20006100	-3.73849400
C	2.33071000	1.72258300	-3.63253500
C	1.30169900	4.28152200	-3.94360900
H	-0.63095300	3.37624600	-3.72258100
C	3.18849700	2.79887800	-3.84055200
H	2.74430800	0.72188000	-3.52413600
C	2.68386900	4.09573000	-3.99822900
H	0.88301300	5.27766700	-4.07603800
H	4.26195900	2.62465000	-3.89360300
H	3.35218300	4.93564200	-4.16902300
H	-1.31316200	1.16196500	-5.07348700

14-I

Cartesian coordinates:

P	-1.62191600	-0.42544100	0.41366600
P	1.87544300	-0.05805800	-0.33012300
O	-0.03189900	-5.02994900	0.18319700
O	0.89570800	-5.79092200	-1.78561900

O	1.73493200	-4.05220500	2.45735600
O	0.86655500	-3.93031800	4.59053200
O	5.11191600	0.25786900	4.72176500
O	5.34252600	2.53421500	-4.49331800
O	-4.22948100	-3.79400600	-3.82066900
O	-5.96195600	3.02813500	2.67041400
C	1.63244400	-1.84713300	-0.75585300
C	0.81602100	-2.70349200	0.05653300
C	0.67355400	-4.00364900	-0.41183600
C	1.23220500	-4.47196200	-1.59909400
C	1.98677400	-3.65262500	-2.40695300
C	2.17616400	-2.33666800	-1.95336700
C	0.35181600	-6.20655900	-0.53043800
C	-0.91339600	-1.56489300	1.69425200
C	-1.41946700	-1.51176500	3.00164300
C	-0.89264000	-2.26399000	4.06466300
C	0.16728400	-3.08743900	3.76091500
C	0.68818300	-3.15285800	2.47045900
C	0.20770000	-2.41138000	1.39876100
C	1.65743600	-4.73316000	3.71096600
C	2.93188800	-0.03710700	1.17921200
C	3.82582200	-1.04708200	1.53322600
C	4.66046000	-0.94996100	2.66172900
C	4.47159300	0.17942400	3.49413500
C	3.66342200	1.28303300	3.10835400
C	2.89375600	1.13108300	1.95181600
C	3.67795100	2.63671200	3.86529000
C	3.11430700	2.52218600	5.30183400
C	5.13120800	3.17112000	3.92288900
C	2.82914900	3.70162800	3.13563100
C	5.74292500	-2.05350900	2.84969500
C	6.89583200	-1.68516700	3.81330200
C	6.42619600	-2.31936700	1.47985500
C	5.08857400	-3.37408800	3.31849700
C	4.48519200	-0.49699700	5.75904700
C	3.00107500	0.57932300	-1.65135400
C	2.40977900	1.27271700	-2.71516400

C	4.38435100	0.40747800	-1.65579000
C	5.20943000	0.95941500	-2.65109500
C	4.57847600	1.78534200	-3.61139000
C	3.16507400	1.86963000	-3.72880300
C	2.46143700	2.52484200	-4.94532200
C	0.93085000	2.32116200	-4.88711400
C	2.70761500	4.05025200	-5.02793600
C	5.86349700	3.73707800	-3.92498100
C	2.96590800	1.85124400	-6.24604700
C	6.71334500	0.56200100	-2.61851400
C	7.40173100	1.19717800	-1.38682400
C	7.52871200	0.91362900	-3.88470000
C	6.80150800	-0.98451600	-2.49362600
C	-2.48225100	-1.50736000	-0.80244000
C	-2.68585100	-0.97521800	-2.08226600
C	-3.32820800	-1.69507300	-3.09331400
C	-3.73896900	-3.01930400	-2.78022900
C	-3.69445100	-3.53629400	-1.46266800
C	-3.00791200	-2.76496100	-0.50721000
C	-4.37678300	-4.84720600	-0.97178900
C	-5.47622800	-5.40222100	-1.90811800
C	-3.31368300	-5.94282800	-0.72363300
C	-5.09378200	-4.56753700	0.37752300
C	-5.16813500	-1.05767700	-4.70167600
C	-3.29942200	-4.74828200	-4.33354400
C	-3.63875700	-1.02183400	-4.45569500
C	-3.20988700	0.46239600	-4.46432700
C	-4.97405300	2.11375900	2.32812700
C	-5.35619800	0.85669400	1.79477900
C	-7.20509800	0.31275000	3.41517800
C	-4.33470700	0.06112400	1.25183000
C	-2.99550800	0.45903900	1.27833500
C	-2.65654000	1.62331400	1.97740900
C	-3.61755000	2.45513800	2.56390200
C	-6.27390500	3.94859800	1.61264800
C	-7.85332300	1.08808800	1.10745600
C	-3.49871500	5.02170400	2.97988500

C	-3.17791500	3.60481300	3.51215000
C	-1.65341000	3.56208800	3.76551800
C	-6.87790700	-1.16784200	1.43925400
C	-2.91093400	-1.70367900	-5.63898000
C	-6.80031900	0.29782400	1.91931200
C	-3.87504100	3.40703600	4.88181300
H	2.42594900	-4.00603300	-3.33349600
H	2.78600400	-1.67678900	-2.55795800
H	-0.52639700	-6.83030700	-0.70220300
H	1.12193100	-6.74590300	0.04141500
H	-2.26687600	-0.86870700	3.20635300
H	-1.30926600	-2.20970100	5.06455300
H	2.66038700	-4.84801900	4.12484500
H	1.16900800	-5.70868200	3.56731700
H	3.88107600	-1.93156800	0.90841900
H	2.23830800	1.93114500	1.62923900
H	2.12750000	2.04397900	5.30428900
H	2.99784000	3.52462400	5.73162600
H	3.77882800	1.96065900	5.95901000
H	5.79158900	2.47993900	4.45030700
H	5.15342900	4.13605800	4.44479200
H	5.52683000	3.32804900	2.91243100
H	3.16608200	3.86694900	2.10650800
H	2.92065700	4.65447300	3.66867100
H	1.76451400	3.44276500	3.11071200
H	7.68363500	-2.44201300	3.71486100
H	6.59863900	-1.66280200	4.86142700
H	7.33163900	-0.71219100	3.56792000
H	7.21891300	-3.06603500	1.60486600
H	6.88491900	-1.40494000	1.08707600
H	5.73729700	-2.70624900	0.72410300
H	4.30878900	-3.69734300	2.62170700
H	4.62968600	-3.26535100	4.30793200
H	5.84320000	-4.16803200	3.38603000
H	3.42402700	-0.24081700	5.85431000
H	5.00660200	-0.23963600	6.68477700
H	4.57176700	-1.57548000	5.58733600

H	1.33117300	1.37117800	-2.71834600
H	4.83846900	-0.16821400	-0.85743600
H	0.48233000	2.73870000	-5.79536400
H	0.47362300	2.83011100	-4.03135400
H	0.65875400	1.26024700	-4.84336600
H	3.73914200	4.28324600	-5.29425400
H	2.46536600	4.54326700	-4.07919100
H	2.06271800	4.48530500	-5.80119400
H	6.56156400	3.53066300	-3.10607500
H	5.06039100	4.37946000	-3.54662500
H	6.39443800	4.25249400	-4.72949600
H	4.04366300	1.97602000	-6.36919600
H	2.46548100	2.29618100	-7.11528800
H	2.73821900	0.77849400	-6.24180000
H	6.90936400	0.90464400	-0.45293400
H	7.38776700	2.29178400	-1.43763900
H	8.45001500	0.87826500	-1.33024600
H	8.50475900	0.41821800	-3.81246100
H	7.71929700	1.98111200	-3.99749300
H	7.03805200	0.56049600	-4.79580700
H	6.32208200	-1.47120300	-3.35082800
H	6.33360800	-1.36892900	-1.58394900
H	7.85333400	-1.29333000	-2.47520800
H	-2.32414200	0.02671200	-2.27933600
H	-2.88625600	-3.15193900	0.49815600
H	-5.08842500	-5.83386500	-2.83027300
H	-6.20184300	-4.62958300	-2.17940200
H	-6.01375400	-6.19742700	-1.37728900
H	-3.78892600	-6.84847100	-0.32566900
H	-2.56115600	-5.60356000	-0.00474300
H	-2.79360600	-6.21730000	-1.64848500
H	-5.60641900	-5.47667100	0.71253900
H	-5.84504500	-3.77850200	0.26652600
H	-4.40829000	-4.27283800	1.17655600
H	-5.40412600	-0.57353000	-5.65763900
H	-5.70059500	-0.51526000	-3.91148600
H	-5.54443400	-2.08214000	-4.73305800

H	-3.11173000	-5.55833100	-3.62046500
H	-2.34385000	-4.27726300	-4.58978300
H	-3.75331500	-5.16602800	-5.23611200
H	-2.12447200	0.58396400	-4.37074500
H	-3.68952600	1.03874900	-3.66593700
H	-3.50691300	0.91236400	-5.41804700
H	-6.52028400	-0.30236600	4.01073600
H	-8.21610000	-0.09700200	3.53492400
H	-7.19667500	1.32826400	3.81707800
H	-4.58463000	-0.88135500	0.78349100
H	-1.60970600	1.89384800	2.03912900
H	-6.96285800	4.68149000	2.04060300
H	-6.75784700	3.44114000	0.77304700
H	-5.37997700	4.45689000	1.24273800
H	-8.79670000	0.52861700	1.08815700
H	-7.53380700	1.23403900	0.06885500
H	-8.06337200	2.06082900	1.55300500
H	-4.56586800	5.24380700	3.02441200
H	-3.14888500	5.15668000	1.95037100
H	-2.98926200	5.76685100	3.60318800
H	-1.39759900	4.32115100	4.51307400
H	-1.07662300	3.78606700	2.86103500
H	-1.32618000	2.59117700	4.15463600
H	-6.18159600	-1.81694700	1.98058100
H	-6.67559700	-1.26415300	0.36613300
H	-7.88986600	-1.54825200	1.61760600
H	-1.83604500	-1.79772600	-5.44308400
H	-3.03107300	-1.09516800	-6.54367300
H	-3.31647800	-2.69239400	-5.85472500
H	-3.56153200	4.19589100	5.57708300
H	-3.60180300	2.44155100	5.32437500
H	-4.96202800	3.44780800	4.78432900
Cu	-0.07730100	1.20924100	-0.30559600
H	-1.88012900	3.09107200	-2.23829000
C	-1.81873100	3.47836100	-1.20769300
C	-0.43989700	3.13591300	-0.62213400
H	-0.33345300	3.63536500	0.35749000

H	-2.60366800	2.93791900	-0.65974700
H	0.34951100	3.57364600	-1.25414900
C	-2.24341800	4.94789100	-1.25038600
C	-1.35110700	6.00155100	-1.01673200
C	-3.57936600	5.27761200	-1.53965300
C	-1.77234600	7.33387400	-1.07431000
H	-0.31588400	5.77049500	-0.78413500
C	-4.00713200	6.60382100	-1.59881200
H	-4.29174900	4.47449900	-1.72556900
C	-3.10101200	7.64273100	-1.36553100
H	-1.05711700	8.13240500	-0.88880200
H	-5.04688400	6.82867900	-1.82694300
H	-3.42925700	8.67830400	-1.40887700

20-TS

Cartesian coordinates:

C	3.02660800	-0.91029900	-1.11239800
C	2.92876100	-1.96395000	-2.03464800
H	1.97171800	-2.44630400	-2.17844900
C	4.04177100	-2.43775100	-2.74075900
C	5.26175000	-1.72884900	-2.57762200
C	5.31984700	-0.49453800	-1.89201200
C	4.20597400	-0.16480500	-1.10286500
H	4.26122400	0.71291100	-0.47081000
C	2.52407800	0.41639500	1.38495700
C	3.41362300	-0.33139900	2.15898900
H	3.55855200	-1.37455900	1.90793300
C	4.12952900	0.21353700	3.23386400
C	3.83448800	1.55985500	3.56835900
C	3.01968500	2.38396400	2.74873200
C	2.37157000	1.77591400	1.66347500
H	1.72776300	2.36019700	1.02071800
C	1.05159400	-1.94693900	0.84768900
C	1.57602300	-3.20324600	0.51272700
H	2.32318200	-3.27357900	-0.26417300
C	1.22785300	-4.39414000	1.17339400
H	1.66438500	-5.34666700	0.89313500

C	0.33619000	-4.27732700	2.21416500
C	-0.73133300	-4.51977300	4.13615500
H	-1.64897400	-5.00610900	4.46648100
H	0.00784400	-4.44942700	4.94863800
C	-0.18895700	-3.03982400	2.57171100
C	0.11306700	-1.84802100	1.92563100
C	-0.45314900	-0.60992900	2.55135000
C	-0.05974800	-0.35196600	3.85843400
C	0.71492800	-0.57311800	5.93295200
H	1.69594700	-0.44120400	6.39087000
H	0.09751400	-1.28198900	6.50531900
C	-0.56399100	0.68937700	4.63086200
C	-1.52983000	1.53898200	4.14089000
H	-1.94436900	2.34382500	4.73803600
C	-1.96810900	1.29425900	2.82864200
H	-2.74507900	1.93470800	2.43159900
C	-1.46242200	0.25949300	2.02784900
C	-3.51126900	1.20821700	0.14773300
C	-4.79637400	0.67792300	0.05843100
H	-4.92135300	-0.39500500	0.12027500
C	-5.93666700	1.48020900	-0.12517400
C	-5.71771500	2.86608500	-0.28123300
C	-4.45223400	3.46450500	-0.03197800
C	-3.36294800	2.60372000	0.13094000
H	-2.36904300	3.02159500	0.23086300
C	-2.67435500	-1.55768600	0.06258000
C	-3.31052300	-2.23324600	1.11396400
H	-3.37019800	-1.74535100	2.07804500
C	-3.85056000	-3.51245900	0.95069500
C	-3.71306700	-4.11481000	-0.32997000
C	-3.24043500	-3.40302600	-1.45488600
C	-2.67008500	-2.14088700	-1.20399400
H	-2.21628100	-1.59312600	-2.02404700
O	-0.16604100	-5.25348100	3.04554100
O	-1.03139800	-3.21033000	3.65290300
O	0.87317800	-1.04808400	4.59691900
O	0.04563700	0.68969500	5.86550500

P	1.61736900	-0.38773400	-0.02196700
P	-1.99687500	0.14709000	0.25052600
C	-0.53137200	1.74554000	-3.05842000
H	-0.17050700	2.64360700	-3.56122100
Cu	-0.14252300	0.88812900	-0.99511000
C	0.36090000	5.23043000	-2.33682400
C	1.75646400	4.52527800	-2.66588200
B	0.31970300	2.99193800	-1.62468000
H	0.18757700	2.53197200	-0.45750200
O	1.67196500	3.26339400	-1.97704900
O	-0.45812600	4.17096400	-1.80991200
C	0.46103200	6.31660600	-1.25280800
H	1.07549200	7.16393600	-1.57747900
H	-0.54257000	6.69254100	-1.03074800
H	0.87871900	5.91660300	-0.32574700
C	-0.35536800	5.82656800	-3.55754500
H	-1.32578300	6.22539700	-3.24301800
H	0.21982900	6.64878600	-3.99979000
H	-0.53890000	5.07648600	-4.33044900
C	2.98846900	5.26702300	-2.12801600
H	3.88251200	4.66825900	-2.33226500
H	3.11511800	6.23968100	-2.61804100
H	2.93268400	5.42793000	-1.04984000
C	1.99323800	4.26881100	-4.16676600
H	2.09853600	5.20930000	-4.71922500
H	2.92228200	3.70168400	-4.28640800
H	1.19334600	3.68881000	-4.63233300
C	-2.06220100	1.84676800	-3.14622700
H	-2.58385300	0.98419000	-2.71665400
H	-2.40427100	2.73300200	-2.60657800
H	-2.40426600	1.93958500	-4.19019200
C	0.06737900	0.63761400	-3.89338300
C	-0.71932000	-0.33839000	-4.53596400
C	1.44821200	0.63993700	-4.19194400
C	-0.16892700	-1.23383700	-5.45847600
H	-1.78949500	-0.36510800	-4.35983100
C	1.99453700	-0.24179300	-5.11871500

H	2.08377200	1.36745500	-3.69738400
C	1.18849000	-1.18214900	-5.77187400
H	-0.81600800	-1.95401900	-5.95470000
H	3.05781100	-0.18910500	-5.34090900
H	1.61039900	-1.85468800	-6.51406000
C	-4.27254800	4.99622300	0.13074100
C	-2.85521400	5.33833000	0.63933200
H	-2.63323500	4.84379200	1.59280800
H	-2.07843000	5.06864400	-0.08215900
H	-2.79227500	6.41934500	0.81066900
C	-4.47266800	5.76084800	-1.19907500
H	-3.83213700	5.35128800	-1.98858800
H	-5.51034800	5.73495500	-1.53482500
H	-4.19951100	6.81453200	-1.06130000
C	-5.27732100	5.52115100	1.18681800
H	-5.11009500	5.03599300	2.15622100
H	-5.13726500	6.60046700	1.32597500
H	-6.31142400	5.34447400	0.88572600
C	-7.31428300	0.75898000	-0.09190200
C	-7.35493300	-0.15585300	1.16339600
H	-6.58107200	-0.92792300	1.15471900
H	-7.23297900	0.43360500	2.07938400
H	-8.32404400	-0.66581700	1.21591000
C	-8.54893700	1.68122700	0.03569100
H	-8.44477400	2.38768900	0.86386300
H	-8.76022200	2.25239300	-0.86851700
H	-9.42696700	1.05437300	0.23420500
C	-7.47635700	-0.12590300	-1.35118800
H	-7.47571700	0.47472800	-2.26771200
H	-6.66664700	-0.85917200	-1.43560100
H	-8.42537400	-0.67503100	-1.31085300
C	-3.34737900	-3.85351200	-2.93952100
C	-1.93765200	-4.12822400	-3.51423300
H	-1.29447800	-3.24434100	-3.46037800
H	-1.43694800	-4.94190200	-2.97678700
H	-2.01132600	-4.42161500	-4.56887700
C	-4.24425100	-5.08495400	-3.20730700

H	-4.38700500	-5.17137300	-4.29133900
H	-3.80821100	-6.02490600	-2.86745300
H	-5.22987800	-4.98199700	-2.74538700
C	-4.00089100	-2.69440300	-3.74193900
H	-5.01206100	-2.48788400	-3.37196900
H	-3.42994200	-1.76492400	-3.69277600
H	-4.07918300	-2.97594700	-4.79855400
C	-4.65270500	-4.18451100	2.09534300
C	-4.05167200	-5.54247600	2.53544900
H	-4.50204100	-5.85434100	3.48608400
H	-4.25088600	-6.32782000	1.80603400
H	-2.96830100	-5.47361600	2.67930800
C	-4.70966800	-3.28343800	3.34858100
H	-3.71446000	-3.09859900	3.76734800
H	-5.18017700	-2.31592600	3.14174200
H	-5.31258100	-3.77945400	4.11753100
C	-6.10878000	-4.41442500	1.61828300
H	-6.14063100	-5.06311600	0.73985000
H	-6.69437200	-4.88796900	2.41655300
H	-6.59354600	-3.46398000	1.36694800
C	2.89548200	3.91427500	2.96896100
C	5.18285500	-0.69742400	3.92948100
C	6.32028700	0.07693100	4.63711600
H	5.99613900	0.62040100	5.52308500
H	7.09119200	-0.63740900	4.95044700
H	6.78787300	0.79890000	3.95936200
C	4.48994100	-1.65047200	4.93348800
H	3.69242300	-2.22201000	4.44675400
H	5.21791900	-2.35902500	5.34845700
H	4.04284000	-1.10844100	5.77293300
C	5.88886200	-1.58274300	2.86538400
H	5.22257800	-2.32007800	2.40902200
H	6.32104200	-0.97414700	2.06394000
H	6.70136300	-2.14167100	3.34342500
C	4.30170500	4.55828300	2.87962200
H	4.22614400	5.64316600	3.02654400
H	4.97594000	4.15483500	3.63789300

H	4.74489000	4.38479000	1.89186200
C	2.24583300	4.27625700	4.32661600
H	2.90917700	4.07944900	5.16860300
H	2.00779700	5.34691800	4.34287700
H	1.30970400	3.72596000	4.47829200
C	2.02170300	4.56627900	1.87746800
H	2.40397000	4.37211700	0.87121700
H	0.98171800	4.22260100	1.91674500
H	2.01561200	5.65158800	2.02927900
C	3.91611000	-3.67807800	-3.66570500
C	4.74169000	-4.87166300	-3.12514000
H	5.81479400	-4.70047400	-3.21478500
H	4.50539100	-5.07717300	-2.07372900
H	4.50397800	-5.77434200	-3.70158900
C	2.45278000	-4.16132100	-3.77427900
H	2.06239500	-4.52314100	-2.81515700
H	1.78620600	-3.37937500	-4.15043600
H	2.40904200	-5.00067900	-4.47769100
C	4.39776800	-3.33712000	-5.09705500
H	5.43931300	-3.01120900	-5.10190800
H	4.31034900	-4.22294600	-5.73906800
H	3.78123700	-2.54529100	-5.53257500
C	6.46588100	0.55427900	-1.96067900
C	7.17288900	0.67826300	-0.59011300
H	6.46951300	0.94882400	0.20487200
H	7.65982200	-0.25993700	-0.29937600
H	7.94586700	1.45566000	-0.63117400
C	5.82688000	1.92746000	-2.31201200
H	5.33234900	1.88430400	-3.28895900
H	5.08454300	2.25634400	-1.58053000
H	6.60884100	2.69485000	-2.36066300
C	7.52966100	0.30537900	-3.05469800
H	8.19391600	-0.53169700	-2.83632400
H	7.07188500	0.12697700	-4.03160400
H	8.15664800	1.20178300	-3.13450600
O	4.38830300	2.14385000	4.69832600
O	6.40799700	-2.26821900	-3.14289700

O	-4.09220700	-5.44157700	-0.45586400
O	-6.75618000	3.69799600	-0.67045200
C	-7.00528400	3.68471000	-2.07726000
H	-7.78392500	4.43020100	-2.25846500
H	-6.10556300	3.94936500	-2.64405500
H	-7.35783900	2.70462300	-2.41803000
C	-2.99145000	-6.35364600	-0.47368500
H	-3.42319700	-7.35466400	-0.55265100
H	-2.33216600	-6.17550900	-1.32992700
H	-2.39966100	-6.28140600	0.44580900
C	7.30654900	-2.84782400	-2.19787300
H	8.13548700	-3.26344000	-2.77680900
H	7.69577400	-2.10462900	-1.49395200
H	6.82300000	-3.64947800	-1.62697800
C	3.73903200	1.84065900	5.93175000
H	4.03678500	0.85705100	6.31313300
H	4.05970800	2.60205700	6.64811300
H	2.64856700	1.87477700	5.83161200

20'-TS

Cartesian coordinates:

C	-2.71302900	-1.05147200	1.56630200
C	-2.10908800	-1.86681500	2.53266700
H	-1.07325000	-2.15948600	2.39540500
C	-2.80142100	-2.33839100	3.65840700
C	-4.11470500	-1.83946000	3.86275800
C	-4.78927700	-1.07839600	2.88106000
C	-4.05148000	-0.70233800	1.74852400
H	-4.53567500	-0.09733000	0.99400100
C	-3.12248400	0.09708400	-1.03839100
C	-3.50877100	1.42688800	-1.19526200
H	-2.95627900	2.19499500	-0.66346000
C	-4.60792700	1.79445900	-2.00123300
C	-5.23043200	0.76442300	-2.74376000
C	-4.93949200	-0.61020400	-2.52544500
C	-3.87414600	-0.90165500	-1.67344900
H	-3.61192400	-1.93391300	-1.49334700

C	-1.14061400	-1.90527900	-0.75538800
C	-1.55313100	-3.18235700	-0.34934200
H	-2.14342500	-3.28468200	0.55160200
C	-1.29038200	-4.34820400	-1.08884800
H	-1.63134300	-5.32278500	-0.75694500
C	-0.61831400	-4.17533800	-2.27766400
C	0.15413500	-4.35608400	-4.34945700
H	1.03697400	-4.81288300	-4.79770700
H	-0.68187400	-4.29967300	-5.06193400
C	-0.18482600	-2.91721800	-2.68679800
C	-0.38962900	-1.75122600	-1.96127000
C	0.09780800	-0.47878200	-2.58423700
C	-0.44835100	-0.13788000	-3.81537800
C	-1.76656700	0.02465800	-5.61341500
H	-2.71406000	0.55036300	-5.43037200
H	-1.82799200	-0.59593900	-6.51175600
C	-0.00190100	0.92632900	-4.59416500
C	1.04983000	1.71617300	-4.18949500
H	1.42055000	2.53365700	-4.79804700
C	1.62388400	1.40384200	-2.94596700
H	2.44445400	2.02111000	-2.60223000
C	1.18300200	0.34731900	-2.13709700
C	3.46948200	1.17922600	-0.48609600
C	4.68037900	0.52979200	-0.73920800
H	4.67178600	-0.53716500	-0.91346000
C	5.91352200	1.19509800	-0.75350400
C	5.89363900	2.58193800	-0.48157000
C	4.68321000	3.31064300	-0.36610900
C	3.48966000	2.56930500	-0.31330500
H	2.55498300	3.08972400	-0.13072700
C	2.48719600	-1.49428800	-0.23161300
C	2.74404800	-1.98457800	1.04951900
H	2.50237400	-1.35899700	1.90437800
C	3.33782300	-3.24391300	1.26660700
C	3.56134600	-4.04267400	0.12427600
C	3.46108800	-3.52743500	-1.19587600
C	2.89962400	-2.25432800	-1.33771100

H	2.78492300	-1.82934000	-2.32660400
O	-0.24895600	-5.11936300	-3.20614700
O	0.47657800	-3.04343600	-3.89010800
O	-1.45406600	-0.79673900	-4.48702500
O	-0.71397800	0.98013700	-5.76638000
P	-1.75187600	-0.38161100	0.12237700
P	1.86125900	0.23975200	-0.40492900
C	-0.25584500	2.27369100	2.66716400
H	-0.11109000	3.32608100	2.89409000
Cu	-0.06057800	1.16400700	0.74285200
C	0.01930600	5.64360400	1.39600200
C	-1.50132200	5.42835400	1.01606600
B	-0.36433100	3.39065300	0.86709100
H	-0.21242600	2.68467000	-0.16198400
O	-1.64875700	3.99465700	0.98985000
O	0.63489000	4.41152300	0.95898500
C	0.68572800	6.81176000	0.65873800
H	0.17473600	7.75560100	0.88348000
H	1.72523000	6.91053500	0.98372800
H	0.68435800	6.66370900	-0.42284100
C	0.26348800	5.84806800	2.90479500
H	1.33592800	5.76065900	3.10627800
H	-0.06102000	6.84605200	3.22127700
H	-0.25521900	5.11745400	3.52922400
C	-1.83738700	5.96186200	-0.38580900
H	-2.86338200	5.68495800	-0.63638900
H	-1.76083500	7.05335800	-0.43822500
H	-1.17447200	5.53015300	-1.14229100
C	-2.50159600	6.00269100	2.02474300
H	-2.39407800	7.09041600	2.11440300
H	-3.52252800	5.79257000	1.68878500
H	-2.37786900	5.55739600	3.01447100
C	-1.61937700	1.90698300	3.26892700
H	-2.40549800	2.47784700	2.76651600
H	-1.86886100	0.84800200	3.17204200
H	-1.66394400	2.14887300	4.34419400
C	0.92935100	1.61904400	3.33285500

C	2.21957400	2.17811000	3.19077500
C	0.80831500	0.51870300	4.20427800
C	3.31698400	1.67517400	3.88195000
H	2.34269400	3.03458600	2.53556900
C	1.90927700	0.01648600	4.90527700
H	-0.16654800	0.07169700	4.36587200
C	3.17207800	0.59062000	4.75511800
H	4.29081200	2.14230100	3.75133600
H	1.76991600	-0.81672700	5.59102000
H	4.02349800	0.21106800	5.31363700
C	7.16285000	0.33497400	-1.09926900
C	4.57480700	4.86063900	-0.31347700
C	3.46631600	5.30294500	-1.30697600
H	3.71223000	4.98370600	-2.32711000
H	2.48198500	4.90997200	-1.04555100
H	3.38993100	6.39662000	-1.30808600
C	4.17718600	5.30498900	1.11353800
H	3.20719500	4.89113700	1.40143900
H	4.92175100	4.98853200	1.85326600
H	4.10785800	6.39934400	1.16184000
C	5.84470600	5.63756300	-0.73428300
H	6.64835300	5.58349200	0.00085700
H	6.24169000	5.28998800	-1.69247300
H	5.57388300	6.69500700	-0.84464900
C	8.50188200	1.08922300	-1.26001900
H	8.43214500	1.91075700	-1.97654200
H	8.87942500	1.49187600	-0.31816300
H	9.24977500	0.37639300	-1.62993300
C	7.35846700	-0.74590800	-0.00777000
H	7.55248000	-0.28694700	0.96894600
H	6.48025600	-1.39128500	0.09736100
H	8.21617700	-1.38355600	-0.25593600
C	6.90458700	-0.35975800	-2.46296300
H	6.01106400	-0.98958900	-2.45300700
H	6.78229200	0.38293000	-3.25986300
H	7.75696100	-0.99856600	-2.72400500
C	3.77615000	-3.58620600	2.71883900

C	4.06153700	-4.27822300	-2.41417000
C	3.97367200	-3.42928500	-3.70137500
H	2.94006300	-3.21583400	-3.99048900
H	4.50194600	-2.47466000	-3.60234100
H	4.44836400	-3.97838800	-4.52258700
C	5.56429900	-4.54779200	-2.14574800
H	6.11080900	-3.60880500	-2.00093200
H	5.70621700	-5.17191600	-1.26103400
H	6.00919300	-5.06441200	-3.00568900
C	3.35667700	-5.62668200	-2.70038400
H	3.69676000	-6.02028400	-3.66681200
H	3.59550400	-6.37432700	-1.94335400
H	2.26803400	-5.51525600	-2.74516900
C	4.61423300	-4.87301200	2.89767000
H	4.98886600	-4.88960600	3.92855100
H	4.04070700	-5.78991200	2.75229600
H	5.47585900	-4.90070400	2.22615500
C	2.53796200	-3.68026700	3.63823600
H	1.86859000	-4.49040400	3.32501900
H	2.84789300	-3.88289100	4.67103000
H	1.96519800	-2.74849500	3.64157000
C	4.68735300	-2.42808200	3.20979800
H	4.18594200	-1.45840100	3.20464700
H	5.01074200	-2.62538900	4.23927000
H	5.58420500	-2.35260500	2.58378300
C	-2.08452500	-3.39139900	4.55371300
C	-6.27813400	-0.62966300	2.91619500
C	-6.33950900	0.91497900	3.00601300
H	-5.87628500	1.27528000	3.93188000
H	-5.82296100	1.39620500	2.16891400
H	-7.38318500	1.25317100	2.99744100
C	-6.95866400	-1.08773300	1.59752900
H	-6.48423800	-0.67331600	0.70387800
H	-6.94108300	-2.18062000	1.51209700
H	-8.00681800	-0.76595800	1.59198400
C	-7.14428800	-1.20801600	4.05779100
H	-7.09622900	-2.29876900	4.10239400

H	-6.87220700	-0.81678800	5.03960700
H	-8.18672900	-0.92051900	3.87196100
C	-0.91951800	-2.72690400	5.32192200
H	-0.19742500	-2.26527400	4.64257000
H	-1.28264900	-1.94793100	6.00207700
H	-0.38650800	-3.47421400	5.92293600
C	-2.98141300	-4.12893300	5.57548100
H	-3.29599700	-3.49630300	6.40601700
H	-3.87925900	-4.54510400	5.11041700
H	-2.40270800	-4.95944000	5.99867900
C	-1.50743000	-4.50162100	3.63331600
H	-0.78085600	-4.12482300	2.90859500
H	-0.99770200	-5.25681700	4.24308100
H	-2.31032000	-5.00293400	3.07969900
C	-5.05973100	3.28165100	-1.95598600
C	-5.79166400	-1.75896700	-3.12648800
C	-7.27784500	-1.57003100	-2.73264800
H	-7.39615400	-1.59531800	-1.64301300
H	-7.67379300	-0.62235800	-3.10139900
H	-7.88140600	-2.38441400	-3.15299100
C	-5.67027600	-1.83034400	-4.66737900
H	-6.14744300	-2.74728500	-5.03475200
H	-6.16320400	-0.98929400	-5.15591300
H	-4.61834000	-1.85504000	-4.97728300
C	-5.35068600	-3.13601900	-2.58133700
H	-4.32811900	-3.39575400	-2.87796100
H	-5.41517500	-3.18657700	-1.48893200
H	-6.01556700	-3.90720900	-2.98604200
C	-5.06710500	3.74442400	-0.47201700
H	-5.76723700	3.13835800	0.11561000
H	-4.08796900	3.69423800	0.00788200
H	-5.40608000	4.78613500	-0.41957400
C	-6.49411400	3.55482300	-2.46920200
H	-6.76593700	4.58086500	-2.19341800
H	-6.59862800	3.47690300	-3.55130300
H	-7.22349400	2.88046900	-2.01073200
C	-4.06058000	4.15626900	-2.74940200

H	-4.05522600	3.90158100	-3.81508600
H	-4.33058400	5.21616100	-2.66497500
H	-3.03986300	4.03648500	-2.37496500
O	7.09774000	3.24637300	-0.33576600
O	3.92535800	-5.37283000	0.26794900
O	-6.20393500	1.06436800	-3.68567200
O	-4.75855700	-2.11678100	5.05365500
C	-5.71251900	1.54598500	-4.93322000
H	-6.58821100	1.70515200	-5.56799700
H	-5.17089600	2.49080400	-4.82551200
H	-5.05094100	0.81329900	-5.41133000
C	-4.49461200	-1.16735700	6.08313300
H	-5.07923900	-1.48075800	6.95184300
H	-3.43021500	-1.14611600	6.34936800
H	-4.79927900	-0.15610000	5.78415100
C	7.55781600	3.31525500	1.00970300
H	7.67173600	2.31455000	1.44718500
H	8.53198000	3.81035000	0.98040600
H	6.87470100	3.89702800	1.64139700
C	2.81909600	-6.23295300	0.54492800
H	3.22815300	-7.24248000	0.63606400
H	2.31824900	-5.95867400	1.48048300
H	2.08292000	-6.20758300	-0.26717400

20-I-TS

Cartesian coordinates:

C	2.93175100	-1.02417900	1.28980000
C	2.39505300	-1.93433200	2.21407500
H	1.32829600	-1.91192700	2.39657800
C	3.19149800	-2.85227200	2.90374400
C	4.58295200	-2.85309300	2.60781700
C	5.12370000	-2.10202700	1.54146000
C	4.27599900	-1.14872900	0.94803400
H	4.67659800	-0.50123600	0.17893900
C	2.91405400	1.17140400	-0.62169900
C	3.79973500	2.09897800	-0.06936300
H	3.82704200	2.20137200	1.00796100

C	4.65590000	2.88714000	-0.85331800
C	4.51485100	2.76397800	-2.26105900
C	3.71300900	1.75433400	-2.85706400
C	2.91510700	0.98044700	-2.00507300
H	2.27024100	0.21371600	-2.41312500
C	1.28511200	1.37045600	1.73533000
C	1.68020900	1.18689100	3.06767900
H	2.28581100	0.32564500	3.32132600
C	1.35412900	2.08512700	4.09882600
H	1.67870700	1.92182800	5.12080700
C	0.62897300	3.19653100	3.73363200
C	-0.21082700	5.24064800	3.57684800
H	-1.11543300	5.73576600	3.93036600
H	0.61514100	5.95440900	3.43699400
C	0.22505000	3.39532100	2.41610300
C	0.49570900	2.51238600	1.37968500
C	0.04664800	2.92458000	0.00946100
C	0.58803400	4.09821800	-0.49947300
C	1.56127400	6.09011800	-0.69121100
H	2.58880800	6.42458300	-0.83462600
H	0.95563600	6.85672100	-0.18432900
C	0.23279200	4.64940600	-1.72794700
C	-0.72345000	4.06484700	-2.52668200
H	-1.01392600	4.49085100	-3.48080900
C	-1.31962700	2.89480800	-2.02793500
H	-2.09078700	2.42535700	-2.62646700
C	-0.96922500	2.31672600	-0.79867600
C	-3.14002800	0.48584600	-1.52498400
C	-4.40716800	0.99854600	-1.25113100
H	-4.55300000	1.56007100	-0.33673500
C	-5.50388600	0.80172100	-2.10598400
C	-5.28452300	-0.01946600	-3.23606800
C	-3.98365900	-0.42990700	-3.63466900
C	-2.93760900	-0.18865100	-2.73697600
H	-1.94141200	-0.54556500	-2.96718500
C	-2.54692600	0.90228700	1.26256100
C	-3.02454900	2.13810300	1.71856000

H	-2.85600200	3.01483500	1.10671500
C	-3.69567100	2.26360800	2.93973600
C	-3.85208800	1.08489300	3.71917000
C	-3.53923200	-0.19994800	3.22063700
C	-2.83141900	-0.24258700	2.00669000
H	-2.50478900	-1.20203800	1.61972100
O	0.18362400	4.23767600	4.51725800
O	-0.48069200	4.57942300	2.33995000
O	1.55442700	4.89063000	0.08354100
O	0.97564300	5.78527300	-1.95961900
P	1.79045900	0.14729100	0.42589600
P	-1.71147200	0.67149600	-0.36419900
C	-0.48330200	-2.94909300	-0.15550500
H	0.26993000	-3.73819800	-0.19592700
Cu	-0.06177700	-0.93216300	-0.54634000
C	0.79237000	-4.07141400	-3.64796800
C	2.06310400	-4.03673900	-2.70187900
B	0.56241700	-2.37346200	-2.08056000
H	0.39295700	-1.13899400	-2.25784700
O	1.91229600	-2.77872400	-2.01272100
O	-0.14676000	-3.20837200	-2.97285900
C	1.05659300	-3.46329500	-5.03560600
H	1.73993600	-4.08051100	-5.62960000
H	0.10839100	-3.38725700	-5.57685900
H	1.47779400	-2.45694500	-4.95416400
C	0.14956800	-5.45114400	-3.81583900
H	-0.73271800	-5.36617300	-4.45941000
H	0.84423400	-6.15636300	-4.28778700
H	-0.17386500	-5.86679000	-2.85894000
C	3.40794400	-4.01236900	-3.43640500
H	4.22045000	-3.95578700	-2.70412800
H	3.55204000	-4.92266100	-4.03060300
H	3.49335400	-3.14755600	-4.09810900
C	2.09526900	-5.17779000	-1.66997200
H	2.33936900	-6.13606500	-2.14293100
H	2.86692100	-4.95616400	-0.92526000
H	1.14372800	-5.29179800	-1.14649000

C	-1.87030600	-3.48435800	-0.52403400
H	-2.61918900	-2.68852400	-0.39777100
H	-1.88085800	-3.71432200	-1.59683800
C	-3.69562500	-1.05120100	-5.02587600
C	-2.17813800	-1.20427500	-5.26665000
H	-1.65194500	-0.24594600	-5.18279300
H	-1.71017300	-1.91552200	-4.57880300
H	-2.01904300	-1.57486100	-6.28610700
C	-4.32222800	-2.45622300	-5.19081300
H	-4.03276300	-3.11779300	-4.36609900
H	-5.41080400	-2.41542500	-5.24682300
H	-3.96290100	-2.91084900	-6.12225900
C	-4.24296000	-0.10950900	-6.12785900
H	-3.76116300	0.87417400	-6.07190700
H	-4.02596100	-0.53111000	-7.11734300
H	-5.32252500	0.02825200	-6.04235900
C	-6.82232700	1.54138400	-1.73898500
C	-6.48056800	3.02838500	-1.44385700
H	-5.79450800	3.15130700	-0.60143300
H	-6.02658100	3.50572300	-2.31975900
H	-7.39858400	3.57494400	-1.19833100
C	-7.89612500	1.58362800	-2.85103800
H	-7.48441600	1.93824800	-3.80007100
H	-8.37390100	0.62049600	-3.03133900
H	-8.68376000	2.28181400	-2.54218500
C	-7.44059700	0.91779000	-0.46471800
H	-7.72217400	-0.12924500	-0.62375400
H	-6.74179600	0.94731800	0.37860400
H	-8.34477600	1.46661000	-0.17298400
C	-3.95325600	-1.56180600	3.84807000
C	-2.70278000	-2.31126000	4.36532600
H	-1.97542600	-2.48213700	3.56504400
H	-2.19860900	-1.75430300	5.16386400
H	-2.98875600	-3.29075400	4.76726100
C	-4.99807700	-1.48399400	4.98560900
H	-5.33841300	-2.50311900	5.20497600
H	-4.60383800	-1.07144100	5.91489900

H	-5.87163300	-0.89268800	4.69705000
C	-4.61759800	-2.42052700	2.73670800
H	-5.49875200	-1.91246000	2.32765400
H	-3.94326500	-2.65149200	1.90968600
H	-4.94214300	-3.37902100	3.15690100
C	-4.32668300	3.61698700	3.35845600
C	-3.74482700	4.16358700	4.68561300
H	-4.05318500	5.20784200	4.82211500
H	-4.10666600	3.60167000	5.54697100
H	-2.64963200	4.12986800	4.68755900
C	-4.10487700	4.70218900	2.28183600
H	-3.04327200	4.92225600	2.12793600
H	-4.53880100	4.41975600	1.31597000
H	-4.59898300	5.62691100	2.60084300
C	-5.85671800	3.43033100	3.51662500
H	-6.09006000	2.68755200	4.28246900
H	-6.32259900	4.38111300	3.80550600
H	-6.30991300	3.10933100	2.57115900
C	3.72935500	1.45831800	-4.37901600
C	5.69433900	3.78878400	-0.12342800
C	7.01526800	3.94741000	-0.91349700
H	6.89674800	4.47566600	-1.85767700
H	7.73640000	4.50092500	-0.30015900
H	7.45133600	2.96763300	-1.13966900
C	5.09189400	5.17725500	0.20059300
H	4.17185000	5.07011600	0.78470000
H	5.80517200	5.77041000	0.78681200
H	4.85483500	5.74765100	-0.70135800
C	6.09610800	3.15653800	1.23585700
H	5.28323900	3.16372900	1.96819700
H	6.43848600	2.12342100	1.11549000
H	6.91929600	3.73506900	1.66988900
C	5.17675200	1.15615200	-4.84047800
H	5.18700800	0.93929400	-5.91608800
H	5.84485300	1.99804400	-4.65174000
H	5.57170700	0.27603900	-4.31904300
C	3.14795800	2.63274500	-5.20181500

H	3.79595400	3.50887100	-5.18751100
H	3.03219500	2.32761200	-6.24920500
H	2.15927400	2.92371400	-4.82736700
C	2.87817100	0.21511600	-4.71976000
H	3.20378000	-0.67293800	-4.16831400
H	1.81275900	0.36999800	-4.51489400
H	2.97798100	-0.00007800	-5.78965900
C	2.54752000	-3.88471300	3.86542800
C	3.06368400	-3.75169800	5.31862500
H	4.10132100	-4.07079500	5.41496100
H	2.97591100	-2.71955600	5.67965900
H	2.46157000	-4.38565100	5.98101500
C	1.01308600	-3.72577200	3.92528900
H	0.71312000	-2.75557300	4.33897300
H	0.54248600	-3.84179100	2.94383600
H	0.59926900	-4.50133800	4.57912300
C	2.84555900	-5.31271300	3.34397900
H	3.91962200	-5.50719100	3.30737400
H	2.38264300	-6.05740200	4.00385200
H	2.43291900	-5.45138000	2.33790100
C	6.54370200	-2.26336200	0.92535400
C	7.41462800	-1.02818600	1.25464700
H	6.95433100	-0.10584400	0.88434100
H	7.56801900	-0.91311100	2.33362500
H	8.40144700	-1.12224000	0.78457000
C	6.39618000	-2.35902900	-0.61874000
H	5.77451100	-3.21724700	-0.89644300
H	5.94991400	-1.46711100	-1.06560300
H	7.38473000	-2.49337900	-1.07348300
C	7.30633600	-3.54278800	1.34229900
H	7.65929500	-3.52491000	2.37370300
H	6.69460000	-4.43967100	1.21087000
H	8.19050100	-3.64020700	0.70056300
O	5.21592400	3.59473000	-3.12230900
O	5.40346200	-3.66056700	3.38232000
O	-4.36029500	1.22961100	5.00090500
O	-6.35549100	-0.43446100	-4.01233400

C	-7.07073900	-1.54212700	-3.46271700
H	-7.83790000	-1.80644900	-4.19510500
H	-6.41049700	-2.40132800	-3.29893400
H	-7.55240400	-1.28430700	-2.51287600
C	-3.36563200	1.15707700	6.02413100
H	-3.88701000	1.31536500	6.97175400
H	-2.87308600	0.17895600	6.04190000
H	-2.60190400	1.93219800	5.89255200
C	6.15834400	-2.94991500	4.36274600
H	6.71416400	-3.70209300	4.92881400
H	6.86532000	-2.24964000	3.90466400
H	5.50430200	-2.39229500	5.04357100
C	4.70995700	4.91612900	-3.31138000
H	5.23338100	5.63279600	-2.66844800
H	4.89986700	5.19051900	-4.35329600
H	3.63302000	4.96901900	-3.11648400
H	-0.48375200	-2.64704700	0.90859700
C	-2.38603800	-4.71814000	0.21526600
C	-1.58392300	-5.51020300	1.04648200
C	-3.72714100	-5.10595200	0.04617000
C	-2.09670800	-6.64512000	1.68337800
H	-0.54426200	-5.23772300	1.19920700
C	-4.24612800	-6.23424700	0.67901900
H	-4.37106800	-4.50712700	-0.59637400
C	-3.42957200	-7.01303100	1.50476400
H	-1.44848600	-7.24077000	2.32228000
H	-5.28819600	-6.50764800	0.52892200
H	-3.82954100	-7.89383700	2.00076000

21

Cartesian coordinates:

C	3.32934400	-1.37433200	-0.81647500
C	2.26924400	-0.47234600	-0.90918800
C	2.09949000	0.54423300	0.04538400
C	3.02095300	0.61871200	1.09911300
C	4.08123200	-0.28417300	1.19677200
C	4.24124700	-1.28451600	0.23730800

H	3.44136200	-2.15182900	-1.56832100
H	1.55859000	-0.55913300	-1.72685700
H	2.90611300	1.39634000	1.85110100
H	4.78310900	-0.20340200	2.02319300
H	5.06677800	-1.98771300	0.30994400
C	0.95038500	1.54295200	-0.06065100
H	1.00444600	2.19781200	0.81853300
C	1.06456700	2.42236300	-1.32813400
H	0.97189000	1.82255000	-2.23910800
H	0.27274800	3.18075900	-1.35269300
H	2.03046000	2.93979800	-1.36050500
B	-0.43009700	0.77298100	0.00604500
O	-1.02396200	0.18935700	-1.08847100
O	-1.14960400	0.59935500	1.16148700
C	-2.12297300	-0.63799100	-0.60682300
C	-2.42816400	-0.00097400	0.80625600
C	-2.81271700	-0.99575700	1.89995200
H	-3.74608500	-1.51264200	1.64867100
H	-2.03171900	-1.74243800	2.05941100
H	-2.96532800	-0.46155800	2.84321000
C	-3.44851500	1.14419500	0.75394700
H	-3.45435000	1.65790700	1.72025200
H	-3.18638600	1.87713300	-0.01566300
H	-4.46034000	0.77661800	0.55296200
C	-1.58885900	-2.07438600	-0.52756100
H	-2.36798100	-2.77855200	-0.21719100
H	-1.22959900	-2.37445100	-1.51689900
H	-0.75029300	-2.15111600	0.17141900
C	-3.26471900	-0.55814700	-1.61842400
H	-2.94008300	-0.98764300	-2.57161700
H	-4.13550800	-1.12585800	-1.27078800
H	-3.57190800	0.47381000	-1.80225700

22

Cartesian coordinates:

C	5.03290600	0.86739400	-0.89166400
C	3.67531700	1.04253100	-0.61959700

C	3.00162000	0.19816500	0.27356300
C	3.73082200	-0.82726400	0.89123800
C	5.08846500	-1.00763500	0.62371500
C	5.74509900	-0.16013700	-0.27059200
H	5.53571200	1.53713100	-1.58501700
H	3.12865900	1.84963200	-1.10361600
H	3.22782700	-1.48948900	1.59340600
H	5.63483900	-1.80747100	1.11750400
H	6.80324100	-0.29643900	-0.47801400
C	1.51947300	0.36639400	0.53482300
H	1.24363300	1.42313600	0.43858000
H	1.29732100	0.08798200	1.57300500
C	0.63355600	-0.47290700	-0.41566700
H	0.88642000	-0.22110900	-1.45763500
H	0.87720900	-1.53950400	-0.31927300
B	-0.91524500	-0.26790300	-0.22169700
O	-1.47126900	0.86184500	0.33043800
O	-1.85785100	-1.19278400	-0.60370500
C	-2.89421000	0.61456500	0.51612500
C	-3.16616400	-0.56280200	-0.50065000
C	-3.65060400	1.91098600	0.23154700
H	-4.73318100	1.75720300	0.30777200
H	-3.36460400	2.67081800	0.96593600
H	-3.42320300	2.30237000	-0.76255600
C	-3.07946600	0.20965300	1.98483800
H	-2.67993300	1.00288300	2.62426900
H	-4.13565600	0.06439600	2.23513900
H	-2.53834300	-0.71359200	2.21501400
C	-3.53321500	-0.07999900	-1.91061000
H	-3.50611400	-0.93322400	-2.59538900
H	-4.53764900	0.35526700	-1.94163900
H	-2.82043200	0.66674800	-2.27474700
C	-4.17113800	-1.61253400	-0.02949300
H	-3.85939300	-2.07918900	0.90760500
H	-5.16317000	-1.16875300	0.11346600
H	-4.25875700	-2.40023500	-0.78465200

15

Cartesian coordinates:

C	2.56321900	-0.54912700	1.33936900
C	3.17244000	-1.76471100	1.67149300
H	3.15405600	-2.56957700	0.94826000
C	3.78392900	-1.96453700	2.91457200
C	3.74440100	-0.88628300	3.84048200
C	3.29402800	0.40424000	3.48039100
C	2.65087500	0.51458000	2.23689800
H	2.21603600	1.46598700	1.94675800
C	4.55294200	-3.27801900	3.21281700
C	4.55985900	-4.22066100	1.98905700
H	5.02409900	-3.75408100	1.11299800
H	3.55248000	-4.54563900	1.70904900
H	5.14748100	-5.11360300	2.23089900
C	6.02976100	-2.93948200	3.53699300
H	6.58925700	-3.86145200	3.74034100
H	6.10818700	-2.29034400	4.41133900
H	6.50862800	-2.43788200	2.68763100
C	3.94121600	-4.06853300	4.39558400
H	4.38160500	-5.07287500	4.43670500
H	2.85601800	-4.17820000	4.28635200
H	4.14293400	-3.58577400	5.35212200
C	3.14724000	-1.30663400	6.08265200
H	2.54286300	-0.39988300	6.19304900
H	3.63272300	-1.53398500	7.03531200
H	2.48721900	-2.13530000	5.80132600
C	3.49144700	1.71662100	4.29148900
C	4.48808000	1.62726300	5.47046400
H	4.68122400	2.64395600	5.83366100
H	5.44341900	1.19271100	5.16294700
H	4.11299900	1.05070200	6.31652400
C	2.12968600	2.22622700	4.81869900
H	1.42163200	2.39646700	4.00085000
H	2.26072300	3.17623000	5.35146200
H	1.67020200	1.51361400	5.51301300
C	4.08011800	2.79112200	3.33448900

H	3.41959000	3.02803800	2.49648400
H	5.04138600	2.46221200	2.92364900
H	4.24903900	3.72164300	3.88888700
C	3.27631400	0.39656700	-1.26823600
C	3.17454400	1.55969600	-2.02698100
H	2.23289700	2.09524500	-2.02499400
C	4.25245900	2.06464400	-2.78002700
C	5.48341200	1.37974800	-2.65995100
C	5.59851600	0.12852800	-1.98761000
C	4.48047800	-0.32062600	-1.28445100
H	4.53597900	-1.24895400	-0.73233900
C	3.97742500	3.30534600	-3.67478900
C	4.00298400	4.59076000	-2.81242500
H	3.79070500	5.46598500	-3.43949100
H	4.97465100	4.75208600	-2.33436000
H	3.23887800	4.54257600	-2.03064400
C	2.55371200	3.19080200	-4.28926100
H	2.42418700	2.24016500	-4.82020900
H	2.41154400	4.00139800	-5.01341700
H	1.76206000	3.28946000	-3.54268600
C	4.94206800	3.44492000	-4.87613000
H	4.99064300	2.51803800	-5.45809800
H	5.96018000	3.71252900	-4.59652300
H	4.56441300	4.23508300	-5.53585000
C	7.28580300	2.92594300	-2.51775900
H	6.77399900	3.88504900	-2.64271600
H	8.29520900	3.00719100	-2.93028100
H	7.34740600	2.69208000	-1.44895600
C	6.86703100	-0.75952700	-2.08489600
C	8.10377800	-0.10621300	-1.42270000
H	8.92385100	-0.83343000	-1.37530600
H	7.88246000	0.21212500	-0.39699400
H	8.46380400	0.75450200	-1.98588000
C	7.17299900	-1.05548700	-3.57454200
H	7.35422900	-0.13675000	-4.13508000
H	6.33733200	-1.58885200	-4.04331100
H	8.06345500	-1.69188200	-3.65448600

C	6.65948900	-2.12187200	-1.38591800
H	7.55415700	-2.73713200	-1.53207400
H	5.80894900	-2.67476500	-1.80011800
H	6.50940600	-2.01519300	-0.30504300
C	1.34222700	-1.78725900	-1.07528600
C	1.86325300	-2.07619900	-2.34646600
H	2.56110100	-1.38150700	-2.79629400
C	1.54361200	-3.23795800	-3.06675300
H	1.97026200	-3.43868900	-4.04332500
C	0.68204100	-4.11745100	-2.45200000
C	-0.39373400	-5.92770400	-1.76202700
H	-1.31446800	-6.42928400	-2.06077100
H	0.31430300	-6.62828000	-1.29413600
C	0.13253700	-3.83833800	-1.20321500
C	0.39583300	-2.68285700	-0.47681500
C	-0.24488200	-2.58361600	0.87585100
C	0.07876800	-3.57904200	1.78879800
C	0.73795200	-5.50019300	2.69826600
H	1.68420500	-5.88245200	3.08203900
H	0.08154400	-6.31301300	2.35286900
C	-0.47484500	-3.68079200	3.06237500
C	-1.41510800	-2.77964100	3.50702300
H	-1.85519600	-2.84874600	4.49580600
C	-1.79184600	-1.77549200	2.59960300
H	-2.54812000	-1.06767100	2.91538800
C	-1.25037600	-1.65718800	1.31062000
C	-3.12722100	0.59149500	1.23084800
C	-4.46996100	0.19065900	1.21907800
H	-4.74881800	-0.66695000	0.62178200
C	-5.45211100	0.88429900	1.93461900
C	-5.03578200	2.02728600	2.67182200
C	-3.67378300	2.35899300	2.84602400
C	-2.75388000	1.65361300	2.05293200
H	-1.71093400	1.94912300	2.06589400
C	-6.91186400	0.36195500	1.98156200
C	-7.06032900	-0.96666400	1.21143000
H	-8.08898300	-1.32895600	1.31735600

H	-6.39564600	-1.74603900	1.59902200
H	-6.86302100	-0.84637800	0.14008400
C	-7.30681100	0.08412600	3.45377300
H	-8.33463900	-0.29762400	3.50028400
H	-7.24908200	0.99009900	4.06006900
H	-6.64818800	-0.67298600	3.89604300
C	-7.92298000	1.35289200	1.35609400
H	-7.60718100	1.66154500	0.35248900
H	-8.05665700	2.24250100	1.97129100
H	-8.90265400	0.86819700	1.26176100
C	-6.30082900	4.01824500	2.54238400
H	-5.44726100	4.70292000	2.55901100
H	-7.14774100	4.48463000	3.05250900
H	-6.56785300	3.81666300	1.49887900
C	-3.09245300	3.39933800	3.84444000
C	-4.05826600	3.84657300	4.96630800
H	-4.87024800	4.48324200	4.61577000
H	-3.48749900	4.42563200	5.70250500
H	-4.50230500	2.99033200	5.48368100
C	-2.57988200	4.64046700	3.07652500
H	-3.40469800	5.20904000	2.63351900
H	-1.90912700	4.36020700	2.25839100
H	-2.04255100	5.31159500	3.75880100
C	-1.88724900	2.74774700	4.57798100
H	-1.49012400	3.44860700	5.32130200
H	-1.06517200	2.49180800	3.90519300
H	-2.19284300	1.83497400	5.10284200
C	-2.67547800	-0.98300300	-1.18434300
C	-3.33943300	-2.20989400	-1.14628500
H	-3.31634700	-2.78335000	-0.22651200
C	-4.03607700	-2.72125700	-2.25706500
C	-3.94748300	-1.97467600	-3.45759200
C	-3.39168300	-0.66790900	-3.50359700
C	-2.74531400	-0.21208800	-2.35125400
H	-2.26993700	0.76100900	-2.34744500
C	-4.86856800	-4.02274100	-2.05680400
C	-5.61643800	-3.94630200	-0.69868500

H	-6.28552300	-3.08069600	-0.66675300
H	-4.94383600	-3.88798300	0.16134400
H	-6.22587200	-4.84803900	-0.56844000
C	-5.97358600	-4.25536800	-3.11500500
H	-6.61848800	-5.07212400	-2.76851900
H	-5.58922800	-4.53875700	-4.09414600
H	-6.59828600	-3.36656400	-3.24576900
C	-3.93664400	-5.25563400	-2.00703700
H	-4.52286500	-6.16555400	-1.82559000
H	-3.19910800	-5.15386500	-1.20500700
H	-3.39216300	-5.39070500	-2.94816800
C	-3.58484600	-3.42968500	-5.29035400
H	-2.56482800	-3.04007500	-5.38050700
H	-4.00158400	-3.59317100	-6.28775200
H	-3.55100700	-4.38614500	-4.75759800
C	-3.54505900	0.26614700	-4.73230800
C	-5.05045200	0.43560200	-5.05755100
H	-5.51941000	-0.52059400	-5.29807200
H	-5.17256400	1.10629300	-5.91733600
H	-5.58231700	0.88067700	-4.20833700
C	-2.80397200	-0.26593100	-5.98226400
H	-3.28189700	-1.15380400	-6.39707000
H	-1.75789200	-0.50184300	-5.75294800
H	-2.80615800	0.50315000	-6.76434800
C	-2.97909700	1.67383000	-4.44305000
H	-3.16407600	2.31598300	-5.31135400
H	-1.89735400	1.66253300	-4.26855600
H	-3.45765500	2.14455100	-3.57797900
O	4.19613000	-1.13133900	5.12865100
O	6.63725800	1.88047000	-3.24313500
O	0.21742700	-5.32785400	-2.90655000
O	-0.69916900	-4.87844100	-0.84129100
O	0.98983500	-4.60162700	1.61692400
O	0.07265900	-4.75626500	3.72279100
O	-6.02439300	2.80749700	3.25052200
O	-4.44551900	-2.49190000	-4.64362700
P	1.81092100	-0.16798400	-0.29998100

P	-1.79615200	-0.23093600	0.24998100
Cu	-0.03728600	1.15455800	-0.27082000
H	0.07545400	2.74431400	0.47402000
H	-0.34736300	2.30778200	-1.53985700
C	-1.38470000	5.25831200	-1.16813400
C	0.15797400	5.54884600	-1.05509200
B	-0.26174600	3.29271800	-0.66943800
O	0.72374300	4.23357100	-1.16684600
O	-1.50531100	4.00400000	-0.48787000
C	-1.84119000	5.07117300	-2.62724300
H	-2.85956100	4.66781600	-2.62748700
H	-1.84655600	6.01472000	-3.18539800
H	-1.19488600	4.36103100	-3.15215900
C	0.71874100	6.43882300	-2.16716400
H	0.21506300	7.41341200	-2.17950400
H	1.78706700	6.61675800	-2.00534800
H	0.60071100	5.97358900	-3.14895200
C	0.55307700	6.12972000	0.31498900
H	1.64455200	6.10501500	0.40498900
H	0.22335600	7.16830600	0.43668500
H	0.13225900	5.53345100	1.13030300
C	-2.28732800	6.28569800	-0.48126500
H	-3.33542500	5.98278800	-0.58556900
H	-2.06587800	6.36641100	0.58533800
H	-2.17610700	7.27721800	-0.93738200

23-TS

Cartesian coordinates:

P	1.78858000	-0.34001300	-0.24753200
P	-1.76865500	0.32635400	-0.24135100
O	1.00459800	1.17853000	4.23185100
O	0.27516300	3.34449400	4.51995400
O	-0.99904300	-1.21585200	4.21179500
O	-0.26201000	-3.38042100	4.49550100
O	-4.60409900	-4.32468400	2.31782600
O	-5.61712700	3.43225400	-3.64329700
O	4.48456500	4.39028600	2.31863900

O	5.70530200	-3.31255900	-3.67766200
C	-1.19431800	1.28134700	1.24352900
C	-0.24632500	0.69502200	2.14576200
C	0.13383800	1.50107200	3.21082100
C	-0.31538800	2.80630200	3.39695600
C	-1.21066800	3.38887300	2.52906200
C	-1.64566400	2.59074700	1.45705400
C	0.82942800	2.21428600	5.19859500
C	1.23630200	-1.29026600	1.24964600
C	1.69554900	-2.59654800	1.46267700
C	1.25322000	-3.40229500	2.52624700
C	0.34115200	-2.83143800	3.38438200
C	-0.11351200	-1.52758500	3.20031000
C	0.27559200	-0.71391100	2.14470900
C	-0.83687500	-2.26004500	5.17219300
C	-2.73356000	-1.04805500	0.53055100
C	-3.55598700	-0.85711000	1.64296100
C	-4.26424600	-1.90716400	2.24758700
C	-4.04845100	-3.20642200	1.71346100
C	-3.31991200	-3.42138600	0.51320500
C	-2.65625300	-2.31931700	-0.04006400
C	-3.25855100	-4.79547600	-0.20316800
C	-2.45101800	-5.82866400	0.61786400
C	-4.68929700	-5.32762400	-0.46541700
C	-2.56582800	-4.68319800	-1.58031700
C	-5.23069500	-1.56494400	3.41918100
C	-6.49604600	-2.45566700	3.42837400
C	-5.74728300	-0.10733200	3.29532800
C	-4.49918100	-1.64915400	4.78097800
C	-3.96011100	-4.84086500	3.48253400
C	-3.05369600	1.37611800	-1.06181700
C	-2.63680300	2.54135900	-1.72467200
C	-4.39253000	1.00400400	-1.16227200
C	-5.31955100	1.70839100	-1.95485600
C	-4.81804500	2.79517000	-2.70465400
C	-3.50021100	3.29840600	-2.51939000
C	-3.03693200	4.66032500	-3.09970400

C	-1.62090700	5.03173200	-2.60622200
C	-2.98654100	4.67091100	-4.64626700
C	-5.69882300	2.75281100	-4.89689700
C	-3.99908700	5.77132800	-2.60929600
C	-6.80047000	1.23366100	-1.90251500
C	-6.95567400	-0.09675500	-2.67858800
C	-7.83888400	2.25507400	-2.42389100
C	-7.19108600	0.97325700	-0.42210600
C	2.71550500	1.06548100	0.51489200
C	2.60472400	2.33656200	-0.05260500
C	3.23022800	3.45667900	0.50959000
C	3.96460800	3.25816000	1.70944700
C	4.22062700	1.96408500	2.23633400
C	3.53979300	0.89728100	1.62982100
C	5.20581000	1.64419000	3.39873900
C	6.43893200	2.57906800	3.41067900
C	4.48152500	1.68479500	4.76622200
C	5.77474200	0.20853800	3.25174300
C	4.54642200	5.40102000	-0.46372800
C	3.83644400	4.86931600	3.49730700
C	3.12994400	4.83531000	-0.19354400
C	2.42760000	4.72184900	-1.56469200
C	4.87463000	-2.73692300	-2.72193100
C	5.36856500	-1.66582300	-1.93784300
C	7.64286200	-2.59713600	-1.38762500
C	4.43974000	-0.98825000	-1.13013200
C	3.09519000	-1.36409700	-1.06746800
C	2.69565100	-2.52529200	-1.74268500
C	3.57493700	-3.27411100	-2.53387900
C	5.56463700	-2.72638000	-4.97885300
C	7.50274300	-0.81246800	-3.15977300
C	3.06259600	-4.80617400	-4.57899600
C	3.15258700	-4.68177500	-3.03980800
C	1.76778500	-5.08191200	-2.48179000
C	7.14464700	-0.23370400	-0.77776700
C	2.30729100	5.84310600	0.64411700
C	6.88188900	-1.32457300	-1.83853500

C	4.17742400	-5.71779800	-2.51252400
H	-1.57704900	4.39934900	2.67474100
H	-2.37667600	3.01084100	0.77684000
H	1.79613300	2.48258700	5.62435500
H	0.12685900	1.87458400	5.97501000
H	2.43394400	-3.00896900	0.78543500
H	1.62413000	-4.41119700	2.67152200
H	-1.81058300	-2.53792800	5.57571000
H	-0.15321300	-1.92275200	5.96643900
H	-3.64559200	0.14296500	2.04788100
H	-2.03475700	-2.43638600	-0.92024000
H	-1.45821500	-5.43808100	0.87079200
H	-2.31179500	-6.74381500	0.02877800
H	-2.95659100	-6.10931000	1.54193900
H	-5.24835100	-5.46277300	0.46134600
H	-4.63720700	-6.29278100	-0.98493600
H	-5.24642900	-4.63400600	-1.10677000
H	-3.06354500	-3.95775400	-2.23337000
H	-2.60632300	-5.65909500	-2.07743700
H	-1.51093900	-4.39980200	-1.49922400
H	-7.17386400	-2.11196700	4.21901100
H	-6.28311500	-3.51004300	3.59471500
H	-7.02950700	-2.37684100	2.47391600
H	-6.51737700	0.06313300	4.05607800
H	-6.19610300	0.08326600	2.31539100
H	-4.96460200	0.63851800	3.46458200
H	-3.62730300	-0.98658400	4.78531400
H	-4.15655700	-2.66100000	5.01014600
H	-5.17219400	-1.33745700	5.58986600
H	-2.92179000	-4.49968800	3.55768400
H	-3.97411000	-5.93292200	3.41169800
H	-4.50681600	-4.55124400	4.38714400
H	-1.60082900	2.83955700	-1.62690300
H	-4.72624100	0.12903700	-0.61970100
H	-1.36494100	6.03015500	-2.97792500
H	-0.85621000	4.33944400	-2.97611600
H	-1.55857900	5.06197800	-1.51264500

H	-3.98296900	4.64517900	-5.08794100
H	-2.40661600	3.82337800	-5.03038400
H	-2.49850600	5.59063300	-4.99182600
H	-6.24060200	1.80470900	-4.81126400
H	-4.70332400	2.55192400	-5.30835500
H	-6.24487200	3.41703000	-5.57212100
H	-5.02269400	5.58813700	-2.94199500
H	-3.67738700	6.74461500	-3.00101500
H	-3.99548400	5.83333200	-1.51443700
H	-6.29381300	-0.87157200	-2.27604200
H	-6.71845500	0.02095700	-3.74143400
H	-7.98759100	-0.46238500	-2.60453200
H	-8.84084600	1.89355800	-2.16231700
H	-7.81688100	2.38818500	-3.50507000
H	-7.70457200	3.23788900	-1.96233400
H	-7.05064500	1.87397300	0.18624700
H	-6.61627300	0.16314300	0.03338300
H	-8.24813400	0.68846900	-0.36707400
H	1.99400100	2.44104700	-0.94070100
H	3.65412300	-0.10036500	2.03452300
H	6.19173300	3.62260900	3.59630700
H	6.96584600	2.53380100	2.45054400
H	7.13540900	2.24697000	4.18994700
H	5.17147600	1.38842100	5.56650500
H	3.63428400	0.99107100	4.76863800
H	4.10409900	2.68085500	5.00967700
H	6.55329400	0.05431400	4.00727100
H	6.22776400	0.05362300	2.26737100
H	5.02123800	-0.56891000	3.40998700
H	4.46869100	6.37084400	-0.97118500
H	5.11175800	4.72685700	-1.11838500
H	5.11104400	5.53771600	0.45943800
H	4.40252100	4.58686900	4.39210200
H	2.81108800	4.49280400	3.57932500
H	3.81355400	5.96198600	3.44027100
H	1.37952100	4.41594700	-1.47420600
H	2.93531500	4.01621700	-2.23102500

H	2.43946500	5.70331900	-2.05185300
H	7.27898300	-2.94462300	-0.41360900
H	8.71393300	-2.37928500	-1.28864800
H	7.52306900	-3.40692200	-2.11083000
H	4.76485400	-0.13794600	-0.54767600
H	1.66069300	-2.83081300	-1.65635800
H	6.23711500	-3.28174800	-5.63816400
H	5.84711500	-1.66998600	-4.97608200
H	4.53935400	-2.80995600	-5.34879100
H	8.50437300	-0.41183700	-2.96134200
H	6.90528400	-0.00487200	-3.59903600
H	7.61483900	-1.61055800	-3.89412700
H	4.04719000	-4.80961900	-5.04835600
H	2.46353100	-3.99727000	-5.01379900
H	2.57661400	-5.75399700	-4.84079200
H	1.54584100	-6.11071100	-2.78671200
H	0.96297600	-4.44429900	-2.86491000
H	1.73809300	-5.04869600	-1.38726200
H	6.77404200	-0.52517700	0.21002300
H	6.69147700	0.72763700	-1.04574600
H	8.22509700	-0.07473500	-0.68981900
H	1.32882800	5.42539700	0.90947400
H	2.13561300	6.75669500	0.06129200
H	2.81881600	6.13280900	1.56181700
H	3.89016700	-6.72665200	-2.83492700
H	4.20945900	-5.71193700	-1.41663700
H	5.18146800	-5.50963900	-2.88883500
Cu	-0.01306000	-0.11488900	-1.61994700
H	-0.21876500	-1.55020100	-2.38931200
C	-0.16658300	-0.59422900	-3.72099200
C	0.10742600	0.79874800	-3.52435500
H	-0.75327400	1.46019600	-3.63214200
H	0.67099700	-1.18045400	-4.10359800
C	-1.51198400	-1.02834700	-4.27907500
H	-2.33041600	-0.49052400	-3.78911100
H	-1.68528900	-2.10264600	-4.14904300
C	1.43810400	1.38253800	-3.96546800

H	2.27084200	0.71127100	-3.71961300
H	1.64870000	2.34383200	-3.48170300
H	-1.55558200	-0.79481300	-5.35294800
H	1.48253400	1.56193600	-5.05499100

24

Cartesian coordinates:

P	-1.78424900	0.28043200	-0.03985700
P	1.73939200	-0.39187300	-0.05411800
O	-1.04295900	-1.77760700	4.30811200
O	-0.14602600	-3.89862300	4.43078600
O	0.75108000	0.62179000	4.65849400
O	-0.15418400	2.66695200	5.21557700
O	4.57285000	4.48592100	2.01291100
O	5.88034900	-3.32610300	-3.26632300
O	-4.97427400	-4.70025100	1.01360800
O	-5.42614100	4.03443100	-2.97546500
C	1.22940400	-1.44163400	1.39018600
C	0.22472700	-1.00930100	2.32082000
C	-0.12519000	-1.94130600	3.29017400
C	0.41353700	-3.22310200	3.37344900
C	1.36063900	-3.66000700	2.47628400
C	1.75471400	-2.73933800	1.49155700
C	-0.84509600	-2.89692600	5.17330100
C	-1.32796100	1.00621200	1.60689400
C	-1.85911100	2.25286500	1.97163900
C	-1.52794200	2.91486500	3.16542100
C	-0.64247100	2.26591800	3.99516400
C	-0.09777000	1.03129700	3.64943900
C	-0.38157800	0.35727300	2.46809100
C	0.47907800	1.50208900	5.75014600
C	2.66842200	1.03731400	0.64701700
C	3.32963100	1.02859500	1.87524700
C	4.07560600	2.12991200	2.33499400
C	4.03585300	3.29869800	1.53810000
C	3.48828200	3.30777800	0.22689600
C	2.79422700	2.16397600	-0.17746300

C	3.71131000	4.48154100	-0.76194200
C	3.02614200	5.78961400	-0.29952900
C	5.23292500	4.72603800	-0.92322100
C	3.15165700	4.15367300	-2.16353900
C	4.91762500	1.93718600	3.63050600
C	6.01769500	2.99854000	3.86830700
C	5.67246000	0.58308100	3.53296000
C	3.99196300	1.88020600	4.86767700
C	3.72422000	5.18421300	2.92454400
C	3.06106100	-1.38486500	-0.88676200
C	2.66119900	-2.27586400	-1.89289600
C	4.41631800	-1.30134500	-0.57388900
C	5.39962100	-2.01547500	-1.28192200
C	4.95809800	-2.77257200	-2.39086100
C	3.58038500	-3.01219400	-2.64524300
C	3.09150600	-4.08576000	-3.65187700
C	1.55882800	-4.26749700	-3.58124500
C	3.43547100	-3.73101600	-5.11804300
C	6.39245200	-2.39366600	-4.22025200
C	3.73080100	-5.44965200	-3.28873300
C	6.85379900	-1.93803500	-0.73499600
C	7.40907800	-0.50473800	-0.91366400
C	7.86028000	-2.94063600	-1.34543000
C	6.81296400	-2.27324200	0.78154000
C	-2.83187100	-1.18485100	0.34491700
C	-2.94011200	-2.16245400	-0.65281300
C	-3.70543800	-3.31903000	-0.47952000
C	-4.34659100	-3.48604500	0.77809100
C	-4.38976200	-2.45762700	1.75065000
C	-3.57363700	-1.33593700	1.51627200
C	-5.29093500	-2.43838000	3.02074100
C	-6.48335700	-3.42377900	2.98864900
C	-4.44074700	-2.70223500	4.28570600
C	-5.93012500	-1.03017700	3.16636400
C	-5.40548800	-4.44925100	-1.96722500
C	-4.23511000	-5.59615000	1.84371900
C	-3.89393700	-4.31345300	-1.65498100

C	-3.20598600	-3.80529100	-2.94160500
C	-4.61301900	3.27479000	-2.14278200
C	-5.21521900	2.33359500	-1.27025700
C	-7.09429500	3.77323900	-0.40840800
C	-4.35474400	1.44264100	-0.60924600
C	-2.96727600	1.50598300	-0.75830500
C	-2.41928400	2.56104400	-1.49612500
C	-3.21282200	3.50175700	-2.16393700
C	-5.62762700	3.43929200	-4.26579900
C	-7.65533400	2.00453100	-2.11278100
C	-2.69137500	4.89562000	-4.30100300
C	-2.56705700	4.78157400	-2.76336900
C	-1.05840600	4.85014600	-2.43563700
C	-7.06249600	1.36040800	0.20667000
C	-3.30258300	-5.71169600	-1.35512100
C	-6.73018800	2.35803000	-0.92440400
C	-3.23607200	6.01777800	-2.11095800
H	1.79131600	-4.65372000	2.53375800
H	2.51282900	-3.05183600	0.78440500
H	-1.81352800	-3.28700400	5.49016000
H	-0.23545600	-2.58885200	6.03608200
H	-2.57309000	2.72884600	1.31081800
H	-1.96104600	3.87456700	3.42569300
H	1.41602500	1.78503900	6.23164300
H	-0.20312100	1.00660800	6.45735600
H	3.27160500	0.13535500	2.48754900
H	2.33307900	2.13163200	-1.15743300
H	1.96628500	5.62371200	-0.07192200
H	3.07988900	6.53574900	-1.10181300
H	3.51124400	6.21798300	0.57799300
H	5.69921900	4.99146000	0.02763100
H	5.40604500	5.54465800	-1.63305700
H	5.72938600	3.83122800	-1.31695900
H	3.59159500	3.24342100	-2.58460900
H	3.39009000	4.97935300	-2.84317900
H	2.06216100	4.03743900	-2.16140500
H	6.66074000	2.65034900	4.68593000

H	5.62746300	3.97391400	4.15845300
H	6.64482100	3.13749900	2.98299800
H	6.28870400	0.44124600	4.42844800
H	6.33748300	0.56879900	2.66224300
H	5.00268300	-0.27810400	3.46291900
H	3.25149100	1.08058600	4.76894600
H	3.44989700	2.82265300	5.00791600
H	4.58275900	1.69509100	5.77392500
H	2.73564700	5.36789600	2.48857800
H	4.21452700	6.13913600	3.13138300
H	3.59635600	4.63520400	3.86392900
H	1.60233800	-2.36422600	-2.10212400
H	4.72248500	-0.65417200	0.23979600
H	1.26743600	-5.08639500	-4.24855700
H	1.01763300	-3.37170500	-3.90508200
H	1.22188900	-4.52895500	-2.57157700
H	4.50644500	-3.79735800	-5.31309200
H	3.08977100	-2.72244000	-5.37341600
H	2.93442900	-4.43489500	-5.79402300
H	6.94836100	-1.58238300	-3.73677100
H	5.58754600	-1.95585800	-4.82135000
H	7.06806500	-2.95698000	-4.86918300
H	4.82054600	-5.40822700	-3.34088200
H	3.38117300	-6.22245400	-3.98484500
H	3.44241500	-5.75673500	-2.27615400
H	6.77662800	0.24052400	-0.41913100
H	7.47590500	-0.23031300	-1.97270100
H	8.41614400	-0.43059400	-0.48450200
H	8.78140000	-2.90549200	-0.75061100
H	8.13536500	-2.70850600	-2.37472400
H	7.48131800	-3.96577600	-1.31999500
H	6.43329300	-3.28867500	0.94374200
H	6.18657600	-1.58581100	1.35489000
H	7.82550700	-2.22085100	1.19914900
H	-2.40339600	-2.00260000	-1.58012700
H	-3.51956300	-0.55445900	2.26542600
H	-6.19062400	-4.46814900	3.09145500

H	-7.05967000	-3.32773600	2.06349100
H	-7.15042200	-3.18816800	3.82687100
H	-5.06625100	-2.62819300	5.18444200
H	-3.62696500	-1.97512000	4.37029300
H	-3.99524700	-3.70339800	4.27137300
H	-6.59681700	-1.02167400	4.03641200
H	-6.52553700	-0.77595700	2.28313800
H	-5.19386000	-0.23653300	3.31909700
H	-5.55263400	-5.14111400	-2.80608500
H	-5.83031300	-3.48015800	-2.25455100
H	-5.95964200	-4.82946400	-1.10673800
H	-4.20054700	-5.25343400	2.88354300
H	-3.20903900	-5.72316000	1.48091900
H	-4.75722200	-6.55579700	1.80242100
H	-2.11651400	-3.74603200	-2.83813300
H	-3.57423400	-2.82065200	-3.24903300
H	-3.41870800	-4.50488900	-3.75756800
H	-6.50910900	4.02568800	0.48368300
H	-8.15657000	3.81132000	-0.13565300
H	-6.90842600	4.53280400	-1.17080500
H	-4.76984500	0.67439900	0.02915400
H	-1.33987000	2.63349800	-1.55656400
H	-6.24818800	4.13994600	-4.83066600
H	-6.14143900	2.47726200	-4.18736800
H	-4.68036100	3.28483000	-4.78870500
H	-8.67809200	1.85147900	-1.74704800
H	-7.33912400	1.07862900	-2.60746800
H	-7.69388800	2.80545500	-2.85171100
H	-3.71075400	5.12647600	-4.61298900
H	-2.36429600	3.97599000	-4.79976900
H	-2.05129500	5.71133700	-4.65869000
H	-0.66004900	5.80554100	-2.79460100
H	-0.49060800	4.05267300	-2.92863100
H	-0.86668100	4.79657100	-1.35813200
H	-6.47429600	1.54991400	1.11064100
H	-6.90152300	0.31961200	-0.09748800
H	-8.12001600	1.46420400	0.47387000

H	-2.26095200	-5.63871500	-1.02013500
H	-3.31513400	-6.31893700	-2.26851800
H	-3.87804200	-6.24720500	-0.59969300
H	-2.78220800	6.93791200	-2.50012100
H	-3.09713400	6.00875500	-1.02337000
H	-4.30716900	6.04721800	-2.32292400
Cu	-0.04399800	-0.02737100	-1.57083300
H	0.79824900	1.93511700	-3.94513400
C	1.10448100	0.89098500	-4.12707100
C	0.02813300	-0.06729300	-3.57127100
H	0.36336800	-1.09114000	-3.82416700
C	-1.33140600	0.13954800	-4.26471900
H	-1.73642300	1.14223100	-4.06601000
H	-2.07998000	-0.57635300	-3.89937700
H	-1.29666300	0.02332500	-5.36265400
H	2.04114000	0.75522400	-3.56578600
C	1.43334700	0.74270500	-5.62654000
H	0.56373200	0.94904400	-6.26097100
H	2.23513200	1.42819100	-5.93425000
H	1.76608800	-0.28031200	-5.85014800

25-TS

Cartesian coordinates:

C	3.00503900	-0.85633700	-1.38090900
C	2.71297700	-1.57096000	-2.55424000
H	1.69378300	-1.89017800	-2.72514900
C	3.69478100	-1.89512200	-3.49543200
C	5.01607800	-1.43781800	-3.23718800
C	5.30397800	-0.53618500	-2.18978600
C	4.28420000	-0.31985500	-1.24580300
H	4.49590300	0.30343000	-0.38685600
C	2.62610700	0.11724400	1.31631200
C	3.45287500	-0.75952800	2.02184500
H	3.52705400	-1.78241200	1.67548600
C	4.19441800	-0.36460000	3.14468800
C	3.99296900	0.96622500	3.59666700
C	3.25184700	1.91734600	2.84658900

C	2.57239700	1.45531900	1.71099700
H	1.98066300	2.13857200	1.11698300
C	1.06309700	-2.11223800	0.45254000
C	1.51816900	-3.30398900	-0.12917800
H	2.23623700	-3.25509300	-0.93694500
C	1.12297800	-4.58018100	0.30863900
H	1.50094200	-5.48360300	-0.15769200
C	0.25992600	-4.61869000	1.37965600
C	-0.79949300	-5.17163400	3.24308100
H	-1.73963700	-5.66633800	3.48706000
H	-0.05501600	-5.29492600	4.04429300
C	-0.19959100	-3.44801800	1.97558200
C	0.14446400	-2.17158300	1.55091500
C	-0.36990800	-1.03669100	2.38441800
C	0.03999600	-1.00591900	3.71123300
C	0.81284000	-1.57777000	5.71880500
H	1.80116400	-1.57149100	6.17931200
H	0.15820000	-2.33076100	6.18337600
C	-0.40387000	-0.06879100	4.63974300
C	-1.32421200	0.89643100	4.29927400
H	-1.68741800	1.62306300	5.01784100
C	-1.78556600	0.87635600	2.97249000
H	-2.52682100	1.61148000	2.68472100
C	-1.34056900	-0.04973200	2.01753500
C	-3.33048200	1.31492500	0.34966900
C	-4.65593000	0.88649900	0.37096200
H	-4.85773600	-0.17672600	0.38913000
C	-5.74073400	1.78028300	0.35300300
C	-5.42785100	3.15331900	0.23975000
C	-4.09964100	3.64141000	0.37716000
C	-3.07235300	2.69304900	0.38982400
H	-2.04186100	3.02470400	0.41304400
C	-2.69754300	-1.45162200	-0.18743900
C	-3.32581200	-2.28017900	0.75190700
H	-3.30206800	-1.98847300	1.79373400
C	-3.96577200	-3.46678800	0.37837400
C	-3.93653300	-3.81562400	-1.00001400

C	-3.46155300	-2.93083200	-1.99452100
C	-2.79476800	-1.78009200	-1.53891300
H	-2.34949300	-1.10747400	-2.26270100
O	-0.27744000	-5.71022800	2.02488300
O	-1.03462400	-3.78034800	3.02403800
O	0.93932900	-1.85279200	4.32376400
O	0.21563500	-0.28489600	5.85052200
P	1.66764300	-0.45448800	-0.16031000
P	-1.89597500	0.14942400	0.25648500
C	-0.38884500	1.70846500	-2.97505500
H	0.09841700	2.53596700	-3.49421500
Cu	-0.08138200	0.95978800	-0.95321200
C	0.86387300	5.16204400	-2.23135400
C	2.18073100	4.30859500	-2.50697200
B	0.56480000	2.96938700	-1.48382900
H	0.32430000	2.55770500	-0.30973300
O	1.94691400	3.09361700	-1.77270900
O	-0.09835000	4.18693000	-1.78893500
C	1.02765500	6.18786400	-1.09676800
H	1.73614500	6.98200400	-1.35815300
H	0.05664500	6.65139200	-0.89553300
H	1.36534800	5.70795800	-0.17403300
C	0.29665400	5.87551700	-3.46460600
H	-0.63002000	6.39073700	-3.18964400
H	0.99847000	6.62463600	-3.85076400
H	0.06165400	5.17251400	-4.26718700
C	3.47157500	4.94255900	-1.97158700
H	4.30978000	4.26192900	-2.15350900
H	3.69001700	5.89012400	-2.47850300
H	3.41950300	5.12897900	-0.89696100
C	2.41068100	3.95829200	-3.98938200
H	2.67053600	4.84645500	-4.57696300
H	3.24325100	3.24976900	-4.05451400
H	1.53983700	3.48695700	-4.44986400
C	-1.90075900	1.97334700	-3.13280400
H	-2.47767500	1.09513700	-2.80769700
H	-2.19258800	2.78889400	-2.46164900

C	-3.77953400	5.14542200	0.57752700
C	-2.28825000	5.35767500	0.91791700
H	-1.99014700	4.80062300	1.81428500
H	-1.62734600	5.07143600	0.09389900
H	-2.12124300	6.42126600	1.12467900
C	-4.07704100	5.98903100	-0.68477500
H	-3.57691600	5.57021700	-1.56555000
H	-5.14669500	6.06366600	-0.88531300
H	-3.69884700	7.00887400	-0.54129200
C	-4.60613100	5.68889200	1.76982000
H	-4.36044800	5.14721900	2.69138700
H	-4.36963100	6.74790900	1.93263500
H	-5.67947200	5.59977300	1.59180900
C	-7.16096500	1.16341000	0.50123900
C	-7.14184000	0.17496700	1.70015200
H	-6.44439500	-0.65523800	1.55932900
H	-6.86830300	0.69128400	2.62743900
H	-8.13991800	-0.25787900	1.83577500
C	-8.29427700	2.16665900	0.81859100
H	-8.04236100	2.80854300	1.66742200
H	-8.55442100	2.80941300	-0.02252600
H	-9.19451400	1.59723700	1.08062100
C	-7.53001100	0.37489700	-0.77829000
H	-7.58080800	1.03029900	-1.65497600
H	-6.79582500	-0.40926700	-0.99375800
H	-8.51021400	-0.10396900	-0.66081200
C	-3.65155700	-3.07993800	-3.53148700
C	-2.29664500	-3.39797700	-4.20757200
H	-1.55237300	-2.62170500	-4.00079900
H	-1.88533000	-4.35371000	-3.86359600
H	-2.42198600	-3.46001400	-5.29563800
C	-4.69546800	-4.13340200	-3.97100900
H	-4.87641700	-4.00874000	-5.04545200
H	-4.37000700	-5.16248600	-3.81790700
H	-5.64912300	-4.00079100	-3.45203400
C	-4.17311400	-1.72742000	-4.09222700
H	-5.12369600	-1.45043700	-3.62208000

H	-3.47298600	-0.90125200	-3.94754800
H	-4.34432900	-1.82107500	-5.17085000
C	-4.75706100	-4.29743300	1.42221700
C	-4.22650200	-5.74574600	1.56383900
H	-4.65547000	-6.21011000	2.46064500
H	-4.50589400	-6.36438100	0.71081000
H	-3.13545100	-5.76511100	1.66058800
C	-4.69420300	-3.65123900	2.82384600
H	-3.67073300	-3.60578500	3.21130700
H	-5.10835200	-2.63689800	2.83060900
H	-5.29260900	-4.25016500	3.51959500
C	-6.24687600	-4.34648000	0.99960200
H	-6.36660400	-4.81270400	0.01909600
H	-6.82498700	-4.92708800	1.72975100
H	-6.67498700	-3.33792600	0.96001300
C	3.21952900	3.42573300	3.20563700
C	5.17982900	-1.39808100	3.76517400
C	6.42061100	-0.74324700	4.41719300
H	6.18615600	-0.14253200	5.29397000
H	7.12148600	-1.52971400	4.72191000
H	6.93784100	-0.09247100	3.70315000
C	4.45391200	-2.30448700	4.78887400
H	3.57969500	-2.78147000	4.33327000
H	5.13124500	-3.09189300	5.14307900
H	4.11276700	-1.74761600	5.66614700
C	5.73735600	-2.33478000	2.65920600
H	4.98064500	-3.00993300	2.24867600
H	6.17261900	-1.76640400	1.83061900
H	6.52519500	-2.96478900	3.08729500
C	4.66378100	3.98408000	3.24735900
H	4.64303500	5.05299000	3.49459700
H	5.27354900	3.46957000	3.99208500
H	5.14697600	3.87744400	2.26880600
C	2.51584300	3.68929700	4.55863200
H	3.10296100	3.33806400	5.40696600
H	2.36467100	4.76790500	4.68995100
H	1.53097100	3.20830100	4.59088500

C	2.44947500	4.23893700	2.14279700
H	2.86642800	4.10703500	1.13958400
H	1.38653900	3.97501300	2.10474000
H	2.51448100	5.30341200	2.39519300
C	3.31583800	-2.63899800	-4.80311300
C	4.02873100	-4.00620800	-4.93802700
H	5.09742900	-3.89325100	-5.11945200
H	3.88572300	-4.62078000	-4.04064900
H	3.60723300	-4.55792800	-5.78731300
C	1.79913800	-2.92019600	-4.88147500
H	1.45969400	-3.59427800	-4.08574400
H	1.20374100	-2.00304100	-4.83572800
H	1.57774100	-3.40745600	-5.83756400
C	3.68228800	-1.74751300	-6.01598200
H	4.75228500	-1.53083700	-6.04188200
H	3.41080900	-2.25539900	-6.95017000
H	3.13549000	-0.79835100	-5.97823100
C	6.61576900	0.28002700	-2.00497900
C	7.37997400	-0.21033000	-0.75239800
H	6.76692900	-0.12323500	0.15122800
H	7.68632100	-1.25848400	-0.84827500
H	8.28564300	0.39000800	-0.60082900
C	6.22982100	1.77028100	-1.79290500
H	5.68667200	2.15611300	-2.66259900
H	5.60328100	1.93211400	-0.91237100
H	7.13887300	2.37001200	-1.66531400
C	7.57989200	0.27614400	-3.21413800
H	8.09034900	-0.67594500	-3.36290600
H	7.06532600	0.53263000	-4.14415900
H	8.35455100	1.03224500	-3.03726100
O	4.57466900	1.41298000	4.77401600
O	6.02692200	-1.87820600	-4.07930200
O	-4.42901100	-5.06241700	-1.35265400
O	-6.43207400	4.08055300	0.00703300
C	-6.83387800	4.16099500	-1.36157500
H	-7.56326700	4.97305600	-1.42056700
H	-5.98289900	4.38504700	-2.01450800

H	-7.30161100	3.23067300	-1.70293800
C	-3.41328300	-6.03307500	-1.61376400
H	-3.93182300	-6.97462400	-1.81246800
H	-2.80943800	-5.76340000	-2.48669400
H	-2.74847900	-6.15635500	-0.75137500
C	6.84548000	-2.90108300	-3.51318400
H	7.57167000	-3.17617300	-4.28263500
H	7.37917800	-2.55033300	-2.62311900
H	6.25228800	-3.78213400	-3.24075800
C	3.92610400	1.04572100	5.99107700
H	4.32669300	0.10559600	6.38709900
H	4.13450700	1.83859600	6.71523600
H	2.84217400	0.95370200	5.85990300
C	0.08473900	0.45964500	-3.74769900
H	-0.36187600	-0.47087400	-3.36950300
H	-0.16434300	0.51369600	-4.82152400
C	-2.34673600	2.35002200	-4.55774000
H	-1.83398900	3.26014200	-4.89535100
H	-2.12792900	1.55900000	-5.28527800
H	1.17175500	0.35013500	-3.67932800
H	-3.42690300	2.54378800	-4.60015800

26

Cartesian coordinates:

C	-2.07435300	0.43541700	0.29331700
H	-2.24621300	0.56588500	1.37799700
C	-2.88254600	-0.81024600	-0.14162600
H	-2.78105200	-0.94105500	-1.22939300
H	-2.42887700	-1.70097300	0.30971400
B	-0.51787000	0.20684900	0.14776900
O	0.38064800	1.21109700	-0.12887000
O	0.09197500	-1.01559900	0.31277600
C	1.72123900	0.67936700	0.06495800
C	1.48874100	-0.87652900	-0.07047400
C	2.33396200	-1.74614500	0.85876600
H	3.40177100	-1.63031700	0.63993800
H	2.16443300	-1.49922900	1.90920500

H	2.07152100	-2.79908900	0.71413700
C	1.59977400	-1.38819400	-1.51331800
H	1.22872100	-2.41696900	-1.55367800
H	0.99483900	-0.78496900	-2.19765000
H	2.63595800	-1.38125800	-1.86779600
C	2.16532800	1.11097700	1.46943900
H	3.19529400	0.80482800	1.68103500
H	2.10889300	2.20169400	1.53934000
H	1.51297600	0.68977400	2.24097900
C	2.64213100	1.29580600	-0.98664200
H	2.70611400	2.37722900	-0.82876100
H	3.65447100	0.88225500	-0.91143500
H	2.27028800	1.12594500	-1.99955600
C	-2.53363000	1.73163100	-0.40345200
H	-2.43849900	1.64636200	-1.49372200
H	-3.58024000	1.96931100	-0.18183000
H	-1.92289600	2.58480800	-0.09101200
C	-4.37118700	-0.76729600	0.22365600
H	-4.89350100	0.05939000	-0.27070100
H	-4.87502800	-1.69566200	-0.07065300
H	-4.50736900	-0.64492600	1.30600400

styrene

Cartesian coordinates:

C	-1.78082400	-1.04627600	-0.00000600
C	-0.40638700	-1.28127300	-0.00000900
C	0.51521900	-0.22033600	-0.00000400
C	0.00880800	1.09260100	0.00000400
C	-1.36231300	1.32954700	0.00000800
C	-2.26534300	0.26169200	0.00000300
H	-2.47191300	-1.88512600	-0.00001000
H	-0.03487800	-2.30369400	-0.00001600
H	0.69383200	1.93554000	0.00000600
H	-1.73063100	2.35222000	0.00001400
H	-3.33546700	0.45037500	0.00000600
C	1.95472200	-0.52927400	-0.00000700
C	2.97742700	0.33492200	0.00001000

H	2.18617900	-1.59467000	-0.00002600
H	4.00441700	-0.01723100	0.00000600
H	2.84060100	1.41297200	0.00003100

HBpin

Cartesian coordinates:

C	0.78885900	-0.19177400	0.04579200
C	-0.78885900	-0.19177600	-0.04578500
B	0.00000000	1.94447000	-0.00003800
O	-1.08500500	1.20039100	-0.37034900
O	1.08500500	1.20040600	0.37030100
C	1.48135400	-0.48083900	-1.29256400
H	2.54982300	-0.26690400	-1.19213600
H	1.36572500	-1.52847700	-1.58968600
H	1.08510500	0.15292300	-2.09211700
C	-1.37858900	-1.07584300	-1.14298200
H	-1.13824000	-2.13053500	-0.96628500
H	-2.46841100	-0.97345100	-1.14866900
H	-1.00957600	-0.79483800	-2.13184300
C	-1.48135400	-0.48078800	1.29258300
H	-2.54982300	-0.26685700	1.19214700
H	-1.36572500	-1.52841400	1.58974600
H	-1.08510500	0.15300500	2.09211100
C	1.37858900	-1.07579800	1.14302400
H	2.46841200	-0.97340500	1.14870800
H	1.00957600	-0.79475400	2.13187400
H	1.13824000	-2.13049600	0.96636900
H	0.00000000	3.13439700	-0.00006200

***trans*-2-butene**

Cartesian coordinates:

C	-0.53810400	-0.39536400	0.00000100
C	0.53810300	0.39536300	0.00000100
H	-0.39243900	-1.47772700	0.00000100
H	0.39243800	1.47772600	0.00000000
C	1.96350900	-0.07922300	0.00000000
H	2.50788200	0.28907400	-0.88043800

H	2.50788300	0.28906900	0.88043900
H	2.02278000	-1.17312500	-0.00000300
C	-1.96350900	0.07922400	0.00000000
H	-2.50788300	-0.28907200	-0.88043800
H	-2.50788400	-0.28906700	0.88043900
H	-2.02277800	1.17312600	-0.00000300

23-TS-propene

Cartesian coordinates:

P	1.80708900	-0.33164900	-0.27561400
P	-1.75019800	0.33522800	-0.24773600
O	1.05353900	1.32889400	4.18240300
O	0.28298300	3.48499900	4.43269900
O	-0.91868800	-1.08072100	4.24904700
O	-0.16668500	-3.23280400	4.58244100
O	-4.46769500	-4.33747500	2.39405900
O	-5.70225300	3.29538000	-3.66099000
O	4.47068700	4.60288100	1.89626100
O	5.69753000	-3.43687100	-3.61666600
C	-1.18158800	1.32337500	1.21827500
C	-0.21138000	0.77452900	2.12156800
C	0.16586000	1.61179200	3.16360400
C	-0.30805300	2.91141100	3.32818800
C	-1.22711400	3.45626600	2.46122300
C	-1.65789100	2.62706700	1.41175300
C	0.86361700	2.38025200	5.13001200
C	1.28201200	-1.22459300	1.26367100
C	1.74757900	-2.52412400	1.50500600
C	1.32241400	-3.30262400	2.59510500
C	0.42036600	-2.71119200	3.44984300
C	-0.04283300	-1.41484600	3.23599500
C	0.32833100	-0.62807500	2.15340800
C	-0.73831900	-2.09697300	5.23577000
C	-2.67709100	-1.04960700	0.54894400
C	-3.49401600	-0.85996800	1.66558800
C	-4.17969000	-1.91478800	2.28728500
C	-3.94207700	-3.21645200	1.76874200

C	-3.22102700	-3.43275400	0.56425300
C	-2.58318000	-2.32553900	-0.00908500
C	-3.14264900	-4.81456700	-0.13504200
C	-2.31032400	-5.82289900	0.69208800
C	-4.56658700	-5.37422900	-0.37645400
C	-2.46523800	-4.70809600	-1.51999500
C	-5.14878500	-1.57505300	3.45728900
C	-6.39346800	-2.49393400	3.48741900
C	-5.69909000	-0.13193500	3.30965700
C	-4.40990300	-1.61917800	4.81690600
C	-3.80650800	-4.81630500	3.56534700
C	-3.06660200	1.34201900	-1.07209700
C	-2.69362800	2.52209600	-1.73508400
C	-4.38998100	0.91878400	-1.17506500
C	-5.34178400	1.58598200	-1.97004700
C	-4.88119200	2.69060900	-2.71987200
C	-3.58435100	3.24466500	-2.53190700
C	-3.17367200	4.62419500	-3.11057900
C	-1.77627100	5.05300000	-2.61040600
C	-3.11643000	4.63646100	-4.65686400
C	-5.75353700	2.61222100	-4.91418300
C	-4.18200700	5.69566500	-2.62491200
C	-6.80308200	1.05376300	-1.91988700
C	-6.90396300	-0.28313500	-2.69377500
C	-7.87951700	2.03252900	-2.44582300
C	-7.18663900	0.78127100	-0.43970900
C	2.73523700	1.12033300	0.38599400
C	2.62545300	2.33428100	-0.29615400
C	3.24461700	3.50225900	0.16348800
C	3.96918000	3.41658800	1.38214400
C	4.22962800	2.17639600	2.02386000
C	3.55468800	1.05492600	1.51506900
C	5.21786900	1.97153100	3.20946600
C	6.44070400	2.91744000	3.13735100
C	4.49402000	2.12397600	4.56882400
C	5.80392700	0.53579100	3.18754500
C	4.56063200	5.35648000	-0.97023100

C	3.81301600	5.16344900	3.03325700
C	3.14431100	4.80825500	-0.66570400
C	2.45888200	4.56155100	-2.02850600
C	4.86259400	-2.83830500	-2.67884100
C	5.38629400	-1.81959600	-1.84533500
C	7.57482200	-2.91899600	-1.24988500
C	4.46464500	-1.09981400	-1.06646200
C	3.09812000	-1.39315200	-1.07325000
C	2.66075800	-2.51698300	-1.78696300
C	3.52693600	-3.30023000	-2.55933100
C	5.65304200	-2.80232900	-4.90169700
C	7.61857500	-1.04893400	-2.93852600
C	3.00769700	-4.73879800	-4.66722000
C	3.04368800	-4.66549700	-3.12253600
C	1.61697100	-4.99657700	-2.62931900
C	7.19497800	-0.56278600	-0.54505400
C	2.30747200	5.88334000	0.06739200
C	6.91237700	-1.58222700	-1.66952800
C	3.98383400	-5.77610100	-2.58955800
H	-1.61376000	4.46129400	2.59124000
H	-2.40683300	3.01766400	0.73379700
H	1.82710100	2.67644700	5.54423900
H	0.17261000	2.04131100	5.91709800
H	2.47589400	-2.95277100	0.82667300
H	1.69771500	-4.30656900	2.76177200
H	-1.70502900	-2.36840300	5.65985600
H	-0.04571000	-1.73456300	6.01095600
H	-3.59880600	0.14329300	2.05883600
H	-1.97239200	-2.44080500	-0.89700700
H	-1.32188200	-5.41247500	0.93036200
H	-2.16130500	-6.74363100	0.11420800
H	-2.80277800	-6.09877000	1.62468500
H	-5.11444400	-5.50671500	0.55736500
H	-4.50296100	-6.34514100	-0.88381400
H	-5.14144200	-4.69868300	-1.02143400
H	-2.98148400	-3.99987700	-2.17748000
H	-2.49318200	-5.69083500	-2.00430800

H	-1.41478700	-4.40574000	-1.45273700
H	-7.07581900	-2.15150800	4.27468000
H	-6.15641800	-3.54014100	3.67168300
H	-6.93224700	-2.44411200	2.53401100
H	-6.47052400	0.03440900	4.06997600
H	-6.15494100	0.03087200	2.32790800
H	-4.93315800	0.63443700	3.46298000
H	-3.55527500	-0.93455700	4.80643500
H	-4.04049800	-2.61832900	5.06002400
H	-5.08712400	-1.31171800	5.62390100
H	-2.78008000	-4.43999500	3.63533600
H	-3.78451400	-5.90913900	3.50996400
H	-4.36225300	-4.53176300	4.46606000
H	-1.67118500	2.86200200	-1.63442400
H	-4.69101700	0.03208100	-0.63255500
H	-1.55979300	6.06126100	-2.98068300
H	-0.98195100	4.39309900	-2.97713300
H	-1.71982000	5.08506200	-1.51658700
H	-4.10863700	4.56656800	-5.10324300
H	-2.49775700	3.81529900	-5.03784800
H	-2.66785900	5.57677300	-5.00054100
H	-6.25972700	1.64450800	-4.82963000
H	-4.74957900	2.44834900	-5.32153100
H	-6.32148000	3.25483200	-5.59225600
H	-5.19594800	5.47151900	-2.96201200
H	-3.89783200	6.68101200	-3.01549900
H	-4.18572000	5.75791500	-1.53006100
H	-6.21243200	-1.03031900	-2.28887100
H	-6.66977400	-0.15778400	-3.75643900
H	-7.92068100	-0.68929500	-2.62074800
H	-8.86718600	1.63211700	-2.18652900
H	-7.85957800	2.16473200	-3.52716600
H	-7.78550100	3.02060000	-1.98552000
H	-7.08411900	1.68856000	0.16647600
H	-6.58108400	-0.00393800	0.01968300
H	-8.23160300	0.45456600	-0.38661600
H	2.01530300	2.35439800	-1.19098000

H	3.66932800	0.09871700	2.01027900
H	6.18329600	3.97023200	3.23632300
H	6.96467100	2.79752900	2.18203800
H	7.14342500	2.65889200	3.93857100
H	5.19249200	1.92537000	5.39171200
H	3.66865500	1.40798200	4.63876200
H	4.08645200	3.12701200	4.71607800
H	6.57823200	0.45447700	3.95874000
H	6.26622300	0.30553400	2.22274000
H	5.05802300	-0.23460700	3.40520200
H	4.48372900	6.27443600	-1.56650100
H	5.13858900	4.62852200	-1.55223200
H	5.11241900	5.58262200	-0.05680900
H	4.40805900	5.00278300	3.93943300
H	2.81309800	4.73931500	3.17441400
H	3.72506700	6.24210600	2.86975200
H	1.41169000	4.25812500	-1.92273600
H	2.97808600	3.79866400	-2.61913300
H	2.47244900	5.49278800	-2.60592800
H	7.14889100	-3.28617100	-0.30878500
H	8.65167300	-2.77247000	-1.09722100
H	7.43781300	-3.68657200	-2.01447000
H	4.81365900	-0.28185300	-0.45180300
H	1.60665700	-2.76190100	-1.74762800
H	6.33352500	-3.36702000	-5.54463800
H	5.98273300	-1.76106400	-4.84693700
H	4.64609500	-2.82517600	-5.32694900
H	8.63347600	-0.72132900	-2.68188400
H	7.08986500	-0.18624900	-3.36090700
H	7.71316900	-1.81710100	-3.70669100
H	4.00841600	-4.78739000	-5.09861200
H	2.47507300	-3.88279700	-5.09830100
H	2.47758400	-5.64751600	-4.97753700
H	1.34614100	-6.00111200	-2.97319700
H	0.86724300	-4.30063600	-3.02216700
H	1.54743200	-4.99209700	-1.53604200
H	6.75820900	-0.87691300	0.40823000

H	6.81955600	0.43895300	-0.78375400
H	8.27805400	-0.48176600	-0.40064800
H	1.32738400	5.48679600	0.35795000
H	2.13953800	6.74037000	-0.59676400
H	2.80770900	6.25547800	0.96151500
H	3.64961300	-6.75609400	-2.95304900
H	3.97333400	-5.80322600	-1.49357900
H	5.01243200	-5.61905100	-2.92170100
Cu	-0.00671700	-0.08892100	-1.63295600
H	-0.22408500	-1.45026100	-2.52156200
C	-0.02841900	-0.39449300	-3.77454400
C	0.18804400	0.97872300	-3.44003800
H	-0.63769100	1.67493000	-3.56485600
H	0.85282700	-0.94374000	-4.10471700
C	-1.30468900	-0.79682700	-4.49527600
H	-2.17617200	-0.31554500	-4.03929700
H	-1.46518000	-1.88035800	-4.47682700
H	-1.25086300	-0.46824600	-5.54320900
H	1.18556600	1.39540500	-3.54878700

propene

Cartesian coordinates:

C	1.28310000	-0.22039500	0.00000000
C	0.13380200	0.45550100	0.00000000
H	2.24528600	0.28481100	0.00000000
H	1.30569200	-1.30863600	0.00000000
H	0.16404400	1.54625400	0.00000000
C	-1.23504000	-0.16288600	0.00000000
H	-1.81225200	0.15052100	0.88045700
H	-1.81225400	0.15052600	-0.88045300
H	-1.18168600	-1.25679500	-0.00000300

27 (geometry optimized with B3LYP/SDD/6-31G(d))

Cartesian coordinates:

C	2.05412500	3.34808000	-0.79981300
C	1.01912200	3.21409500	-1.73938000
H	0.61409500	2.22568700	-1.93943400

C	0.50086200	4.33466500	-2.39194800
H	-0.30586300	4.21183000	-3.10961400
C	0.99981500	5.60610300	-2.10449100
H	0.59109600	6.47992800	-2.60559700
C	2.01824900	5.75198700	-1.16033300
H	2.40566200	6.73988600	-0.92359500
C	2.54328600	4.63208300	-0.51361900
H	3.32978100	4.76555800	0.22156200
C	3.40001500	2.37730900	1.58601200
C	4.60404900	3.09195300	1.69343600
H	5.20091100	3.28372100	0.80642400
C	5.05200100	3.54308300	2.93689700
H	5.97939400	4.10727600	3.00358100
C	4.31029900	3.27520800	4.09071500
H	4.66159200	3.62488600	5.05817900
C	3.12242600	2.54733000	3.99668900
H	2.54994900	2.31927400	4.89224900
C	2.67116800	2.09904300	2.75288300
H	1.75824500	1.51277500	2.67848500
C	4.20313400	1.41535400	-1.04431000
C	4.39455900	2.06973700	-2.26926000
H	3.71105200	2.85887900	-2.55779700
C	5.43842100	1.74822300	-3.15422600
H	5.56918200	2.27237000	-4.09474900
C	6.28744200	0.73812300	-2.76126500
C	7.81315300	-0.88571700	-2.63680600
H	7.55341200	-1.80875300	-3.17310400
H	8.89000700	-0.82267600	-2.45579100
C	6.11715600	0.08168200	-1.54549400
C	5.09492000	0.36668800	-0.65282900
C	5.09486600	-0.36667300	0.65329400
C	6.11702200	-0.08165600	1.54604800
C	7.81296900	0.88572000	2.63747500
H	7.55328900	1.80878700	3.17374500
H	8.88982700	0.82258600	2.45650400
C	6.28720500	-0.73808900	2.76183700
C	5.43815700	-1.74819400	3.15472800

H	5.56883800	-2.27233400	4.09526600
C	4.39437600	-2.06972000	2.26967100
H	3.71085100	-2.85886800	2.55815000
C	4.20305500	-1.41534400	1.04470200
C	2.05407600	-3.34808500	0.80002600
C	2.54327900	-4.63208500	0.51389400
H	3.32985000	-4.76555900	-0.22120600
C	2.01818900	-5.75198800	1.16056700
H	2.40563800	-6.73988600	0.92387700
C	0.99965900	-5.60610600	2.10462100
H	0.59089900	-6.47993100	2.60569300
C	0.50066300	-4.33467100	2.39201500
H	-0.30613600	-4.21183700	3.10959800
C	1.01897600	-3.21410200	1.73948800
H	0.61391900	-2.22569700	1.93949300
C	3.40016900	-2.37731300	-1.58568600
C	4.60420800	-3.09196500	-1.69299900
H	5.20098800	-3.28373700	-0.80593200
C	5.05227200	-3.54309900	-2.93641900
H	5.97966500	-4.10730000	-3.00301800
C	4.31067700	-3.27521700	-4.09030500
H	4.66205700	-3.62489800	-5.05773700
C	3.12280200	-2.54732900	-3.99638900
H	2.55041000	-2.31926800	-4.89200100
C	2.67143200	-2.09904100	-2.75262400
H	1.75850600	-1.51276600	-2.67831000
C	-3.40016500	-2.37731100	1.58568300
C	-2.67143300	-2.09904300	2.75262500
H	-1.75850400	-1.51277100	2.67831600
C	-3.12281200	-2.54733000	3.99638700
H	-2.55042300	-2.31927200	4.89200200
C	-4.31069200	-3.27521100	4.09029600
H	-4.66207900	-3.62488900	5.05772600
C	-5.05228100	-3.54308900	2.93640600
H	-5.97967800	-4.10728400	3.00300000
C	-4.60420700	-3.09195900	1.69298900
H	-5.20098100	-3.28373100	0.80591900

C	-2.05404400	-3.34807700	-0.80001500
C	-1.01895500	-3.21408800	-1.73948700
H	-0.61391000	-2.22568000	-1.93950100
C	-0.50063300	-4.33465600	-2.39200900
H	0.30615800	-4.21181900	-3.10960000
C	-0.99961000	-5.60609600	-2.10460100
H	-0.59084500	-6.47991900	-2.60567000
C	-2.01813100	-5.75198300	-1.16053600
H	-2.40556400	-6.73988300	-0.92383500
C	-2.54322900	-4.63208100	-0.51386800
H	-3.32979200	-4.76555800	0.22124000
C	-4.20303300	-1.41535300	-1.04471600
C	-4.39433800	-2.06973400	-2.26968400
H	-3.71080300	-2.85887600	-2.55815700
C	-5.43811600	-1.74822000	-3.15475000
H	-5.56878600	-2.27236600	-4.09528700
C	-6.28717600	-0.73812200	-2.76186900
C	-7.81289100	0.88572400	-2.63756000
H	-8.88976400	0.82269900	-2.45665800
H	-7.55307800	1.80875600	-3.17382900
C	-6.11700700	-0.08168300	-1.54608000
C	-5.09485600	-0.36668900	-0.65331700
C	-5.09493000	0.36666800	0.65280800
C	-6.11717000	0.08164600	1.54546200
C	-7.81323100	-0.88572900	2.63671600
H	-8.89006900	-0.82257900	2.45563200
H	-7.55362200	-1.80880400	3.17300800
C	-6.28747100	0.73807300	2.76123700
C	-5.43846200	1.74817700	3.15421500
H	-5.56923400	2.27231300	4.09474200
C	-4.39459600	2.06970900	2.26925900
H	-3.71110000	2.85885500	2.55780800
C	-4.20315700	1.41533800	1.04430600
C	-3.40001900	2.37732100	-1.58600000
C	-2.67116700	2.09906000	-2.75286900
H	-1.75824600	1.51278700	-2.67846900
C	-3.12241600	2.54735600	-3.99667500

H	-2.54993600	2.31930200	-4.89223300
C	-4.31028400	3.27524200	-4.09070200
H	-4.66156900	3.62492900	-5.05816600
C	-5.05199200	3.54311300	-2.93688700
H	-5.97938100	4.10731200	-3.00357200
C	-4.60405000	3.09197100	-1.69342600
H	-5.20091700	3.28373400	-0.80641600
C	-2.05415600	3.34808300	0.79984500
C	-1.01914500	3.21409700	1.73940300
H	-0.61410500	2.22569100	1.93944100
C	-0.50089300	4.33466400	2.39198300
H	0.30583900	4.21182800	3.10964100
C	-0.99986300	5.60610000	2.10454800
H	-0.59115000	6.47992300	2.60566200
C	-2.01830600	5.75198500	1.16040000
H	-2.40573400	6.73988300	0.92367900
C	-2.54333500	4.63208400	0.51367400
H	-3.32983700	4.76556100	-0.22149900
O	7.39386100	0.24506200	-3.40786600
O	7.11820900	-0.85002700	-1.38855900
O	7.11807300	0.85006800	1.38920100
O	7.39355400	-0.24500900	3.40854100
O	-7.39353400	-0.24506100	-3.40857500
O	-7.11807900	0.85002300	-1.38924000
O	-7.11820300	-0.85008000	1.38851400
O	-7.39388100	0.24498800	3.40783400
P	2.69839400	1.79181800	-0.02452300
P	2.69840500	-1.79182200	0.02478700
P	-2.69838900	-1.79181700	-0.02478400
P	-2.69841000	1.79182300	0.02453700
Cu	1.19759800	-0.00001400	0.00007600
Cu	-1.19759800	0.00001500	-0.00003800
H	0.00005900	0.00000400	-1.26301400
H	-0.00006000	0.00000000	1.26304700

28

Cartesian coordinates:

C	-3.27685700	-1.73625100	-0.92580700
C	-3.09858000	-2.97038600	-1.56946700
H	-2.12643800	-3.45630800	-1.52803400
C	-4.16729500	-3.58605100	-2.22618400
H	-4.01598300	-4.54344300	-2.71766200
C	-5.42450300	-2.98156100	-2.23804400
H	-6.25748100	-3.46376500	-2.74318800
C	-5.61467900	-1.75842600	-1.58803600
H	-6.59489500	-1.28857400	-1.58560500
C	-4.54892800	-1.13978700	-0.93524600
H	-4.71129000	-0.19475500	-0.42538600
C	-2.54025300	-0.33029300	1.48228600
C	-3.16987500	0.92068900	1.57312200
H	-3.19344200	1.58009000	0.71067200
C	-3.75182800	1.33191200	2.77421600
H	-4.24905100	2.29753200	2.82890200
C	-3.70650000	0.50332600	3.89830300
H	-4.16031400	0.82560300	4.83179000
C	-3.07389000	-0.73889400	3.81886700
H	-3.03004100	-1.38614300	4.69067300
C	-2.49257000	-1.15294000	2.61933100
H	-1.99979200	-2.12048200	2.56048800
C	-1.39017000	0.49470200	-1.09188600
C	-1.98519800	0.67317100	-2.34829300
H	-2.76692400	-0.00770800	-2.66267900
C	-1.61251900	1.70177200	-3.23186900
H	-2.08963900	1.82338200	-4.19810300
C	-0.61428500	2.54707000	-2.80337300
C	1.01010600	4.06880100	-2.62264900
H	1.95735100	3.81187600	-3.11527200
H	0.93248000	5.14602000	-2.44993200
C	-0.01135500	2.38563800	-1.55747700
C	-0.34241900	1.37629100	-0.66739600
C	0.34242300	1.37634800	0.66727700
C	0.01135200	2.38576600	1.55727500
C	-1.01013500	4.06899600	2.62231300
H	-1.95737000	3.81207400	3.11495900

H	-0.93254400	5.14620400	2.44951800
C	0.61428200	2.54730900	2.80315700
C	1.61252700	1.70205800	3.23172000
H	2.08964800	1.82375500	4.19794200
C	1.98521200	0.67338500	2.34823100
H	2.76694500	-0.00746100	2.66267200
C	1.39018400	0.49480400	1.09184000
C	3.27692400	-1.73611800	0.92593400
C	4.54898100	-1.13962100	0.93525800
H	4.71130200	-0.19464300	0.42528700
C	5.61477300	-1.75816100	1.58807600
H	6.59497700	-1.28828500	1.58555500
C	5.42465200	-2.98122800	2.23822800
H	6.25766200	-3.46335500	2.74339500
C	4.16745800	-3.58575000	2.22648500
H	4.01618800	-4.54308800	2.71807800
C	3.09870200	-2.97018500	1.56974100
H	2.12656700	-3.45613100	1.52840600
C	2.54019800	-0.33044600	-1.48228500
C	3.16981000	0.92053000	-1.57327500
H	3.19340600	1.58002000	-0.71089400
C	3.75171200	1.33163400	-2.77443400
H	4.24892800	2.29725100	-2.82923800
C	3.70634500	0.50293200	-3.89843400
H	4.16012000	0.82511600	-4.83197100
C	3.07374600	-0.73928300	-3.81884600
H	3.02986600	-1.38662100	-4.69058300
C	2.49247600	-1.15320900	-2.61924400
H	1.99970600	-2.12074900	-2.56028300
O	-0.08266500	3.63835200	-3.44129300
O	0.92174900	3.37918500	-1.37283500
O	-0.92176000	3.37929100	1.37255000
O	0.08265400	3.63864100	3.44098400
P	-1.81029600	-0.99458500	-0.07716900
P	1.81031100	-0.99458300	0.07727000
Cu	-0.00000500	-2.47491000	0.00023300
H	-0.00001400	-4.03249400	0.00047700

S8

Cartesian coordinates:

C	-1.53808700	3.46578400	0.21924300
C	-0.45800000	4.30097600	0.54487900
H	0.55272800	3.90779800	0.49317100
C	-0.67280900	5.63000100	0.91678700
H	0.17484200	6.26322300	1.16461200
C	-1.96956400	6.14384300	0.95620700
H	-2.13785100	7.18005900	1.23757900
C	-3.05126500	5.32389100	0.62412400
H	-4.06300300	5.72057500	0.64650000
C	-2.83862800	3.99429400	0.25935100
H	-3.68762900	3.37127500	-0.00389800
C	-2.50393200	1.33971300	-1.46535800
C	-3.79204300	0.92251500	-1.09599400
H	-4.02825900	0.75184300	-0.05002600
C	-4.76876300	0.70300500	-2.06910800
H	-5.76363400	0.38202900	-1.77042100
C	-4.47315300	0.89858200	-3.42018100
H	-5.23546000	0.72685400	-4.17543200
C	-3.19319100	1.30946500	-3.79746600
H	-2.95451200	1.45848900	-4.84713800
C	-2.21383300	1.52468200	-2.82668900
H	-1.21659400	1.83983300	-3.12472700
C	-1.55680000	0.74566200	1.27148900
C	-1.63707600	1.42035500	2.49832400
H	-1.61067400	2.50339800	2.50703100
C	-1.74228000	0.75580600	3.73255900
H	-1.80544800	1.30001200	4.66839700
C	-1.76145300	-0.62006500	3.68909900
C	-1.67043800	-2.80020800	4.13978300
H	-0.65978500	-3.15173100	4.38860100
H	-2.43501100	-3.49292000	4.50033100
C	-1.69537800	-1.30804900	2.47890700
C	-1.58042000	-0.68726800	1.24460700
C	-1.61328200	-1.56434800	0.02979800

C	-2.80838400	-2.20073800	-0.26719900
C	-4.89549500	-3.00676200	-0.20182900
H	-5.83640600	-2.52035600	-0.47384800
H	-5.06764700	-3.82578800	0.51052100
C	-2.96833900	-3.09026000	-1.32652900
C	-1.91761500	-3.41382700	-2.15546600
H	-2.03290300	-4.10709900	-2.98140000
C	-0.68338000	-2.80406900	-1.86957200
H	0.16346000	-3.05451500	-2.49692800
C	-0.50559000	-1.90311300	-0.81046300
C	2.21037600	-1.83831700	-1.83698100
C	2.98332100	-2.98624500	-1.60827200
H	2.96142200	-3.47064100	-0.63733700
C	3.79303400	-3.50765400	-2.61975900
H	4.39168200	-4.39371500	-2.42508900
C	3.83630700	-2.89494300	-3.87329400
H	4.46889900	-3.30149000	-4.65789600
C	3.07081800	-1.75121400	-4.11208400
H	3.10617400	-1.26169500	-5.08164000
C	2.27091800	-1.22277700	-3.09850900
H	1.69715100	-0.31806200	-3.28217800
C	1.75564700	-1.76209300	1.03095300
C	1.35130300	-3.01133700	1.52932200
H	0.60995400	-3.59623000	0.99347300
C	1.89234400	-3.50355000	2.71894800
H	1.58038300	-4.47708400	3.08988300
C	2.83946000	-2.75436900	3.42314300
H	3.26088200	-3.14072300	4.34772800
C	3.24300400	-1.51047900	2.93473800
H	3.97995700	-0.91868400	3.46978900
C	2.70308300	-1.01273800	1.74718200
H	3.02598100	-0.04371200	1.37844400
O	-1.88382600	-1.51075100	4.72467100
O	-1.78725000	-2.65915200	2.72132400
O	-4.01276600	-2.04477700	0.38055500
O	-4.26905200	-3.52303700	-1.38059700
P	-1.16428900	1.71541200	-0.25543200

P	1.12648400	-1.06333600	-0.55524700
Cu	1.08491000	1.28924600	-0.78059200
C	2.64581400	2.52974300	-1.14625700
H	2.28023400	3.53454200	-0.89207800
C	3.73124600	2.17966200	-0.18852300
C	4.80749600	1.32288300	-0.51648700
C	3.72373900	2.69047400	1.13240800
C	5.79185800	0.98802800	0.41497700
H	4.87260400	0.91097500	-1.51953200
C	4.70503900	2.35800800	2.06298800
H	2.92377200	3.37015400	1.42404500
C	5.75289500	1.49712900	1.71515500
H	6.60227700	0.32560400	0.11667200
H	4.65910300	2.78258100	3.06420900
H	6.52586000	1.24273600	2.43577100
C	3.05817900	2.54110600	-2.62708900
H	3.94520100	3.17160500	-2.81520300
H	3.29711300	1.54314000	-3.01451200
H	2.24286800	2.93307300	-3.24888100

S5

Cartesian coordinates:

C	2.63843500	-1.37966700	-1.90688000
C	2.51044600	-1.00148100	-3.25684800
H	1.67971900	-0.36441400	-3.54908000
C	3.44414700	-1.42145400	-4.20528900
H	3.32277100	-1.12322000	-5.24372400
C	4.53282700	-2.20865000	-3.82362000
H	5.26378000	-2.52882400	-4.56178700
C	4.67881200	-2.57478200	-2.48532000
H	5.52560400	-3.18156800	-2.17428500
C	3.73969000	-2.16720800	-1.53475400
H	3.87559400	-2.46244100	-0.50067600
C	2.08955400	-1.30430500	0.93068800
C	2.06715300	-2.65219300	1.32902300
H	1.59072200	-3.39504200	0.69617300
C	2.65209100	-3.04610600	2.53355300

H	2.63981000	-4.09504100	2.82057500
C	3.25772000	-2.09756800	3.36378100
H	3.71437700	-2.40532900	4.30114500
C	3.27410100	-0.75550200	2.98225400
H	3.74091900	-0.00912800	3.61900900
C	2.69449900	-0.36159100	1.77378500
H	2.71447400	0.68388600	1.48699900
C	-0.07348700	-1.87032800	-0.87747500
C	-0.13861900	-2.77841200	-1.94056900
H	0.69454300	-2.84474800	-2.62994800
C	-1.24556900	-3.61787600	-2.15977000
H	-1.27423700	-4.31747700	-2.98799900
C	-2.28592700	-3.51069400	-1.26426700
C	-4.23563000	-3.61860700	-0.18166600
H	-5.05240000	-3.03656300	-0.62881400
H	-4.61969400	-4.39727800	0.48365100
C	-2.23554500	-2.61770100	-0.19699900
C	-1.16916000	-1.76490800	0.03947500
C	-1.20089500	-0.91206200	1.27078400
C	-1.07177000	-1.54251500	2.49927600
C	-0.69468300	-3.03263200	4.12886200
H	0.34639900	-3.33663900	4.29551500
H	-1.39439300	-3.76664400	4.54042200
C	-1.06631000	-0.86699100	3.71701100
C	-1.20087800	0.50207000	3.77754300
H	-1.18690900	1.03668900	4.72103600
C	-1.36703300	1.17128700	2.55220600
H	-1.47934700	2.24860400	2.57595600
C	-1.39543800	0.50570500	1.31880200
C	-2.20234800	3.11627000	0.20939100
C	-3.29750900	3.29063900	1.07366700
H	-3.74649200	2.43268400	1.56321300
C	-3.81756800	4.56062800	1.31999500
H	-4.66168700	4.67420100	1.99535500
C	-3.26288000	5.68210300	0.69689500
H	-3.67177400	6.67067900	0.88808900
C	-2.18754300	5.52351500	-0.17592400

H	-1.75413000	6.38699000	-0.67356900
C	-1.66275700	4.25048900	-0.41501800
H	-0.83599200	4.13457400	-1.10798700
C	-2.94852000	0.72998000	-1.14724800
C	-4.11098000	0.31074000	-0.48086900
H	-4.15096700	0.31593200	0.60411600
C	-5.21654100	-0.13877700	-1.20352300
H	-6.11521300	-0.44942800	-0.67561700
C	-5.17239400	-0.18250400	-2.60052300
H	-6.03551700	-0.53071700	-3.16230600
C	-4.01501200	0.21856400	-3.26851500
H	-3.96892400	0.17687500	-4.35371700
C	-2.90739600	0.67267300	-2.54772800
H	-1.99491400	0.96545900	-3.06123300
O	-3.45834800	-4.22289800	-1.22118000
O	-3.37880300	-2.74385200	0.55679000
O	-0.92825300	-2.88956000	2.72551200
O	-0.92289300	-1.76025500	4.74719000
P	1.38644300	-0.73642500	-0.69097300
P	-1.49243700	1.46321200	-0.25988200
Cu	0.55569500	1.40726100	-1.46971600
H	0.23904100	1.09527600	-2.98048600
C	1.69860500	3.12034100	-2.08418300
H	2.46195300	2.75546100	-2.76372400
H	0.88813700	3.66509300	-2.55615300
C	1.91659200	3.21351300	-0.72797500
H	1.20021900	3.77174700	-0.12926400
C	3.15855900	2.85924000	-0.02279100
C	3.34388800	3.31224000	1.29785100
C	4.20728700	2.13025100	-0.61947000
C	4.52446900	3.05347300	1.99420600
H	2.54971500	3.88103000	1.77689000
C	5.38337000	1.86831400	0.07788700
H	4.09426400	1.75195900	-1.63101700
C	5.55244900	2.32817800	1.38818800
H	4.64148700	3.42283400	3.01013100
H	6.17307700	1.29725400	-0.40351500

H	6.47328600	2.12324400	1.92731400

S5'

Cartesian coordinates:

C	-2.72742900	-1.98522600	-1.95149800
C	-2.11315100	-1.99443000	-3.21672000
H	-1.10896000	-1.59063700	-3.33216800
C	-2.77655700	-2.52877500	-4.32306200
H	-2.28674500	-2.52642300	-5.29351000
C	-4.05363000	-3.07531200	-4.18194300
H	-4.56560600	-3.49935500	-5.04203600
C	-4.66726900	-3.08216700	-2.92755900
H	-5.65945500	-3.51035000	-2.80793900
C	-4.01108500	-2.54011800	-1.82052800
H	-4.50076600	-2.55449900	-0.85185500
C	-2.63086000	-1.99864700	0.92864100
C	-3.75154700	-1.41701600	1.54199000
H	-4.14381200	-0.47685500	1.16710800
C	-4.36510300	-2.03502000	2.63503300
H	-5.23886600	-1.57605900	3.09175900
C	-3.86729700	-3.24160900	3.13354800
H	-4.34736100	-3.72203400	3.98219800
C	-2.74959200	-3.82777000	2.53504400
H	-2.35294900	-4.76431800	2.91823700
C	-2.13589900	-3.20778500	1.44590000
H	-1.26278100	-3.66893100	0.98968400
C	-2.28076600	0.49716100	-0.50530600
C	-3.26745900	0.98717500	-1.37061100
H	-3.74912400	0.30483700	-2.06136300
C	-3.66983800	2.33466700	-1.37893700
H	-4.43634900	2.69685600	-2.05538300
C	-3.04864700	3.16890400	-0.47537800
C	-2.33975000	4.89434300	0.76474000
H	-1.63075700	5.62210800	0.35284300
H	-2.88952500	5.31729500	1.61324000
C	-2.06637500	2.69916200	0.39166500
C	-1.62549700	1.38660600	0.40294700

C	-0.61090100	0.97128500	1.42342200
C	-1.05045700	0.81128800	2.72994600
C	-2.31839800	0.55020600	4.55370600
H	-2.85330700	-0.40703200	4.60940400
H	-2.77737100	1.30253300	5.20103400
C	-0.22812300	0.41890800	3.78262000
C	1.11290000	0.17124400	3.58678400
H	1.76232400	-0.13809400	4.39844400
C	1.59904100	0.34721600	2.28022200
H	2.64912500	0.14812400	2.10228200
C	0.78845800	0.75820000	1.20932900
C	3.32984600	1.22216600	-0.20837200
C	3.78268500	2.13981800	0.75469400
H	3.08554000	2.57648400	1.46286600
C	5.13185300	2.48414900	0.82761000
H	5.46604400	3.19212300	1.58171200
C	6.04999700	1.92466900	-0.06498300
H	7.10091100	2.19554900	-0.00693000
C	5.61191600	1.01528300	-1.02690400
H	6.31873900	0.57040900	-1.72186000
C	4.26196000	0.66427600	-1.09612600
H	3.92849800	-0.04523100	-1.84808400
C	0.94526700	2.31335500	-1.31640100
C	1.00777200	3.57645200	-0.70590900
H	1.33634900	3.67148400	0.32401100
C	0.64227900	4.72070400	-1.41360000
H	0.71103100	5.69519600	-0.93574600
C	0.20192600	4.61805000	-2.73715300
H	-0.08109900	5.51166500	-3.28751300
C	0.13450700	3.36651600	-3.34840700
H	-0.20392500	3.27875800	-4.37748300
C	0.50958600	2.21830200	-2.64512900
H	0.47960900	1.24294800	-3.12389700
O	-3.26559600	4.50500400	-0.25603700
O	-1.63037500	3.72793600	1.19200000
O	-2.32431900	1.01976900	3.20300900
O	-0.95230100	0.35806700	4.94475900

P	-1.75188000	-1.28048300	-0.54016800
P	1.55234200	0.77748800	-0.47746200
Cu	1.32079100	-1.17667200	-1.70626300
H	1.07096700	-0.95311600	-3.23250700
C	1.44000800	-3.24378200	-1.66158800
H	0.40068300	-3.49754400	-1.84616300
H	2.13792000	-3.56518900	-2.42851600
C	1.85976500	-2.89049200	-0.38921700
H	1.10830000	-2.80337400	0.39253500
C	3.25575800	-2.87228300	0.08381500
C	3.51166700	-2.73739600	1.46209500
C	4.36205500	-3.02362400	-0.77567800
C	4.81278500	-2.75062000	1.96195300
H	2.67206800	-2.62763800	2.14454500
C	5.66210400	-3.03625200	-0.27539200
H	4.20375500	-3.13322700	-1.84481900
C	5.89776900	-2.89926700	1.09546900
H	4.97943700	-2.64992200	3.03167400
H	6.49763000	-3.15740900	-0.96056900
H	6.91304600	-2.91201800	1.48234200

S5-l

Cartesian coordinates:

C	-1.21810300	3.53709400	0.55867100
C	-0.24461400	4.01496800	1.45676100
H	0.55748900	3.34846700	1.76455400
C	-0.30609900	5.32181700	1.94208700
H	0.45103600	5.66993200	2.64036200
C	-1.32662300	6.18095900	1.52821500
H	-1.36926100	7.20110900	1.90115000
C	-2.28843600	5.72173700	0.62783200
H	-3.08482600	6.38285100	0.29527600
C	-2.23780600	4.41062700	0.14836500
H	-2.99570100	4.07540300	-0.55099600
C	-2.31629400	1.74328400	-1.42188500
C	-3.69178000	1.62766800	-1.16046200
H	-4.03938600	1.53472000	-0.13583400

C	-4.61532500	1.62516400	-2.20764300
H	-5.67787700	1.54859100	-1.98898300
C	-4.17873100	1.73053900	-3.53147700
H	-4.89905600	1.72819800	-4.34540200
C	-2.81382400	1.83676600	-3.80360900
H	-2.46633500	1.91296600	-4.83062000
C	-1.89136700	1.84127800	-2.75527800
H	-0.82878100	1.91271200	-2.97183100
C	-1.73888300	0.72229400	1.23489000
C	-2.00529400	1.23995200	2.50791700
H	-1.90530200	2.30566300	2.67554700
C	-2.38019900	0.43293700	3.59662700
H	-2.58463000	0.85541200	4.57437700
C	-2.46974400	-0.92018200	3.35727900
C	-2.59256700	-3.14038100	3.50037900
H	-1.66387900	-3.60223200	3.86356200
H	-3.44700700	-3.81068300	3.62411100
C	-2.22637300	-1.44967000	2.09196000
C	-1.85516200	-0.68358500	0.99766400
C	-1.74501800	-1.38514200	-0.32281100
C	-2.92476100	-1.81029000	-0.91436700
C	-5.07254400	-2.09053500	-1.47780200
H	-5.54102600	-1.24847500	-2.00452700
H	-5.82484000	-2.74348200	-1.02584100
C	-2.97627600	-2.57114100	-2.07950100
C	-1.82682900	-2.97883500	-2.71803700
H	-1.85579100	-3.59080100	-3.61300400
C	-0.61061400	-2.56960900	-2.14299200
H	0.30511400	-2.88682700	-2.62578800
C	-0.54034700	-1.78623300	-0.98331600
C	2.34859800	-1.94821300	-1.44319200
C	2.40804200	-1.53004000	-2.78692400
H	1.66067500	-0.84006800	-3.16866800
C	3.40572400	-1.99749500	-3.64191600
H	3.42422400	-1.66899200	-4.67788900
C	4.38234200	-2.87694700	-3.16588400
H	5.16566600	-3.23506800	-3.82842500

C	4.34384000	-3.28787600	-1.83378100
H	5.09856500	-3.97042900	-1.45169200
C	3.33517300	-2.83195500	-0.98026700
H	3.32254300	-3.16552900	0.05140600
C	1.27464100	-2.16987800	1.23735800
C	0.85587800	-3.50803600	1.32490200
H	0.37804100	-3.98380200	0.47327900
C	1.04586200	-4.23098500	2.50317600
H	0.72399200	-5.26815200	2.55773100
C	1.65273400	-3.62411200	3.60775600
H	1.80261400	-4.18892500	4.52464300
C	2.06361100	-2.29240200	3.52960800
H	2.52792400	-1.81311500	4.38752200
C	1.87427200	-1.56505400	2.35149900
H	2.16247400	-0.51849900	2.29157600
O	-2.83493300	-1.92523200	4.21859200
O	-2.44636000	-2.80741200	2.11802400
O	-4.20360300	-1.59000900	-0.45952200
O	-4.28045300	-2.84634700	-2.40178200
P	-1.02949100	1.80590400	-0.08693700
P	1.08659700	-1.18703800	-0.31865800
Cu	1.31308500	1.15397200	-0.06475800
H	1.56666800	1.44044600	1.46023300
C	2.88664400	2.48841300	-0.80780000
C	2.23057800	1.96477200	-1.90199000
H	2.65268000	1.15484600	-2.48646700
H	1.42398100	2.52298300	-2.36491000
H	2.52190100	3.42828500	-0.39917600
C	4.20933800	2.07334400	-0.29278500
C	4.92277500	0.97259300	-0.80026600
C	4.81093800	2.83957300	0.72061500
C	6.18325200	0.64862100	-0.30254100
H	4.49088500	0.35944600	-1.58500900
C	6.07324400	2.51934300	1.21541700
H	4.27139200	3.69180400	1.12701700
C	6.76675700	1.41851000	0.70733500
H	6.71254500	-0.20994500	-0.70813300

H	6.51513800	3.12866600	1.99981100
H	7.75108400	1.16443900	1.09170200

S6-TS

Cartesian coordinates:

P	1.66318100	-0.46775800	-0.15609000
P	-1.89024200	0.35746300	-0.10102300
O	0.55335400	-0.72523600	4.50344900
O	-0.13595400	1.19878700	5.56719000
O	-1.54429000	-2.78763900	3.42397600
O	-0.91681400	-4.94175500	2.89705400
O	-5.12216400	-4.69949000	0.30413500
O	-5.31042400	4.77404300	-2.29555100
O	4.29866700	2.71910400	4.21350200
O	5.76448400	-2.22073000	-4.16274500
C	-1.40382000	0.64603100	1.66553400
C	-0.54265000	-0.29279000	2.32229000
C	-0.22302700	0.01614200	3.63759000
C	-0.65050300	1.17052600	4.28996800
C	-1.46354000	2.08926400	3.66654300
C	-1.83784700	1.79204600	2.34472200
C	0.33660700	-0.13341800	5.78493000
C	0.93834700	-1.87517200	0.81996000
C	1.32781200	-3.19205400	0.54274100
C	0.76521800	-4.31149800	1.18042300
C	-0.19769300	-4.05247200	2.12880100
C	-0.58470400	-2.74961000	2.43332600
C	-0.07310700	-1.62239100	1.80433300
C	-1.51336000	-4.12955000	3.91145600
C	-2.97081800	-1.13457800	0.02259100
C	-3.88133800	-1.31530700	1.06557000
C	-4.68433200	-2.46093200	1.17598900
C	-4.47460100	-3.47716200	0.20505200
C	-3.65268000	-3.27754200	-0.93610900
C	-2.89667100	-2.09987900	-0.98295900
C	-3.58690500	-4.28149300	-2.11625900
C	-2.89699700	-5.60268600	-1.70122900

C	-5.01095700	-4.57286700	-2.65138200
C	-2.77491200	-3.70806100	-3.29993200
C	-5.73664300	-2.51180100	2.32194400
C	-7.02418200	-3.27070100	1.92156900
C	-6.19777400	-1.07963600	2.70173800
C	-5.12360400	-3.12650000	3.60380200
C	-4.59319300	-5.65387700	1.22496800
C	-3.05453400	1.72420400	-0.54472000
C	-2.56537000	3.03861400	-0.61923700
C	-4.37294300	1.48906000	-0.92872500
C	-5.20461400	2.49806200	-1.45080600
C	-4.62303500	3.77273200	-1.62589400
C	-3.33678700	4.09499700	-1.10944800
C	-2.82281300	5.55513100	-1.00574200
C	-1.48424100	5.62998900	-0.23806900
C	-2.58620800	6.21035200	-2.38735300
C	-5.23908200	4.67548300	-3.71902000
C	-3.85202900	6.39565900	-0.20844300
C	-6.68099300	2.11025700	-1.75215100
C	-6.74283000	1.21269800	-3.01181600
C	-7.65430500	3.30005200	-1.92511700
C	-7.23875100	1.29613600	-0.55247200
C	2.56321500	0.47901900	1.14802700
C	2.55356000	1.87513500	1.11106100
C	3.16526300	2.64455300	2.10969500
C	3.78426500	1.94801100	3.18234500
C	3.94208600	0.53615600	3.18028700
C	3.27493100	-0.16373800	2.16384200
C	4.81211600	-0.27485200	4.18532200
C	6.08139500	0.49239000	4.62715100
C	3.98235400	-0.70660700	5.41867000
C	5.32526600	-1.58420900	3.53072700
C	4.63685200	4.71256700	2.03508100
C	3.58010900	2.75135700	5.44650200
C	3.17862800	4.19123100	1.99707900
C	2.56795500	4.66661200	0.66146100
C	4.87199600	-1.97960900	-3.12437000

C	5.32827800	-1.30244200	-1.96702800
C	7.51190800	-2.50910400	-1.63202200
C	4.35379000	-0.91067400	-1.03363300
C	2.99859800	-1.20074000	-1.20786100
C	2.62275400	-2.00655800	-2.29103300
C	3.54351200	-2.46601900	-3.24025700
C	5.75939700	-1.19927800	-5.16979600
C	7.58955100	-0.20086300	-2.63794500
C	3.16062300	-3.10470900	-5.73779400
C	3.12163700	-3.56072300	-4.26014200
C	1.68159000	-4.05152900	-3.98669500
C	7.03807000	-0.49563900	-0.24173900
C	2.35065700	4.85273300	3.12476100
C	6.83665700	-1.11428000	-1.64201100
C	4.06276200	-4.77962500	-4.08641800
H	-1.81442300	2.98207800	4.17265500
H	-2.50733000	2.47914600	1.84206200
H	1.27667600	-0.10153600	6.33524300
H	-0.42949100	-0.70786900	6.32773400
H	2.10672200	-3.36465700	-0.18994300
H	1.08524200	-5.32154400	0.94830400
H	-2.53096800	-4.47144500	4.10105600
H	-0.89794400	-4.17327600	4.82307100
H	-3.96507800	-0.53681600	1.81329300
H	-2.20511900	-1.92418100	-1.79844700
H	-1.91436700	-5.40849900	-1.25531700
H	-2.74562400	-6.23549200	-2.58464500
H	-3.49222300	-6.17419600	-0.98885300
H	-5.65223100	-5.00693600	-1.88323000
H	-4.95473900	-5.27281600	-3.49453100
H	-5.48216400	-3.65152300	-3.01459000
H	-3.18553800	-2.75725900	-3.65774300
H	-2.81320800	-4.41921800	-4.13282600
H	-1.71981900	-3.55115300	-3.05094200
H	-7.75636900	-3.19138100	2.73405900
H	-6.85922200	-4.32605000	1.71290200
H	-7.47123900	-2.82624600	1.02479100

H	-7.02687100	-1.14972700	3.41477500
H	-6.55193600	-0.52232400	1.82854900
H	-5.41213500	-0.49267100	3.18717200
H	-4.23185400	-2.56725000	3.90625500
H	-4.83716700	-4.17261300	3.46907700
H	-5.84972800	-3.08662800	4.42564500
H	-3.54229000	-5.45179400	1.45978600
H	-4.67329200	-6.64019500	0.75783400
H	-5.17884000	-5.66631400	2.15120200
H	-1.55067400	3.22836500	-0.29265600
H	-4.76638700	0.48556200	-0.83260000
H	-1.19964600	6.68149900	-0.12116200
H	-0.66693800	5.12957800	-0.76905000
H	-1.55836000	5.19628300	0.76556100
H	-3.52199100	6.40891500	-2.91053000
H	-1.95273000	5.58121900	-3.02390200
H	-2.07367000	7.17117800	-2.25575200
H	-5.76866700	3.79210700	-4.09203000
H	-4.20018500	4.63390100	-4.06504700
H	-5.71919300	5.57458400	-4.11415300
H	-4.82469200	6.41185800	-0.70381500
H	-3.49569500	7.42903200	-0.11288400
H	-3.98352200	5.99220400	0.80275200
H	-6.13145800	0.31171800	-2.88967700
H	-6.38401200	1.73781500	-3.90373300
H	-7.77584900	0.89608000	-3.20283700
H	-8.67871100	2.90850400	-1.94157900
H	-7.50675200	3.85397100	-2.85186100
H	-7.57801000	4.00837500	-1.09492000
H	-7.17725100	1.87424500	0.37661500
H	-6.71468900	0.34953000	-0.39810800
H	-8.29286800	1.05541000	-0.73228100
H	2.04378200	2.35927700	0.28726700
H	3.31303800	-1.24561700	2.15519700
H	5.86727500	1.40406000	5.18174100
H	6.68337700	0.77414600	3.75554200
H	6.69487300	-0.15973900	5.26042000

H	4.59234200	-1.33324800	6.08166900
H	3.10926400	-1.28809900	5.10458000
H	3.62954100	0.14523200	6.00475700
H	6.03142900	-2.07074200	4.21289800
H	5.84999500	-1.38639400	2.59074400
H	4.52665800	-2.30589100	3.33371000
H	4.64213600	5.80631700	1.94680100
H	5.21147000	4.30808000	1.19345900
H	5.14195100	4.43835500	2.96251600
H	4.05975600	2.10652200	6.19146800
H	2.53582100	2.44700800	5.31677500
H	3.60908300	3.78010100	5.81848400
H	1.50356300	4.41945800	0.57893400
H	3.08252100	4.25105100	-0.20987300
H	2.65253400	5.75783200	0.60329400
H	7.05144000	-3.16018200	-0.87969300
H	8.57648400	-2.40944600	-1.38482800
H	7.43021400	-2.99499500	-2.60697000
H	4.65260700	-0.34923400	-0.16009100
H	1.57565400	-2.26018400	-2.39551600
H	6.44201200	-1.53956800	-5.95302800
H	6.10943200	-0.24241600	-4.77288700
H	4.76146300	-1.05501800	-5.59163300
H	8.58084200	0.03947200	-2.23470000
H	7.05919700	0.74575900	-2.79506300
H	7.74350700	-0.68711400	-3.60161100
H	4.18113000	-2.99595500	-6.10697400
H	2.62790700	-2.15712900	-5.88117600
H	2.66875700	-3.85804700	-6.36517500
H	1.45407200	-4.88046500	-4.66617200
H	0.93355300	-3.26949900	-4.16022200
H	1.55812800	-4.42103800	-2.96286100
H	6.57343900	-1.09949400	0.54404000
H	6.63979700	0.52316900	-0.17464900
H	8.11093500	-0.44471000	-0.02559100
H	1.34052600	4.42830500	3.17102000
H	2.25316500	5.92769400	2.92839600

H	2.81744300	4.74143300	4.10315000
H	3.77183600	-5.57922900	-4.77937500
H	3.99983900	-5.17909400	-3.06733500
H	5.10179300	-4.51065500	-4.28871400
Cu	-0.05134400	0.29114200	-1.47099900
H	-0.23566700	-0.79494800	-2.66478000
C	-0.17954800	0.62009000	-3.58176000
C	0.12140900	1.87884300	-2.98160200
H	-0.72426300	2.52852300	-2.76984800
H	0.56653500	0.16552600	-4.22950400
H	-1.19821800	0.45907100	-3.92349600
C	1.41686400	2.54935100	-3.10508400
C	1.49291700	3.95495800	-2.97209600
C	2.62244600	1.87556300	-3.41139200
C	2.69186000	4.64531900	-3.13445700
H	0.58167000	4.51041400	-2.75847400
C	3.81995100	2.56843500	-3.57147300
H	2.62258400	0.79344600	-3.50769300
C	3.87213600	3.95923800	-3.43512800
H	2.70282700	5.72835100	-3.03099800
H	4.72628800	2.01253800	-3.80361800
H	4.80876800	4.49515800	-3.56285600

S6'-TS

Cartesian coordinates:

C	-1.30285200	-3.27186900	-1.35154000
C	-1.01882800	-3.26462400	-2.73043200
H	-0.57325000	-2.37945400	-3.17723400
C	-1.29391900	-4.38045600	-3.52095100
H	-1.07270600	-4.35289700	-4.58476000
C	-1.83794500	-5.53182400	-2.94618400
H	-2.04311300	-6.40485400	-3.56001300
C	-2.10814300	-5.55621100	-1.57788700
H	-2.52589800	-6.44916100	-1.12005400
C	-1.84665700	-4.43511400	-0.78598900
H	-2.06517600	-4.47386700	0.27556700
C	-1.18732600	-2.28189800	1.37625400

C	-2.48559900	-2.42369000	1.89331300
H	-3.34425800	-2.19704200	1.26785600
C	-2.67939200	-2.84653500	3.20948500
H	-3.68927300	-2.96382700	3.59520400
C	-1.57973900	-3.12480200	4.02713500
H	-1.73240100	-3.45316300	5.05195500
C	-0.28593800	-2.97661000	3.52467100
H	0.57265600	-3.18340100	4.15791900
C	-0.09110800	-2.55621100	2.20718200
H	0.91553100	-2.42589800	1.81891800
C	-2.20987600	-0.55898400	-0.72791700
C	-3.15171400	-0.81726100	-1.73188900
H	-3.13770500	-1.77543100	-2.23699400
C	-4.12337500	0.12009200	-2.12429100
H	-4.84787000	-0.10142600	-2.90030500
C	-4.10982000	1.33045700	-1.46789700
C	-4.41678300	3.43670200	-0.79489500
H	-3.94470600	4.20296300	-1.42449300
H	-5.21818400	3.86304700	-0.18495100
C	-3.18948000	1.59735700	-0.45703200
C	-2.21522400	0.69995600	-0.04796700
C	-1.37982100	1.07552700	1.13884500
C	-2.02518800	1.11830400	2.36626600
C	-3.47998900	0.83805300	4.04186100
H	-3.54780900	-0.18746600	4.42958400
H	-4.36729600	1.42115200	4.30381300
C	-1.41522600	1.52672400	3.54933300
C	-0.10285500	1.94212000	3.57000100
H	0.37824500	2.27579400	4.48284500
C	0.58240300	1.91540200	2.34315100
H	1.61821800	2.23138700	2.33678300
C	-0.01098800	1.49596300	1.14454100
C	2.58584500	2.25285700	0.05470900
C	2.80043200	3.60852600	-0.24142100
H	2.04201100	4.18043200	-0.76448100
C	3.99303500	4.23305600	0.12724400
H	4.14520100	5.28233100	-0.11282000

C	4.98439600	3.51602400	0.80011000
H	5.91255200	4.00485900	1.08501400
C	4.78426400	2.16614500	1.09305600
H	5.55572400	1.58755900	1.59173200
C	3.59788300	1.53589700	0.71367300
H	3.46538800	0.47900400	0.92177100
C	0.21475100	2.46780500	-1.59646400
C	-0.43557000	3.64949600	-1.20484800
H	-0.51877000	3.89922300	-0.15122400
C	-0.98672200	4.50324100	-2.16225200
H	-1.47745800	5.42102300	-1.84702900
C	-0.90032000	4.18464200	-3.52046700
H	-1.33025200	4.85013700	-4.26466500
C	-0.26363500	3.00737000	-3.91677900
H	-0.19972400	2.74989200	-4.97079100
C	0.28937500	2.15237000	-2.96088000
H	0.76734200	1.22363800	-3.26337700
O	-4.95178000	2.40169900	-1.62720400
O	-3.43110900	2.84926500	0.05809200
O	-3.33892800	0.79936800	2.61979900
O	-2.31642900	1.47431200	4.58212800
P	-0.85458000	-1.76709100	-0.36800400
P	1.03572900	1.34043100	-0.38141000
H	1.35872400	-1.06451500	-2.62525400
C	2.41418100	-2.26512100	-2.08576800
H	1.75874700	-3.04995500	-2.45174700
H	3.13435800	-1.93254300	-2.82826500
C	2.82778800	-2.33478100	-0.72355100
Cu	1.20496300	-0.83703100	-1.02580500
C	4.13111900	-1.89308100	-0.23264800
C	4.55234800	-2.26283900	1.06709600
C	5.04815900	-1.14191300	-1.00484600
C	5.80716900	-1.91590100	1.55944500
H	3.87603000	-2.84684700	1.68921400
C	6.30556400	-0.80080900	-0.51229800
H	4.77183000	-0.81912200	-2.00487500
C	6.70232600	-1.18207900	0.77306300

H	6.09302400	-2.22843800	2.56167300
H	6.98319200	-0.22699200	-1.14083100
H	7.68685500	-0.91974200	1.15096000
H	2.32300100	-3.06858700	-0.09967800

S6-I-TS

Cartesian coordinates:

C	-0.81729900	3.57631900	0.47845400
C	0.22468200	3.95032400	1.34683000
H	0.96433300	3.20802500	1.63633800
C	0.31766800	5.25698400	1.82658000
H	1.12700300	5.52564000	2.50067100
C	-0.61679100	6.21796300	1.43329100
H	-0.53919200	7.23836500	1.79943300
C	-1.64614700	5.86157100	0.56137700
H	-2.37477900	6.60364300	0.24508700
C	-1.74918300	4.55070500	0.08949300
H	-2.55587800	4.29320900	-0.58831400
C	-2.09115000	1.87737900	-1.49910800
C	-3.47560000	1.92078200	-1.26789300
H	-3.85541200	1.88944000	-0.25072300
C	-4.36829200	1.99326000	-2.33910700
H	-5.43792700	2.03734400	-2.14801700
C	-3.88935700	2.01732200	-3.65227800
H	-4.58583900	2.07316000	-4.48491900
C	-2.51477900	1.96538800	-3.89095800
H	-2.13731000	1.97585400	-4.91009600
C	-1.62065600	1.89322000	-2.82070100
H	-0.55013700	1.83473000	-3.00130200
C	-1.68538000	0.87586800	1.20775900
C	-1.93567000	1.47455200	2.44893300
H	-1.73665300	2.53207100	2.57496000
C	-2.42614100	0.75953600	3.55605900
H	-2.61721100	1.24367600	4.50754500
C	-2.65176100	-0.58547800	3.36751200
C	-3.03349200	-2.77082600	3.59398500
H	-2.18976000	-3.33087700	4.02031800

H	-3.97153600	-3.32220900	3.69991500
C	-2.42474400	-1.19306100	2.13429700
C	-1.94071400	-0.52034500	1.02319700
C	-1.86981500	-1.28262600	-0.26637300
C	-3.07593800	-1.61271800	-0.86592500
C	-5.22897200	-1.69158600	-1.46720300
H	-5.58573000	-0.81930100	-2.03156800
H	-6.06119000	-2.24115000	-1.01843600
C	-3.18300900	-2.39859700	-2.01068900
C	-2.06841700	-2.92601400	-2.62273500
H	-2.14213100	-3.55240400	-3.50498400
C	-0.82715400	-2.61277700	-2.04162900
H	0.06448400	-3.01036700	-2.51050300
C	-0.69944800	-1.81173700	-0.89898100
C	2.13957800	-2.33909900	-1.32453500
C	2.48179200	-1.85376700	-2.59976100
H	2.06298000	-0.90961400	-2.93636900
C	3.36009500	-2.56212300	-3.42036900
H	3.61038600	-2.17281900	-4.40378800
C	3.92710600	-3.75807600	-2.97295600
H	4.61976300	-4.30525800	-3.60700400
C	3.60566100	-4.24136600	-1.70404600
H	4.04714900	-5.16762600	-1.34530000
C	2.71562500	-3.54062900	-0.88614500
H	2.47803300	-3.93105200	0.09749000
C	1.10273500	-2.08731300	1.37495500
C	0.48121300	-3.30569400	1.69394800
H	-0.13125800	-3.81218700	0.95359500
C	0.63789800	-3.86689400	2.96287800
H	0.15979300	-4.81542600	3.19582700
C	1.41292000	-3.21612700	3.92738600
H	1.53412700	-3.65436200	4.91477400
C	2.02727900	-2.00079700	3.61982800
H	2.62537100	-1.48666900	4.36756500
C	1.87058500	-1.43677100	2.35192400
H	2.32926300	-0.47965800	2.11457300
O	-3.14815100	-1.50633200	4.25581200

O	-2.78381500	-2.51883400	2.20919300
O	-4.33489400	-1.25921500	-0.43912700
O	-4.50360400	-2.56051200	-2.34449500
P	-0.84195000	1.82821400	-0.13747600
P	0.98391200	-1.31295200	-0.29997900
Cu	1.24445200	0.93364200	-0.49244700
H	2.22742300	1.57447900	0.66356400
C	3.00496500	2.20973000	-0.64772300
C	2.47021200	1.84608800	-1.93222800
H	3.03945000	1.15864200	-2.55049300
H	1.92495300	2.61296100	-2.47576200
H	2.75913500	3.21574800	-0.31206700
C	4.37150500	1.78509300	-0.20879100
C	4.93325400	0.55203100	-0.57495500
C	5.14217000	2.65749300	0.57399900
C	6.22150800	0.20603300	-0.16903300
H	4.35564000	-0.14538600	-1.17389600
C	6.43365900	2.31564700	0.97734400
H	4.72347600	3.61832800	0.86673600
C	6.97994700	1.08539100	0.60858600
H	6.63450400	-0.75629800	-0.46171300
H	7.01225100	3.01216700	1.57940100
H	7.98468800	0.81421300	0.92222100

S7

Cartesian coordinates:

C	-2.16458000	2.26160800	-1.48316700
C	-1.95466700	2.25436300	-2.87202600
H	-0.98207500	1.97030800	-3.26653900
C	-2.98521500	2.60784200	-3.74442300
H	-2.81013700	2.59890000	-4.81676900
C	-4.23699800	2.96739800	-3.24030700
H	-5.03915100	3.24298800	-3.91980300
C	-4.45625600	2.97024700	-1.86035600
H	-5.42735500	3.25543300	-1.46310600
C	-3.42738600	2.61678100	-0.98432200
H	-3.60947300	2.60838800	0.08606000

C	0.00811300	3.45853500	0.03722000
C	1.36184800	3.47559300	0.41290900
H	1.93946900	2.55478700	0.42884700
C	1.98379300	4.67578000	0.75902000
H	3.03005300	4.66925200	1.05024100
C	1.26811300	5.87401000	0.71662700
H	1.75607800	6.80980800	0.97588100
C	-0.07430400	5.86807400	0.33174100
H	-0.63453400	6.79849800	0.29034400
C	-0.70346200	4.66773400	-0.00290400
H	-1.74673300	4.67600200	-0.30288800
C	-1.49569600	1.23129500	1.17938300
C	-1.33730700	1.97373600	2.35688100
H	-0.83751600	2.93386400	2.31247500
C	-1.79545500	1.52501000	3.60783000
H	-1.66528000	2.11570000	4.50777400
C	-2.41933000	0.29791800	3.62800800
C	-3.38529000	-1.63695700	4.19053500
H	-4.42701900	-1.82242500	4.46778400
H	-2.72238000	-2.41308100	4.59451800
C	-2.58991600	-0.45073400	2.46494800
C	-2.14320800	-0.04529600	1.21730200
C	-2.49244700	-0.91230400	0.04336100
C	-3.82215600	-0.93764600	-0.34797500
C	-5.98120200	-0.44765500	-0.66116700
H	-6.85524400	-0.68257400	-0.04816700
H	-6.15919500	0.43469200	-1.29073400
C	-4.31807900	-1.76182400	-1.35711800
C	-3.50004000	-2.63904400	-2.03290500
H	-3.87967200	-3.29262200	-2.81051000
C	-2.14438000	-2.64484700	-1.66025900
H	-1.47656400	-3.31822500	-2.18422800
C	-1.62639400	-1.81785900	-0.65387300
C	0.52433000	-2.16874100	1.34160400
C	1.68803100	-1.65690300	1.93680400
H	2.35046600	-1.00240700	1.37571900
C	2.01160000	-1.98973900	3.25349500

H	2.91431600	-1.57893700	3.69565900
C	1.17910600	-2.83705200	3.98641700
H	1.43171500	-3.09708000	5.01103400
C	0.01786700	-3.34954000	3.40092600
H	-0.62888900	-4.01642000	3.96626800
C	-0.31264400	-3.01506100	2.08655300
H	-1.22889200	-3.39853300	1.64714200
C	0.86854500	-3.18868100	-1.34919100
C	1.48815400	-2.94837100	-2.58581000
H	1.57930000	-1.92876800	-2.95040300
C	2.00596800	-4.00702300	-3.33596700
H	2.48622700	-3.80524300	-4.28949300
C	1.91944000	-5.31390100	-2.85447900
H	2.32966100	-6.13684400	-3.43375500
C	1.31366200	-5.56136300	-1.61961900
H	1.25183600	-6.57639900	-1.23607900
C	0.79124200	-4.50684300	-0.87090000
H	0.33392600	-4.71130200	0.09215700
O	-2.97949500	-0.35860700	4.69176500
O	-3.27014500	-1.60708800	2.76463800
O	-4.85544700	-0.20576500	0.18763000
O	-5.66814200	-1.57059100	-1.49308100
P	-0.74090300	1.83132900	-0.39612100
P	0.20696000	-1.73747900	-0.41758000
Cu	3.16839300	0.62438900	-1.98543100
Cu	0.78006100	0.32924500	-1.27164800
H	1.67132000	0.69278000	-2.59937900
C	5.04686200	0.63344300	-1.38352400
H	5.42833700	1.58225900	-1.79081300
C	5.10061100	0.71627400	0.10472500
C	4.97235900	1.96186000	0.76535800
C	5.29241300	-0.41136500	0.93315000
C	5.01229000	2.07239600	2.15246700
H	4.85150800	2.85840400	0.15839400
C	5.33818700	-0.30149400	2.32577800
H	5.42013100	-1.39003400	0.47902800
C	5.19249500	0.93759600	2.95262800

H	4.91997200	3.05287400	2.61654800
H	5.50765800	-1.19569100	2.92356000
H	5.23767500	1.02324200	4.03522200
C	5.84764700	-0.52310800	-2.00534900
H	6.89163300	-0.55213800	-1.64670700
H	5.41292500	-1.50837600	-1.79503100
H	5.87812800	-0.42263300	-3.09722200

S7'

Cartesian coordinates:

C	0.54635100	3.45092100	0.44757800
C	1.86096600	3.43874000	0.94117800
H	2.43935900	2.51894100	0.92537800
C	2.44382200	4.60710800	1.43529800
H	3.46245700	4.57815500	1.81218500
C	1.72675000	5.80478300	1.42810300
H	2.18344500	6.71686000	1.80335500
C	0.42292500	5.82965200	0.92722400
H	-0.13774700	6.76072700	0.91158800
C	-0.16586600	4.66070100	0.44245800
H	-1.17806700	4.69509000	0.05172900
C	-1.40276900	2.39007800	-1.41353300
C	-2.70799200	2.77618100	-1.07041400
H	-3.03458600	2.72272800	-0.03625100
C	-3.59507900	3.21654300	-2.05509900
H	-4.59954200	3.52543800	-1.77567500
C	-3.19224500	3.27116900	-3.39191500
H	-3.88454400	3.61424800	-4.15622500
C	-1.89821200	2.88143300	-3.74288300
H	-1.57985500	2.91684400	-4.78127600
C	-1.00923600	2.44173600	-2.76062400
H	-0.00258000	2.13701700	-3.03633500
C	-1.12414700	1.20932400	1.25814000
C	-1.01233600	1.82759400	2.51118500
H	-0.43382700	2.73904300	2.60008700
C	-1.61767900	1.31629400	3.67251100
H	-1.52095400	1.81355700	4.63132800

C	-2.34176800	0.15470400	3.52630700
C	-3.50395900	-1.72972700	3.82251200
H	-2.93585000	-2.59033700	4.19991900
H	-4.57604700	-1.85484500	3.99990400
C	-2.46814100	-0.47061400	2.28766300
C	-1.87760400	-0.00144700	1.12463600
C	-2.18354800	-0.73476000	-0.14706700
C	-3.47715000	-0.64339200	-0.63709100
C	-5.58026800	-0.00408200	-1.05679500
H	-5.68115700	0.94192100	-1.60574300
H	-6.50389700	-0.25603900	-0.52826400
C	-3.93362500	-1.34079600	-1.75356500
C	-3.11172700	-2.20085400	-2.44614600
H	-3.46201000	-2.75709100	-3.30866900
C	-1.79348000	-2.32499800	-1.97309400
H	-1.12591900	-2.99323400	-2.50342700
C	-1.31357700	-1.62468300	-0.85752500
C	1.13260900	-3.07105000	-1.49838000
C	1.12380600	-4.42227300	-1.11877000
H	0.72257400	-4.71310300	-0.15321900
C	1.63884900	-5.40084300	-1.97084100
H	1.63033500	-6.44238200	-1.66008600
C	2.16403800	-5.04537900	-3.21498900
H	2.56656000	-5.80893500	-3.87535700
C	2.17903100	-3.70413700	-3.60273200
H	2.59563500	-3.41731200	-4.56456500
C	1.67481100	-2.72339100	-2.74722000
H	1.71197100	-1.67790800	-3.04051300
C	0.55911000	-2.42506000	1.26309000
C	-0.43858100	-3.26381200	1.78519500
H	-1.32735000	-3.47915200	1.19958000
C	-0.30014100	-3.81376200	3.06123500
H	-1.07279000	-4.47251200	3.45072800
C	0.83131100	-3.52958200	3.83064500
H	0.93633100	-3.95825900	4.82387500
C	1.82528500	-2.69285800	3.31984100
H	2.70702700	-2.46505600	3.91254100

C	1.69108700	-2.14092700	2.04433900
H	2.47382400	-1.49550600	1.65237800
O	-3.04972900	-0.53855300	4.47385900
O	-3.26791800	-1.58174400	2.41961400
O	-4.50818800	0.10382600	-0.11655900
O	-5.25604500	-1.05366800	-1.97495200
P	-0.14623700	1.85462200	-0.17474400
P	0.48735600	-1.70280400	-0.43193500
Cu	1.50318600	0.37735800	-0.90765100
C	3.32849800	0.65435700	-1.74012300
C	4.28339100	0.54309800	-0.60313300
C	4.63717600	-0.72573100	-0.07783000
C	4.88465100	1.66197800	0.01894300
C	5.50230400	-0.86419200	1.00361400
H	4.22331300	-1.61572300	-0.54986700
C	5.75065600	1.52266700	1.10684800
H	4.68138100	2.65711300	-0.36644600
C	6.06495200	0.26250000	1.61652400
H	5.75178400	-1.86042000	1.36460400
H	6.19560700	2.41214400	1.54992300
H	6.74398100	0.15605300	2.45841700
H	3.47388600	-0.21863500	-2.39103200
C	3.45386000	1.92833100	-2.58621800
H	4.48518400	2.11118300	-2.93796200
H	2.81605700	1.85911900	-3.47701600
H	3.13921100	2.83147000	-2.04764200

S7-I

Cartesian coordinates:

C	0.09979300	3.47953000	0.78884000
C	1.29296200	3.50450200	1.52798800
H	1.90309300	2.60681600	1.58404900
C	1.71144700	4.67642600	2.16194000
H	2.63883200	4.68058800	2.72835500
C	0.94964800	5.84064500	2.05370200
H	1.27918400	6.75554700	2.53912200
C	-0.23291600	5.83014200	1.30928400

H	-0.82534400	6.73648200	1.21405300
C	-0.65616600	4.65822900	0.68167400
H	-1.57281000	4.66535100	0.09978800
C	-1.21062400	2.43550600	-1.56362400
C	-2.56037900	2.81523100	-1.62790900
H	-3.18670600	2.74266700	-0.74382900
C	-3.10846800	3.27202400	-2.82857700
H	-4.15203400	3.57593900	-2.86291600
C	-2.31856600	3.34959800	-3.97844200
H	-2.74736300	3.70563600	-4.91146900
C	-0.97715000	2.96550700	-3.92535100
H	-0.35829200	3.01798200	-4.81705500
C	-0.42681300	2.50911700	-2.72658100
H	0.61735200	2.20777600	-2.68866300
C	-1.74240700	1.23494200	1.06055500
C	-2.00665400	1.83963700	2.29719800
H	-1.47844100	2.74707800	2.56393700
C	-2.93307100	1.32118400	3.21934100
H	-3.12491700	1.80809400	4.16916800
C	-3.58640400	0.16727300	2.84979100
C	-4.79055000	-1.71219000	2.76512000
H	-4.36316700	-2.57939600	3.28598100
H	-5.86698600	-1.83304700	2.61303400
C	-3.33897800	-0.44603900	1.62337000
C	-2.42441500	0.02851000	0.69631900
C	-2.32687100	-0.69463500	-0.61380500
C	-3.40518200	-0.59822000	-1.47935300
C	-5.27566000	0.04664700	-2.52465400
H	-5.20400900	1.00204200	-3.06171700
H	-6.31699900	-0.21412000	-2.31612800
C	-3.48491800	-1.27531200	-2.69471400
C	-2.47954000	-2.11698200	-3.11384500
H	-2.53740000	-2.65347900	-4.05452600
C	-1.37372600	-2.24868400	-2.25527500
H	-0.56731900	-2.90335800	-2.56317800
C	-1.27371000	-1.57265700	-1.03132600
C	1.26403100	-3.00434800	-0.88929100

C	0.99936200	-4.37088100	-0.70306500
H	0.19749300	-4.68465200	-0.04180400
C	1.76902300	-5.33611500	-1.35317100
H	1.55625900	-6.39035500	-1.19560900
C	2.81143600	-4.95035900	-2.20000100
H	3.41142300	-5.70413200	-2.70311300
C	3.08583700	-3.59511000	-2.38886900
H	3.90146800	-3.28735400	-3.03776700
C	2.32154600	-2.62756000	-1.73252100
H	2.55456300	-1.57322400	-1.85562200
C	-0.15900600	-2.41740500	1.55143200
C	-1.27138500	-3.25579800	1.72511800
H	-1.94366000	-3.44351100	0.89328700
C	-1.52841800	-3.83907100	2.96774800
H	-2.38572700	-4.49748800	3.08654100
C	-0.68276400	-3.58896800	4.05148200
H	-0.88485900	-4.04439100	5.01732600
C	0.42130300	-2.74970000	3.88982300
H	1.08069200	-2.54668000	4.72937800
C	0.68025400	-2.16570200	2.64878900
H	1.53994000	-1.51106900	2.52724500
O	-4.54851000	-0.52954900	3.53470300
O	-4.14601300	-1.55280000	1.49837100
O	-4.55246400	0.13775400	-1.29419900
O	-4.67494900	-0.98696000	-3.31220800
P	-0.37988500	1.88176000	-0.01174400
P	0.30235600	-1.65421300	-0.06423600
Cu	1.44423900	0.41206000	-0.15874100
C	3.38557000	0.76603400	-0.37266500
H	3.60271000	1.83659000	-0.22923000
C	4.33621300	-0.04883300	0.54018200
H	4.12288400	0.18556900	1.59381300
H	4.13838200	-1.12320600	0.42077300
H	3.66291400	0.56320600	-1.42225000
C	5.80938600	0.20291200	0.27707300
C	6.47808100	1.28539500	0.86907200
C	6.53842100	-0.61475700	-0.59927000

C	7.82054400	1.54709500	0.59264400
H	5.93433000	1.93005400	1.55755900
C	7.88162800	-0.35935900	-0.88156200
H	6.04233500	-1.46625100	-1.06220700
C	8.52992700	0.72485300	-0.28637200
H	8.31615500	2.39091000	1.06770000
H	8.42477300	-1.01123700	-1.56234300
H	9.57673800	0.92458700	-0.50127300

S9-TS

Cartesian coordinates:

C	0.33259500	-3.44239600	-0.24672100
C	0.79988700	-3.62355400	-1.55745200
H	0.92181400	-2.77025700	-2.21714500
C	1.11548500	-4.90077100	-2.02578100
H	1.47514600	-5.01646600	-3.04323300
C	0.99578200	-6.00816200	-1.18572100
H	1.25189400	-7.00000500	-1.54937800
C	0.55605000	-5.83459800	0.12809300
H	0.46825000	-6.68983900	0.79328900
C	0.22152600	-4.56276900	0.59369000
H	-0.12701200	-4.44650900	1.61382500
C	-0.22448400	-1.93196700	2.12724100
C	-1.35566400	-2.41927500	2.79992300
H	-2.26403700	-2.63861700	2.24844100
C	-1.32335600	-2.62213500	4.18151800
H	-2.20302600	-3.01182700	4.68838000
C	-0.16270300	-2.34173600	4.90620900
H	-0.13881800	-2.50026200	5.98131100
C	0.96745000	-1.86130700	4.24223300
H	1.87552300	-1.64257900	4.79761400
C	0.94044100	-1.65660800	2.86124600
H	1.82913500	-1.29257500	2.35406000
C	-1.94496200	-1.65501500	-0.22745100
C	-2.45380300	-2.64261600	-1.08341600
H	-1.81822200	-3.46919500	-1.37322400
C	-3.76363800	-2.62085500	-1.59180800

H	-4.13067100	-3.40090000	-2.24965700
C	-4.55515000	-1.56389300	-1.20370100
C	-6.17443000	-0.04656400	-0.92237300
H	-6.33099100	0.70474400	-1.70677300
H	-7.06710700	-0.15464700	-0.29759100
C	-4.07183800	-0.57784700	-0.34959000
C	-2.78174800	-0.55996800	0.16115800
C	-2.46063600	0.54040600	1.12598700
C	-3.10376800	0.52296600	2.35482200
C	-4.22597400	-0.09441800	4.18909100
H	-3.68112500	-0.77946400	4.85254100
H	-5.30298100	-0.13572400	4.37356700
C	-2.98881200	1.53694300	3.30236300
C	-2.22792100	2.65882700	3.06203300
H	-2.14485200	3.46051800	3.78753800
C	-1.57016100	2.71611000	1.82153100
H	-0.96464600	3.58863000	1.61057400
C	-1.66612100	1.70055100	0.86092100
C	-0.07601700	3.55783900	-0.72630900
C	-0.71035100	4.54786300	-1.49254900
H	-1.57430900	4.30095000	-2.09912800
C	-0.23319500	5.86040800	-1.49434300
H	-0.73538500	6.61156000	-2.09861100
C	0.87977700	6.20605900	-0.72720100
H	1.24958500	7.22810400	-0.72986300
C	1.52247100	5.22725600	0.03313000
H	2.40142600	5.47706000	0.62108400
C	1.05760300	3.91150500	0.02731000
H	1.59984700	3.16346400	0.59627200
C	-1.85866600	1.68879300	-2.05486100
C	-3.12487500	2.29426100	-1.99169900
H	-3.43521200	2.80573000	-1.08526900
C	-3.99221700	2.23341600	-3.08325300
H	-4.96404600	2.71794800	-3.02734700
C	-3.61161200	1.55876400	-4.24708300
H	-4.28924800	1.51106300	-5.09539200
C	-2.36138100	0.94272400	-4.31388100

H	-2.06263100	0.40884400	-5.21189600
C	-1.49031800	1.00722000	-3.22390200
H	-0.52308400	0.51519700	-3.27621900
O	-5.86166900	-1.30612800	-1.52775500
O	-5.06593900	0.34073500	-0.10642300
O	-3.96362100	-0.44216000	2.82687300
O	-3.75801900	1.24191800	4.39876600
P	-0.15930500	-1.73927800	0.28977500
P	-0.63435000	1.79054100	-0.67760400
C	2.98370800	0.51727100	-1.51856000
H	4.00950700	0.52100800	-1.15311200
Cu	1.05949700	0.16672200	-0.42240200
C	4.90172400	1.70009400	1.35991900
C	4.82826300	0.20744100	1.88730700
B	2.94981400	0.66766100	0.59905000
H	1.78283900	0.67426900	1.07953400
O	3.79149700	-0.37956600	1.07645300
O	3.57625700	1.92080000	0.84236600
C	5.15827700	2.75133300	2.44605400
H	6.12790200	2.59362600	2.93337100
H	5.16928900	3.74827500	1.99173200
H	4.37659300	2.73974000	3.20915700
C	5.92676000	1.90792400	0.23026600
H	5.76691500	2.89670000	-0.21192800
H	6.95435000	1.86422600	0.60924300
H	5.82881600	1.16623100	-0.56644100
C	4.37943600	0.11279100	3.35657200
H	4.20733900	-0.94064100	3.60303700
H	5.13611000	0.50362300	4.04605500
H	3.44457800	0.65793100	3.52113000
C	6.11147300	-0.60598100	1.69951700
H	6.94265400	-0.17352800	2.26951700
H	5.95138800	-1.62840800	2.05843400
H	6.40301500	-0.66248700	0.64818700
C	2.80216600	1.85653300	-2.25278500
H	1.79873800	2.00015100	-2.66807800
H	2.98596800	2.68563400	-1.56551700

H	3.51063400	1.95025900	-3.09147400
C	2.94823600	-0.68306100	-2.42982600
C	2.25697600	-0.69486900	-3.65904000
C	3.73213200	-1.81964700	-2.13024600
C	2.35319600	-1.77310100	-4.54374700
H	1.66896900	0.17054200	-3.95099800
C	3.83844600	-2.88813500	-3.01565200
H	4.27362900	-1.84020900	-1.18803800
C	3.15254000	-2.87491000	-4.23580100
H	1.81870600	-1.73606800	-5.49094300
H	4.46710400	-3.73682700	-2.75535400
H	3.25047600	-3.70080800	-4.93597800

S9'-TS

Cartesian coordinates:

C	0.65726200	-2.10255100	2.81313800
C	0.56527100	-1.15260200	3.84623700
H	0.52519500	-0.09417100	3.60427700
C	0.51813300	-1.55415300	5.18044200
H	0.45206400	-0.80576800	5.96572000
C	0.54060700	-2.91353100	5.50491700
H	0.49262200	-3.22751500	6.54412000
C	0.61877600	-3.86382200	4.48728600
H	0.63355700	-4.92315700	4.72981100
C	0.68267800	-3.46296900	3.14970500
H	0.74986000	-4.21457900	2.37055900
C	0.75556300	-3.05110200	0.07406000
C	1.96327600	-3.72076000	-0.18058300
H	2.89954000	-3.30843200	0.18156000
C	1.97085300	-4.91436600	-0.90486900
H	2.91269700	-5.42478800	-1.09077700
C	0.77291300	-5.45427300	-1.37997500
H	0.77908100	-6.38466700	-1.94217600
C	-0.43124800	-4.79416500	-1.12875100
H	-1.36702800	-5.20626800	-1.49693100
C	-0.44503500	-3.59632000	-0.41033800
H	-1.39207300	-3.09263900	-0.23619900

C	2.40344100	-0.80705600	0.90321500
C	3.30261400	-0.88159200	1.97679300
H	2.99053200	-1.35840900	2.89696700
C	4.61115600	-0.37297800	1.91748700
H	5.28662100	-0.44001300	2.76317800
C	4.99013500	0.20674300	0.72741800
C	6.10062900	1.07811700	-1.00118300
H	6.41430200	2.11023600	-1.17945000
H	6.73199300	0.37261600	-1.55938800
C	4.11431400	0.27906200	-0.35138000
C	2.81128400	-0.19468000	-0.32145400
C	2.03114400	-0.11064900	-1.59717800
C	2.44745500	-0.92508100	-2.63994100
C	3.34535800	-2.57572400	-3.84106500
H	2.85389000	-3.54132700	-3.65579100
H	4.33852700	-2.71037100	-4.27637500
C	1.90498600	-0.88012600	-3.92188500
C	0.91812900	0.02327500	-4.24752800
H	0.50360100	0.08300200	-5.24788500
C	0.47232400	0.86530100	-3.21420700
H	-0.31888400	1.56896300	-3.44264400
C	0.98929100	0.81992000	-1.91180900
C	-0.83738100	3.06117700	-1.50130500
C	-0.29335500	4.32302800	-1.78992100
H	0.71035800	4.57252000	-1.46342000
C	-1.03810200	5.27552800	-2.48702400
H	-0.60158400	6.24860300	-2.69745100
C	-2.33575100	4.98180500	-2.91004600
H	-2.91509000	5.72508700	-3.45183000
C	-2.88587100	3.73112500	-2.62601100
H	-3.89799400	3.49274800	-2.94246000
C	-2.14845300	2.77758000	-1.92005300
H	-2.60829100	1.81930400	-1.69833100
C	1.38141400	2.73829100	0.30931700
C	2.56179000	3.19660500	-0.29738600
H	2.78527300	2.92491900	-1.32485600
C	3.46167100	3.98719100	0.41891600

H	4.37264100	4.33688200	-0.06065700
C	3.19191600	4.33262900	1.74581900
H	3.89384200	4.94928400	2.30120900
C	2.02013300	3.88140200	2.35499500
H	1.80044400	4.14705100	3.38554100
C	1.11982900	3.08532300	1.64358900
H	0.20940200	2.74162100	2.12605500
O	6.18667200	0.78971900	0.39890600
O	4.73735700	0.91831100	-1.39918300
O	3.45908700	-1.85836300	-2.60944200
O	2.54051000	-1.79131200	-4.72797700
P	0.68574100	-1.49282700	1.06597000
P	0.09997200	1.75473000	-0.57656700
C	-2.96624800	-0.00155500	1.63048000
H	-3.96794700	0.14389600	1.22778600
Cu	-1.05514700	-0.01801200	0.51151000
C	-5.05742300	-0.64564700	-1.38164200
C	-4.57064900	-2.13902500	-1.20761600
B	-2.93029300	-0.70806100	-0.42008700
H	-1.78456000	-0.68467800	-0.93806700
O	-3.48133700	-2.01150100	-0.27347700
O	-3.84736400	0.10293500	-1.14986300
C	-5.56719100	-0.29401200	-2.78287700
H	-6.44219200	-0.89829400	-3.05093300
H	-5.86703600	0.75963100	-2.80930000
H	-4.79382200	-0.44203900	-3.54018900
C	-6.11819000	-0.22859600	-0.34793000
H	-6.22796000	0.86070000	-0.37333200
H	-7.09360700	-0.67573700	-0.57197800
H	-5.83834300	-0.51637600	0.66868200
C	-4.00407000	-2.73592700	-2.50817600
H	-3.52871700	-3.69568400	-2.27891500
H	-4.78624200	-2.91349900	-3.25473400
H	-3.24514800	-2.08093300	-2.94715200
C	-5.60964800	-3.09476000	-0.61756600
H	-6.48528500	-3.18032600	-1.27221600
H	-5.17047500	-4.09258400	-0.51003500

H	-5.94240600	-2.76809000	0.37022400
C	-3.03580900	-1.17655900	2.61464500
H	-3.37811800	-2.07325400	2.09184100
H	-2.07196400	-1.41471400	3.07359800
H	-3.74058200	-0.97334300	3.43750500
C	-2.62683000	1.32748500	2.26003400
C	-2.99886600	2.53346300	1.62057200
C	-2.01909300	1.44794600	3.52771600
C	-2.75445600	3.77618000	2.19630700
H	-3.49290300	2.47779400	0.65421700
C	-1.77638100	2.69706300	4.10887200
H	-1.75690900	0.55221200	4.08053500
C	-2.13536400	3.87241800	3.44887300
H	-3.05730800	4.67779000	1.66862600
H	-1.31774900	2.74549000	5.09488400
H	-1.95376900	4.84266500	3.90363600

S9-l-TS

Cartesian coordinates:

C	-0.23468100	-2.73350700	-2.19479700
C	1.01060100	-2.48992700	-2.79193400
H	1.62447600	-1.67053800	-2.43551600
C	1.47445600	-3.30708400	-3.82597200
H	2.44353200	-3.10698300	-4.27517900
C	0.70367400	-4.38158400	-4.26931600
H	1.06690800	-5.02104200	-5.06965600
C	-0.53402000	-4.64011000	-3.67349100
H	-1.13567300	-5.48130900	-4.00802800
C	-0.99918200	-3.82416500	-2.64293700
H	-1.95696000	-4.04284100	-2.18082300
C	-1.60863100	-2.81922400	0.31523200
C	-2.95629800	-3.19316400	0.20487100
H	-3.59225000	-2.72370700	-0.53919500
C	-3.49258600	-4.15938500	1.05953400
H	-4.53564100	-4.44957700	0.95668600
C	-2.69111700	-4.76028500	2.03273400
H	-3.11016500	-5.51198700	2.69662100

C	-1.34901800	-4.39216500	2.14807000
H	-0.71893000	-4.85576300	2.90253200
C	-0.80894700	-3.42675800	1.29689100
H	0.23821800	-3.15105700	1.38403600
C	-2.17338600	-0.63922000	-1.57333500
C	-2.35936100	-0.67079500	-2.96261500
H	-1.74994500	-1.33713400	-3.56065200
C	-3.30717000	0.12580600	-3.62815800
H	-3.43480200	0.07994800	-4.70406300
C	-4.06770000	0.96020600	-2.84077200
C	-5.44610100	2.52174000	-2.03098000
H	-5.11137400	3.56438700	-2.10882600
H	-6.53077400	2.46371700	-1.89924000
C	-3.89809300	1.00566900	-1.45936200
C	-2.96370500	0.24669300	-0.77038000
C	-2.95848400	0.36504700	0.72502200
C	-4.05028400	-0.14193900	1.41304400
C	-5.90021600	-1.25969500	1.99536700
H	-5.77841400	-2.34585100	2.10269900
H	-6.95017300	-0.99117500	1.84859800
C	-4.21930700	-0.02437300	2.79102600
C	-3.29816800	0.63459900	3.57356200
H	-3.42685800	0.73726600	4.64540400
C	-2.18376500	1.17472100	2.90828800
H	-1.44153000	1.69631200	3.50058100
C	-1.99599200	1.06278500	1.52434400
C	0.38096000	2.66388900	2.10697900
C	-0.03957900	3.96258500	2.43983400
H	-0.85956600	4.42525100	1.90031500
C	0.59790300	4.67698900	3.45400900
H	0.26280700	5.68223800	3.69624900
C	1.66553800	4.10559700	4.15117300
H	2.16350300	4.66504200	4.93888300
C	2.09507300	2.81924100	3.82470000
H	2.93208400	2.36917100	4.35134900
C	1.46175200	2.10270400	2.80630700
H	1.82445200	1.11249300	2.55220300

C	-0.93189600	2.93893500	-0.45493800
C	-2.08828600	3.72101400	-0.30455000
H	-2.76094500	3.53974000	0.52845700
C	-2.39089900	4.72042400	-1.23136100
H	-3.28216100	5.32854500	-1.09588400
C	-1.54856000	4.94601400	-2.32325400
H	-1.78591900	5.72464500	-3.04332300
C	-0.40340400	4.16505100	-2.48774600
H	0.25359900	4.32986600	-3.33736100
C	-0.09817300	3.16665700	-1.56072500
H	0.79181800	2.55848600	-1.69656300
O	-5.07224700	1.81346400	-3.21772800
O	-4.79780900	1.89545900	-0.92062700
O	-5.13220700	-0.80253800	0.87861400
O	-5.40166800	-0.60782700	3.16802800
P	-0.78876600	-1.61726600	-0.82447200
P	-0.41418000	1.65772900	0.77031200
C	2.71715400	0.13129100	-0.78748800
C	3.47328300	1.40637900	-0.39552200
H	2.76262800	2.24595000	-0.34415700
H	3.85977100	1.29959800	0.62446900
C	4.63144800	1.83900600	-1.29106500
C	5.60863000	2.71156900	-0.78360900
C	4.76001600	1.42281000	-2.62283200
C	6.66796300	3.15683600	-1.57354800
H	5.53222000	3.04407700	0.25033400
C	5.81992900	1.86391500	-3.42041000
H	4.02540500	0.73943400	-3.03924900
C	6.77889100	2.73354800	-2.90086100
H	7.41101300	3.83027900	-1.15239200
H	5.89577900	1.52328600	-4.45072600
H	7.60514900	3.07488200	-3.51943100
Cu	0.82049200	-0.16277900	0.06301800
H	1.33501600	-0.98576200	1.53602100
H	2.17051100	0.31609200	-1.73025300
H	3.41565400	-0.67250500	-1.04063800
B	2.48006400	-1.17383300	1.04509400

O	2.77491600	-2.48456900	0.60540700
O	3.50300000	-0.70167800	1.89176200
C	4.59038500	-1.65357200	1.88505700
C	3.88447400	-2.97911300	1.38272400
C	4.74742200	-3.87054300	0.48723500
H	5.62923200	-4.23879700	1.02536000
H	4.16187700	-4.73757500	0.16301200
H	5.08133200	-3.33817300	-0.40625300
C	3.29649000	-3.82072300	2.52903100
H	2.68246000	-4.61900100	2.09854200
H	4.07574200	-4.28317200	3.14523000
H	2.65708300	-3.21272800	3.17732000
C	5.69186500	-1.14885200	0.93944400
H	6.00891100	-0.15108000	1.25884600
H	6.56799200	-1.80695400	0.96099800
H	5.34577000	-1.07021700	-0.09363200
C	5.15356800	-1.72600400	3.30796200
H	5.94050200	-2.48581700	3.38468900
H	5.59296800	-0.75884400	3.57521500
H	4.37458900	-1.95399000	4.03927000

(*S*)-SEGPHOS

Cartesian coordinates:

C	2.92276900	2.13819400	-1.12424100
C	2.17168800	3.18167200	-1.69391700
H	1.10753600	3.25361400	-1.48009500
C	2.77270400	4.12262000	-2.52864100
H	2.17395700	4.91844800	-2.96437600
C	4.14263300	4.05027800	-2.79337300
H	4.61486500	4.78917500	-3.43557700
C	4.90208200	3.02837600	-2.22299400
H	5.96929300	2.96692200	-2.42152500
C	4.29736700	2.07711800	-1.39727600
H	4.90038200	1.28550800	-0.96317600
C	3.39450100	0.02393000	0.79737000
C	3.96248300	-1.14332200	0.26431900
H	3.59763600	-1.53606000	-0.67978000

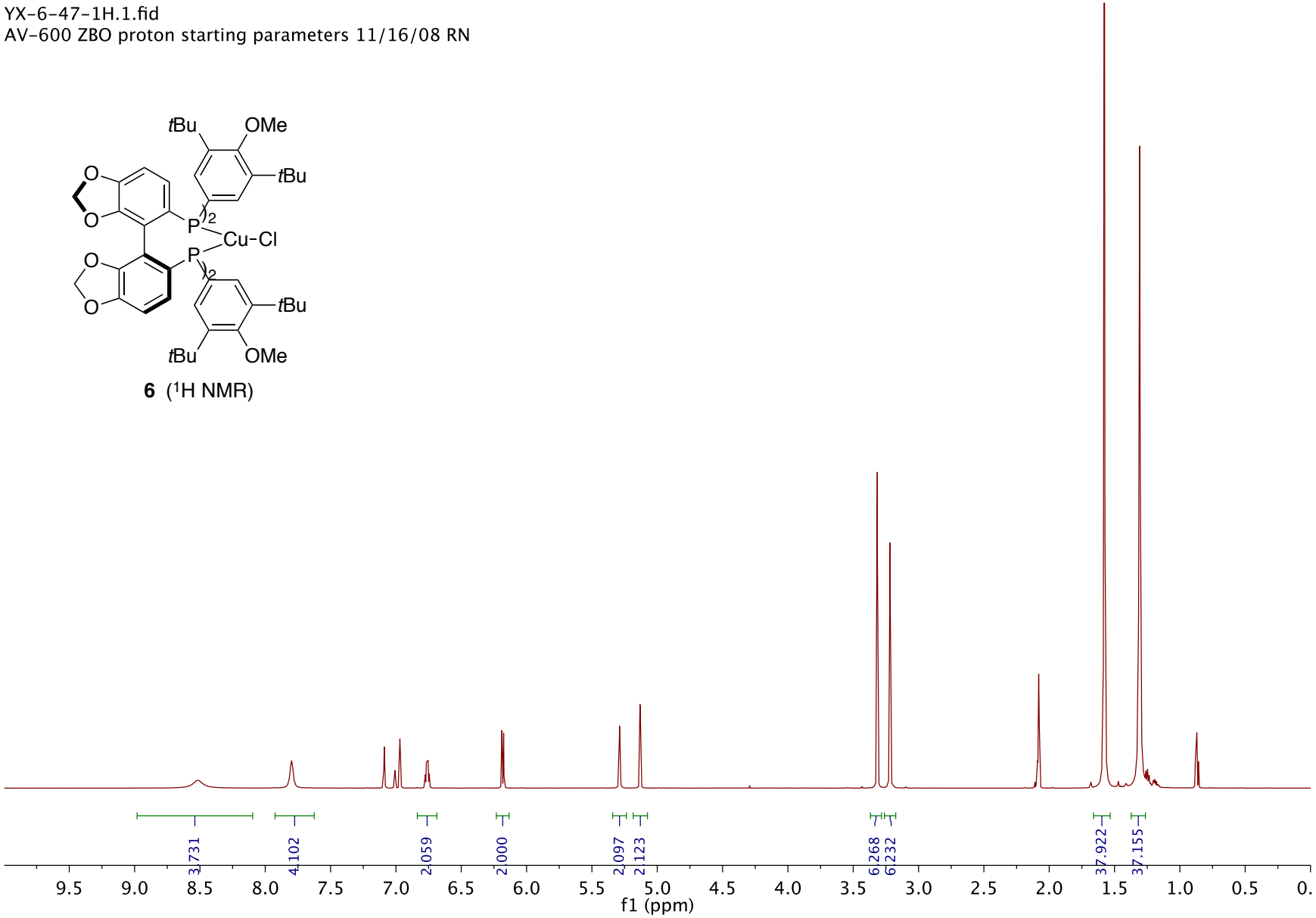
C	4.98554400	-1.81063700	0.94155800
H	5.41507200	-2.71316100	0.51353300
C	5.45840700	-1.32135600	2.16147800
H	6.25631400	-1.84079400	2.68613700
C	4.89892600	-0.16266800	2.70525900
H	5.25683200	0.22197800	3.65686800
C	3.87083700	0.49769100	2.03141300
H	3.42650800	1.38855200	2.46942200
C	1.29136100	-0.24271400	-1.18749900
C	1.68461400	-0.31736500	-2.52908300
H	2.47643300	0.33278100	-2.88474500
C	1.08074100	-1.19550700	-3.44806100
H	1.39376700	-1.23866200	-4.48576000
C	0.07033400	-1.99811600	-2.96398600
C	-1.69280100	-3.34030500	-2.70479800
H	-2.64428300	-2.87346400	-2.99364800
H	-1.77081700	-4.43035100	-2.69417500
C	-0.32460800	-1.94601700	-1.62822100
C	0.23799200	-1.07922700	-0.70824200
C	-0.23798900	-1.07923200	0.70823500
C	0.32461300	-1.94602700	1.62820900
C	1.69280800	-3.34031900	2.70477800
H	2.64429100	-2.87348100	2.99363100
H	1.77082300	-4.43036400	2.69414700
C	-0.07033000	-1.99813400	2.96397300
C	-1.08073900	-1.19553100	3.44805300
H	-1.39376600	-1.23869300	4.48575100
C	-1.68461500	-0.31738600	2.52907900
H	-2.47643600	0.33275500	2.88474400
C	-1.29136100	-0.24272500	1.18749500
C	-2.92277100	2.13818300	1.12425300
C	-4.29736800	2.07710100	1.39729300
H	-4.90038200	1.28549300	0.96318800
C	-4.90208300	3.02835200	2.22301800
H	-5.96929300	2.96689400	2.42155200
C	-4.14263500	4.05025300	2.79340100
H	-4.61486600	4.78914500	3.43561000

C	-2.77270700	4.12260100	2.52866500
H	-2.17396000	4.91842800	2.96440200
C	-2.17169100	3.18165900	1.69393300
H	-1.10754000	3.25360600	1.48010800
C	-3.39450400	0.02393400	-0.79737100
C	-3.96247000	-1.14333300	-0.26433700
H	-3.59761100	-1.53608800	0.67975000
C	-4.98553400	-1.81064300	-0.94157900
H	-5.41504900	-2.71317900	-0.51356800
C	-5.45841400	-1.32134100	-2.16148400
H	-6.25632200	-1.84077400	-2.68614700
C	-4.89894700	-0.16263700	-2.70524800
H	-5.25686600	0.22202600	-3.65684500
C	-3.87085600	0.49771500	-2.03139900
H	-3.42653900	1.38858900	-2.46939500
O	-0.66583000	-2.94823500	-3.62707300
O	-1.31012200	-2.87969300	-1.40666000
O	1.31013000	-2.87969700	1.40664300
O	0.66583800	-2.94825400	3.62705500
P	2.01566300	0.98158100	0.00654100
P	-2.01566400	0.98157800	-0.00653600

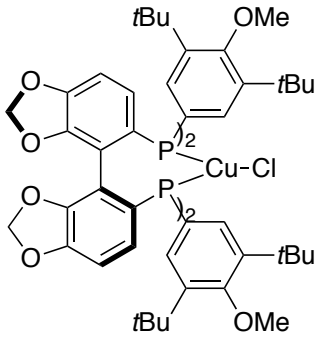
XIV. NMR Spectra

YX-6-47-1H.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN

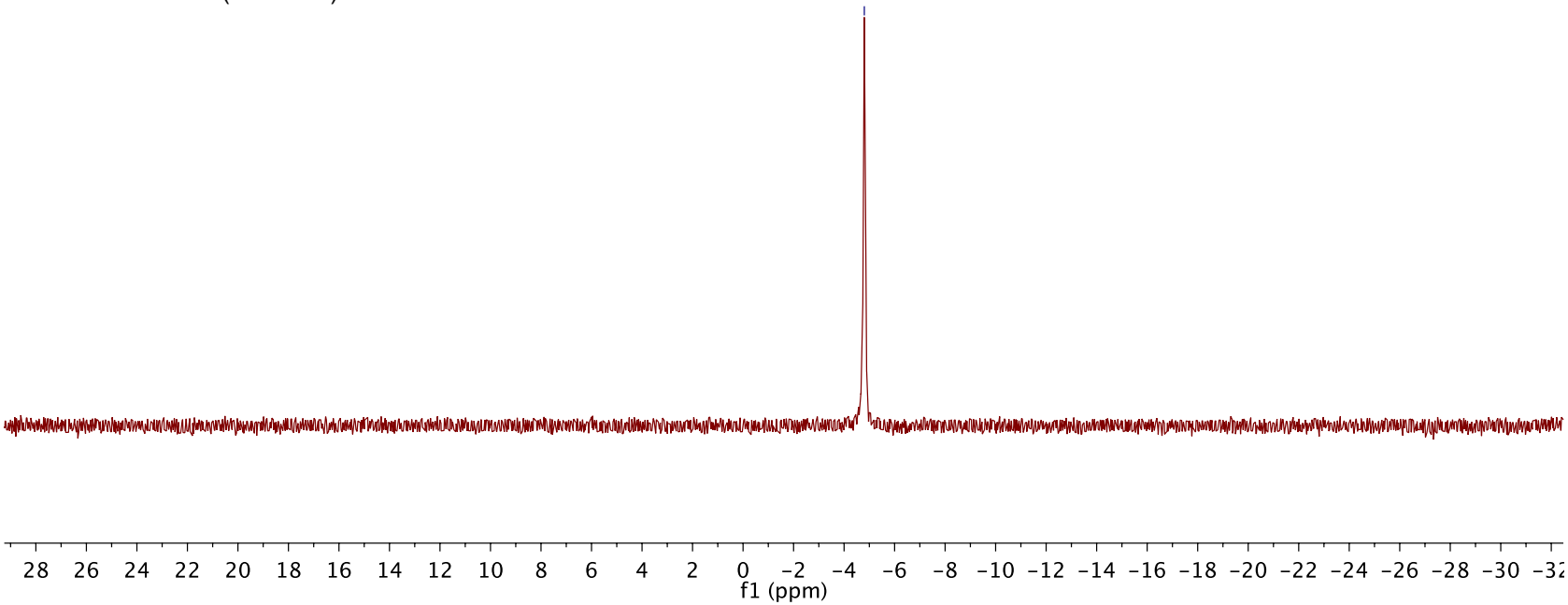
6 (^{1}H NMR)



YX-6-47-31P.1.fid
AV-600 31P starting parameters 11/19/08
31P p1=12.5us at 2dB. SW 400 ppm, O1P -50 ppm
With 1H decoupling

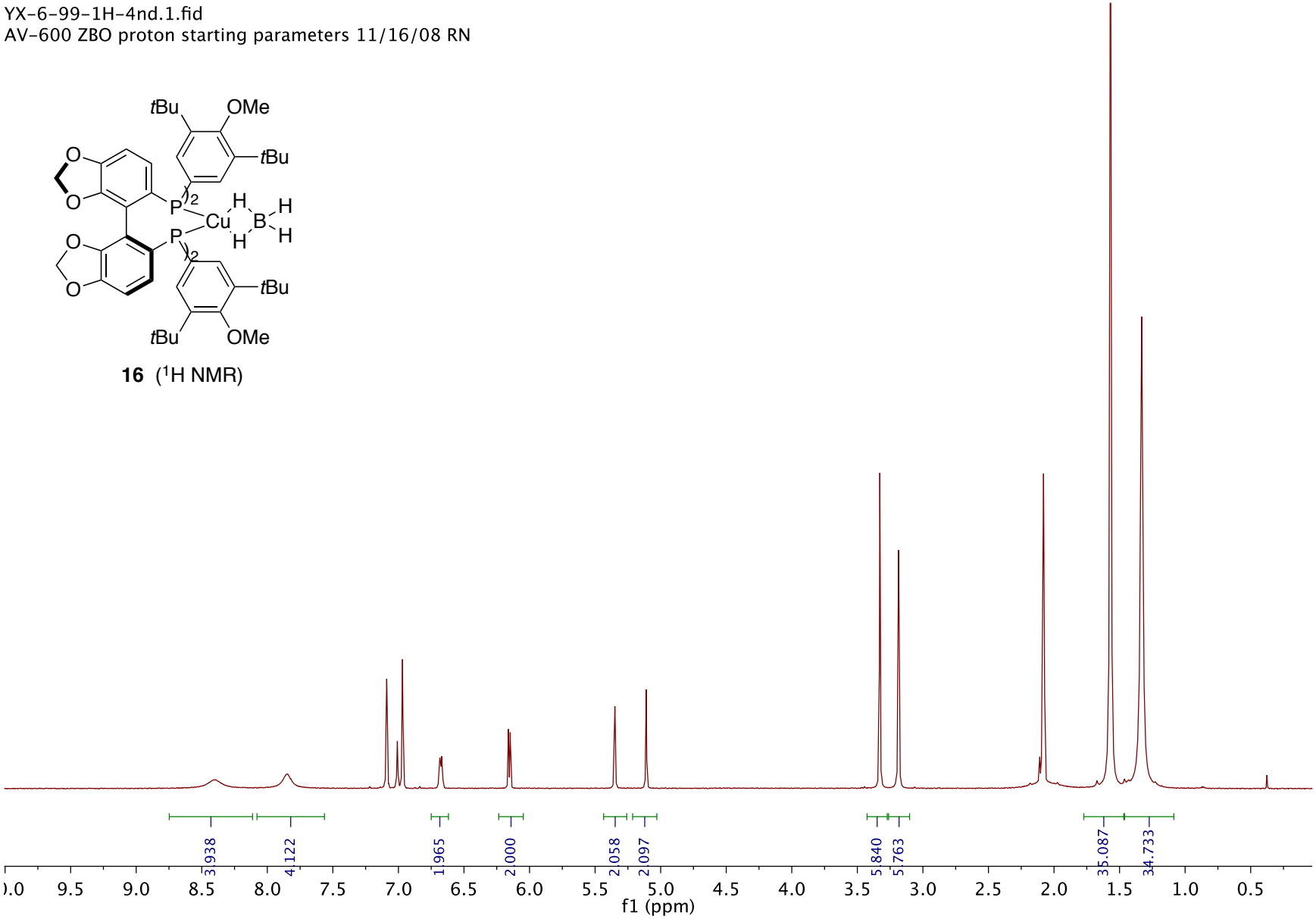


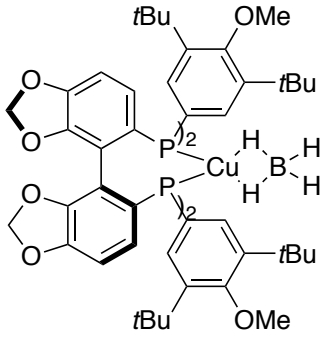
6 (^{31}P NMR)



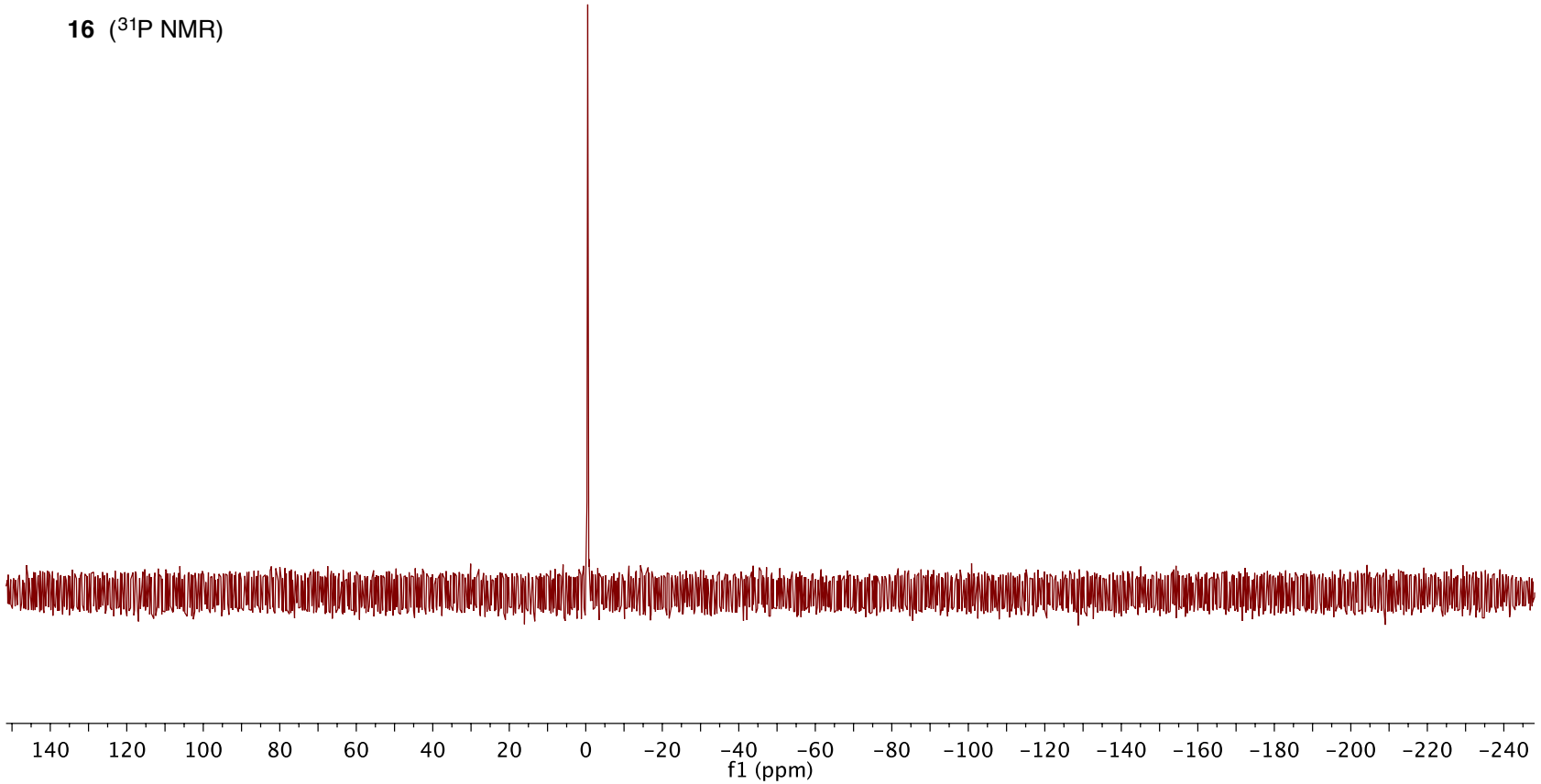
YX-6-99-1H-4nd.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN

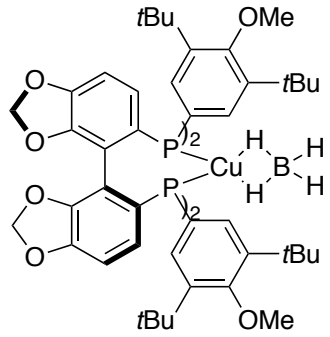
16 (^{1}H NMR)



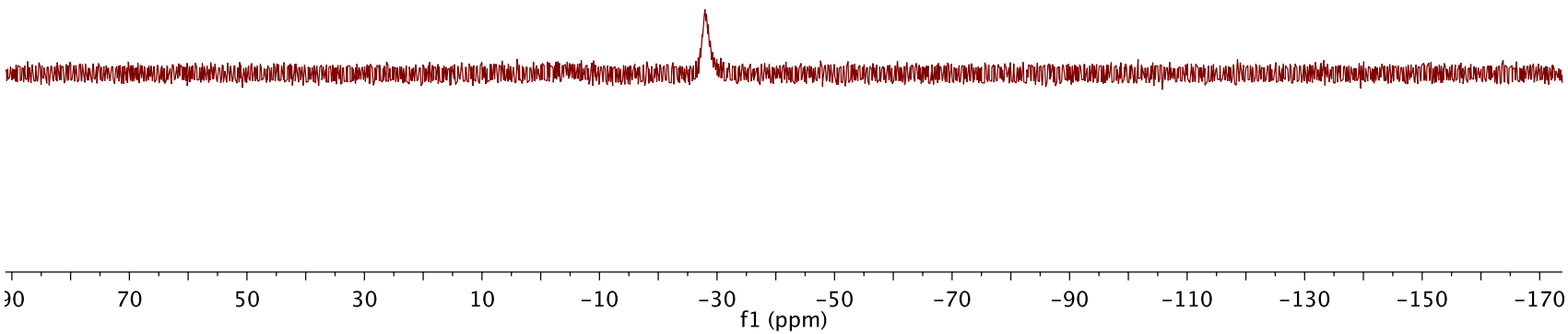

tBu
OMe
tBu
O
O
P
2
Cu
H
B
H
H
H
P
2
O
O
tBu
tBu
OMe

16 (^{31}P NMR)


140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)



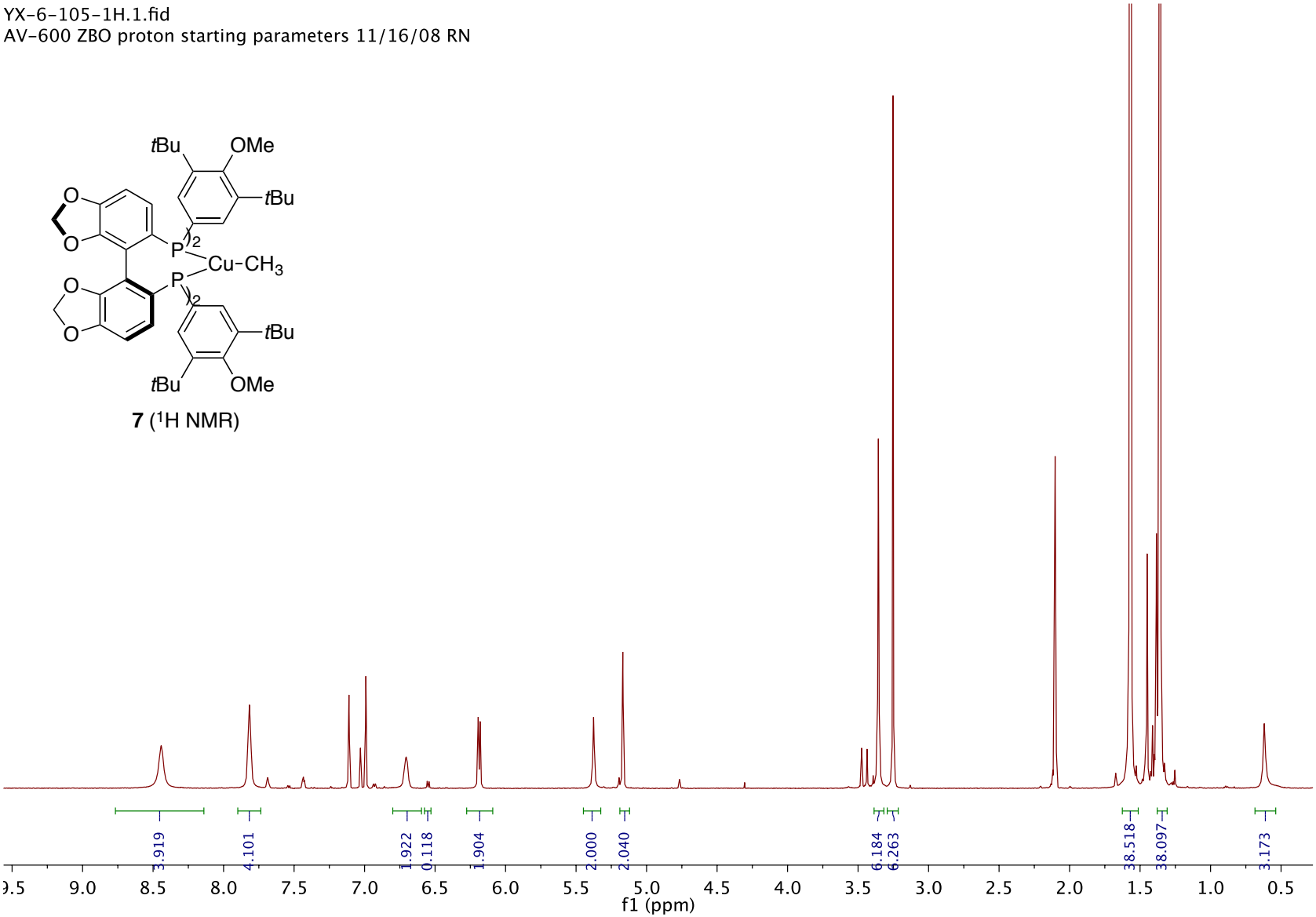
16 (^{11}B NMR)



Note: Multiple baseline corrections were performed to remove the uneven baseline that results from boron in the borosilicate glass NMR tubes.

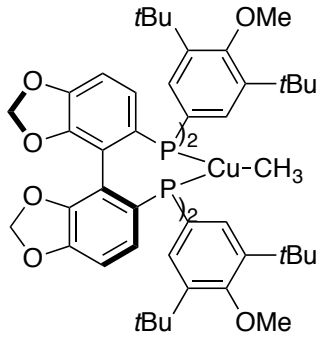
YX-6-105-1H.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN

7 (^{1}H NMR)

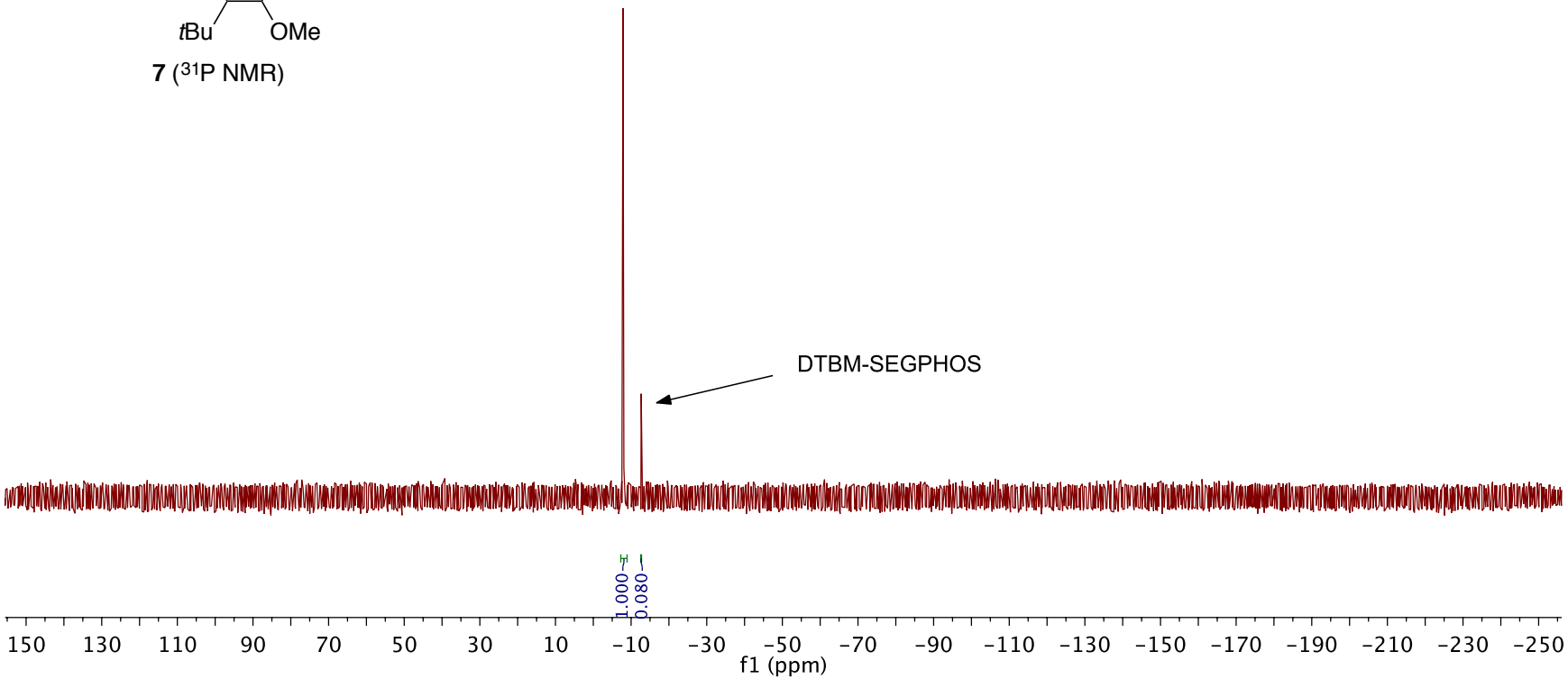


The sample contains 8% DTBM-SEGPHOS as a minor impurity.

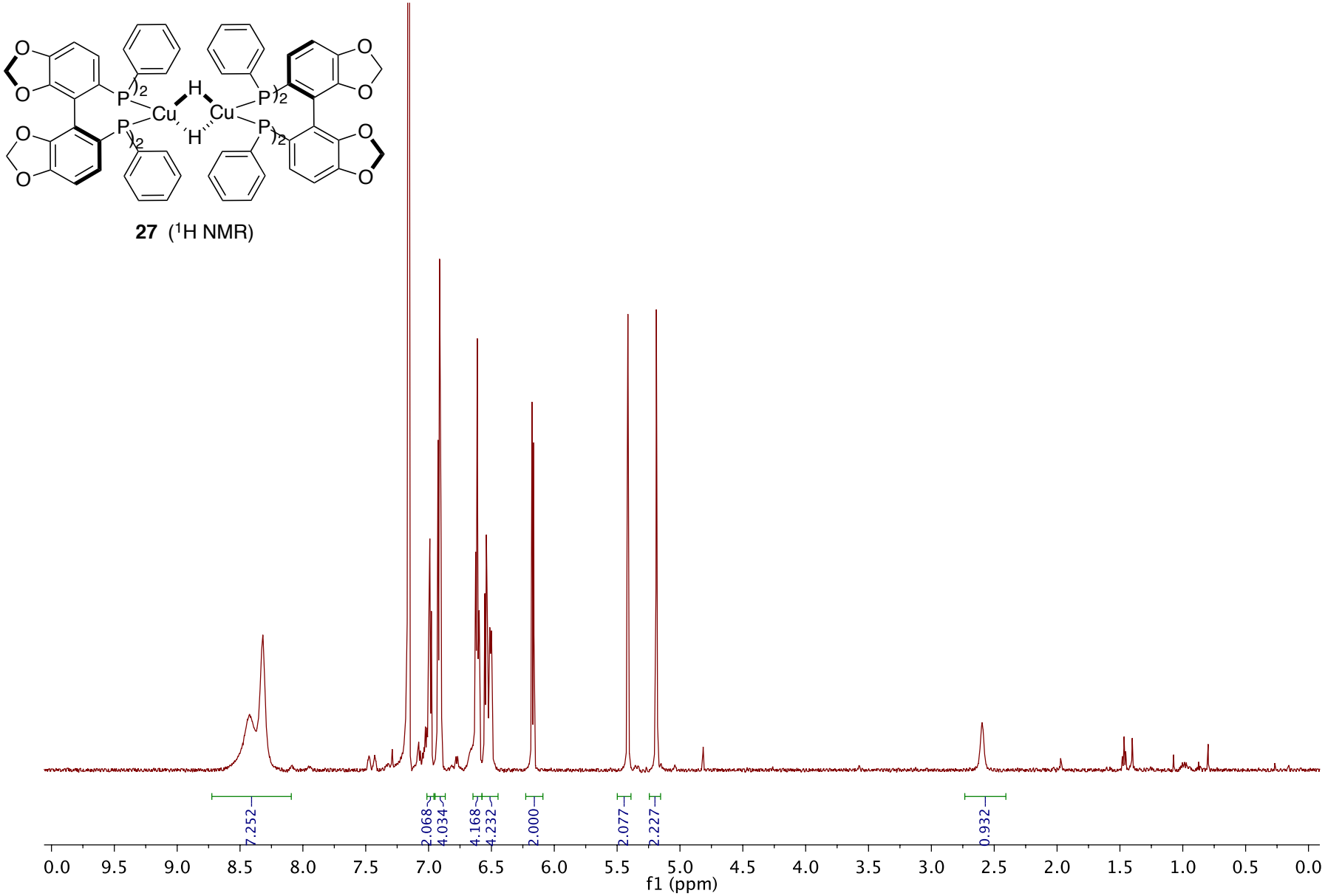
YX-6-105-31P.1.fid
AV-600 31P starting parameters 11/19/08
31P p1=12.5us at 2dB. SW 400 ppm, O1P -50 ppm
With 1H decoupling



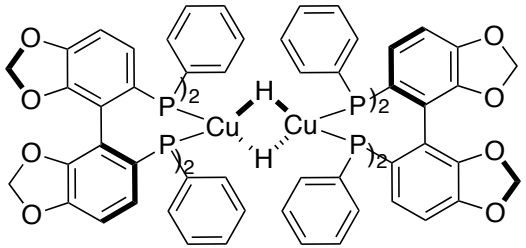
7 (^{31}P NMR)



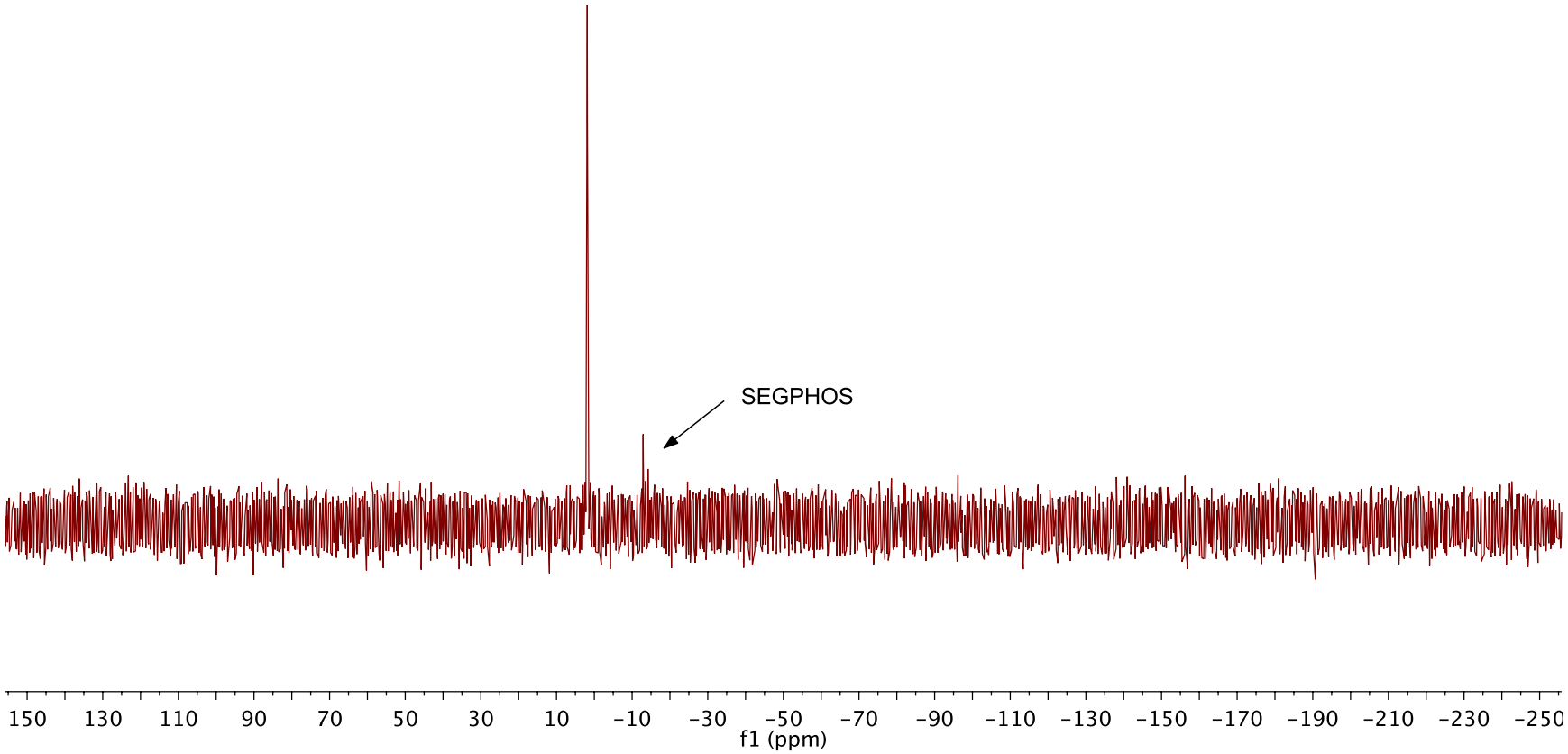
The sample contains 8% DTBM-SEGPHOS as a minor impurity.

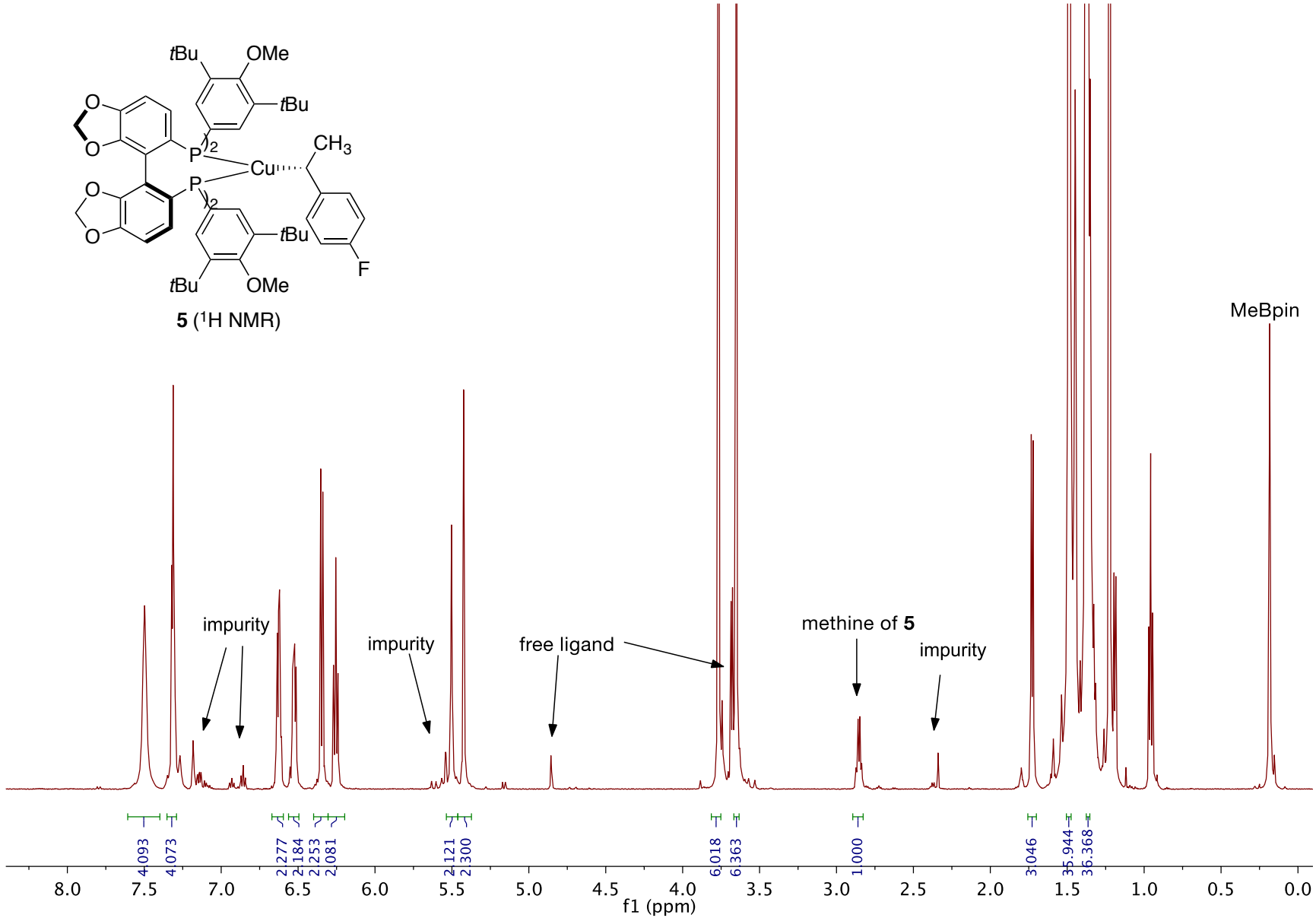

7.252
2.068
4.034
4.168
4.232
2.000
2.077
2.227
0.932
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

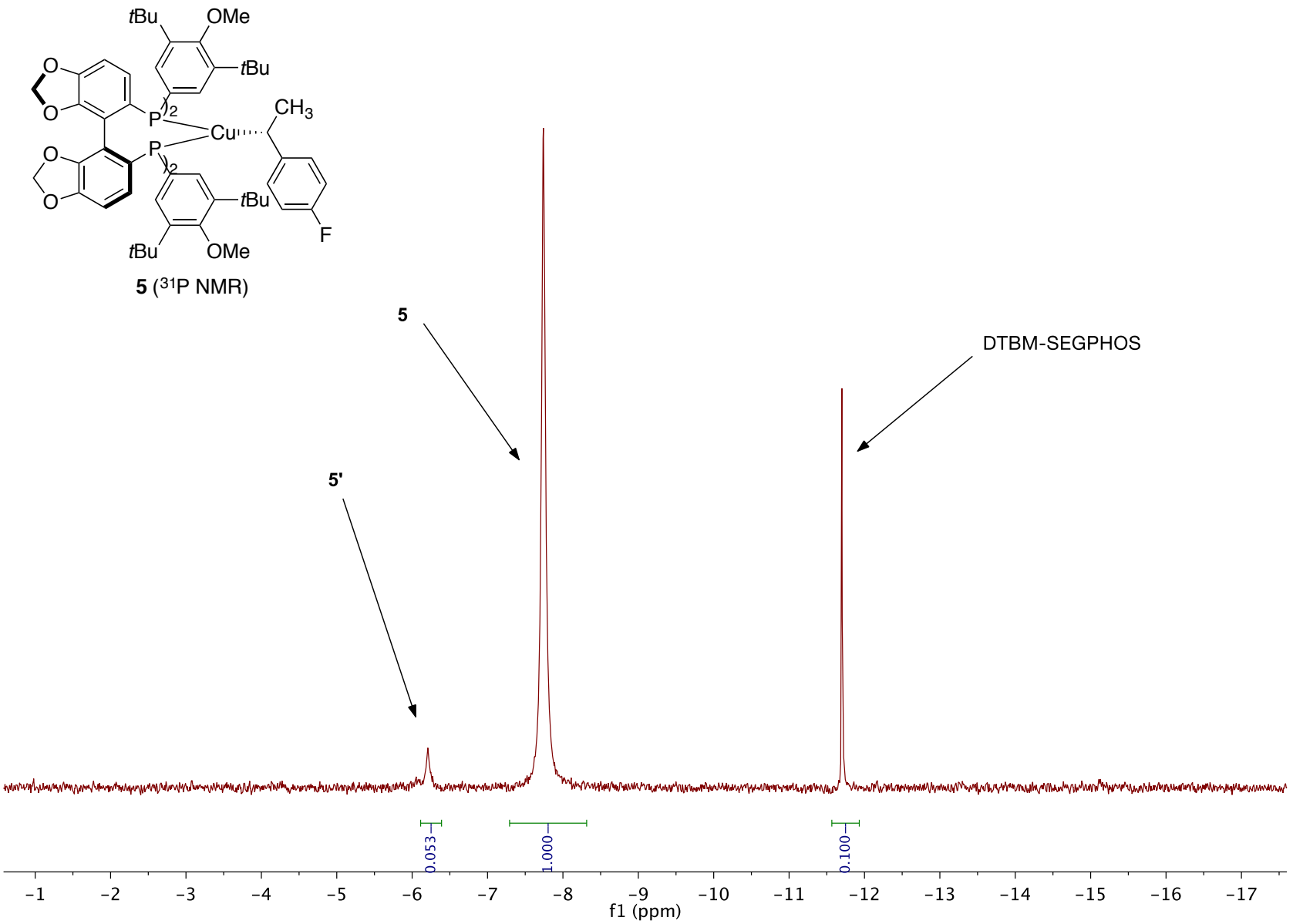
27 (^{1}H NMR)

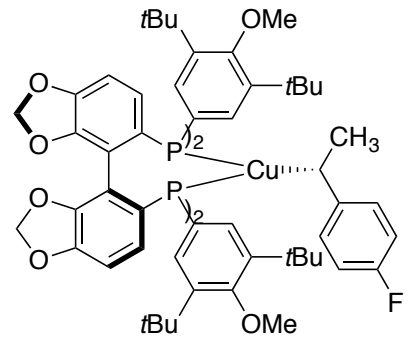

O
O
O
O
P
2
P
2
Cu
H
H
Cu
P
2
P
2
O
O
O
O

27 (^{31}P NMR)

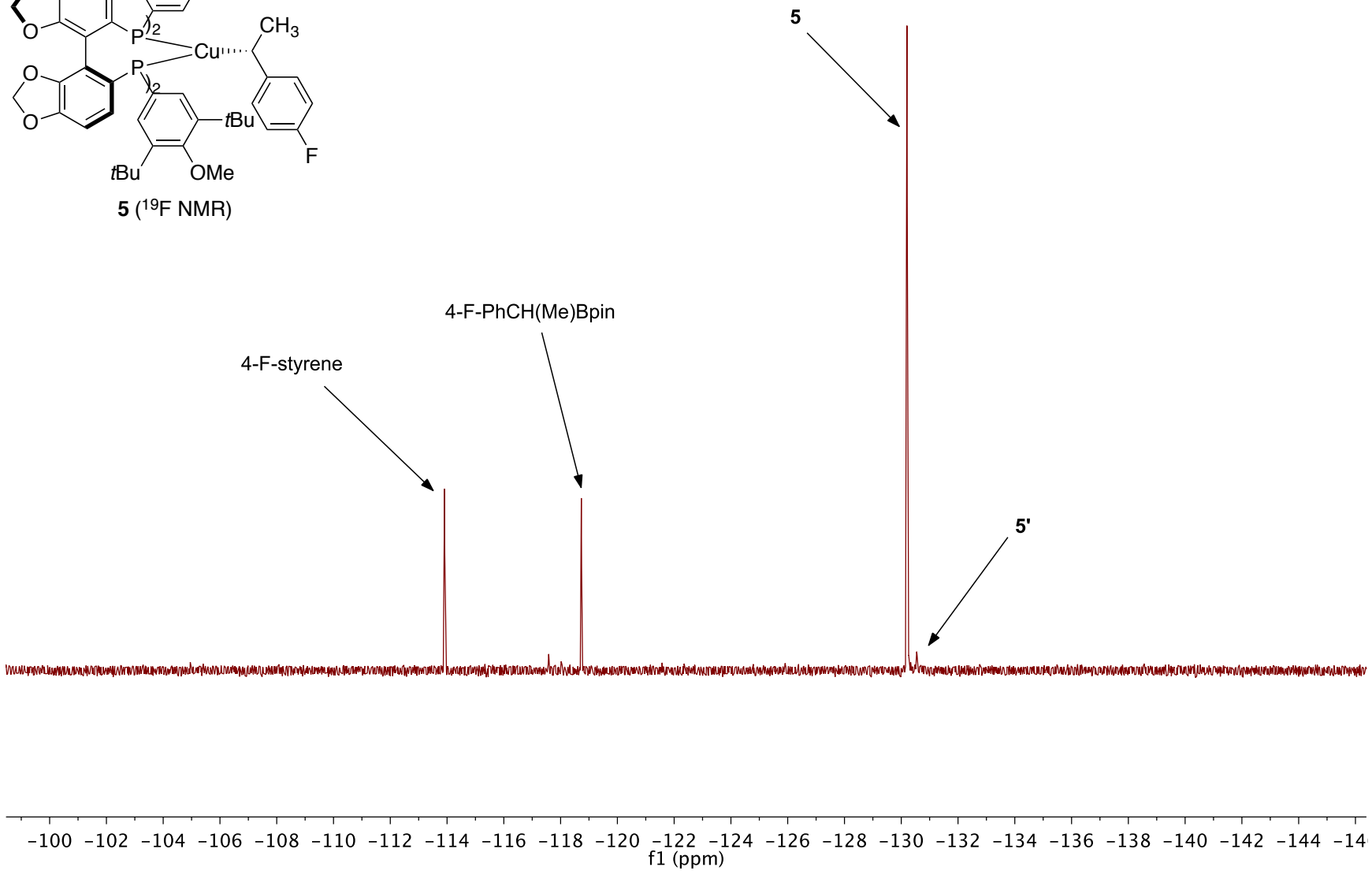

SEGPHOS
150
130
110
90
70
50
30
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
f1 (ppm)

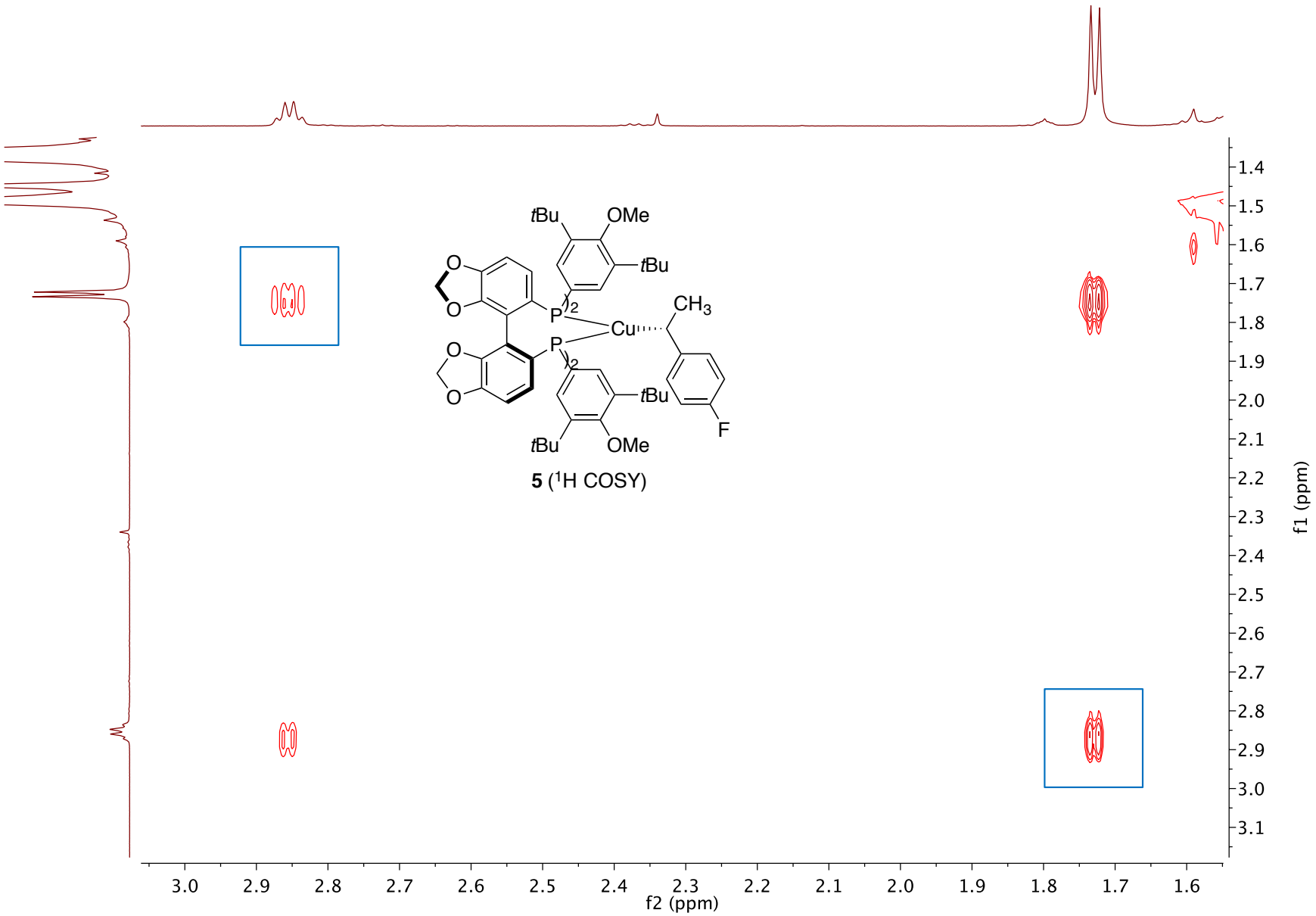

tBu
OMe
tBu
CH3
Cu
P
P
tBu
tBu
OMe
F
O
O
O
O
5 (1H NMR)
MeBpin
impurity
impurity
free ligand
methine of 5
impurity
4.093
4.073
2.277
2.184
2.253
2.081
2.121
2.300
6.018
6.363
1.000
3.046
35.944
36.368
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

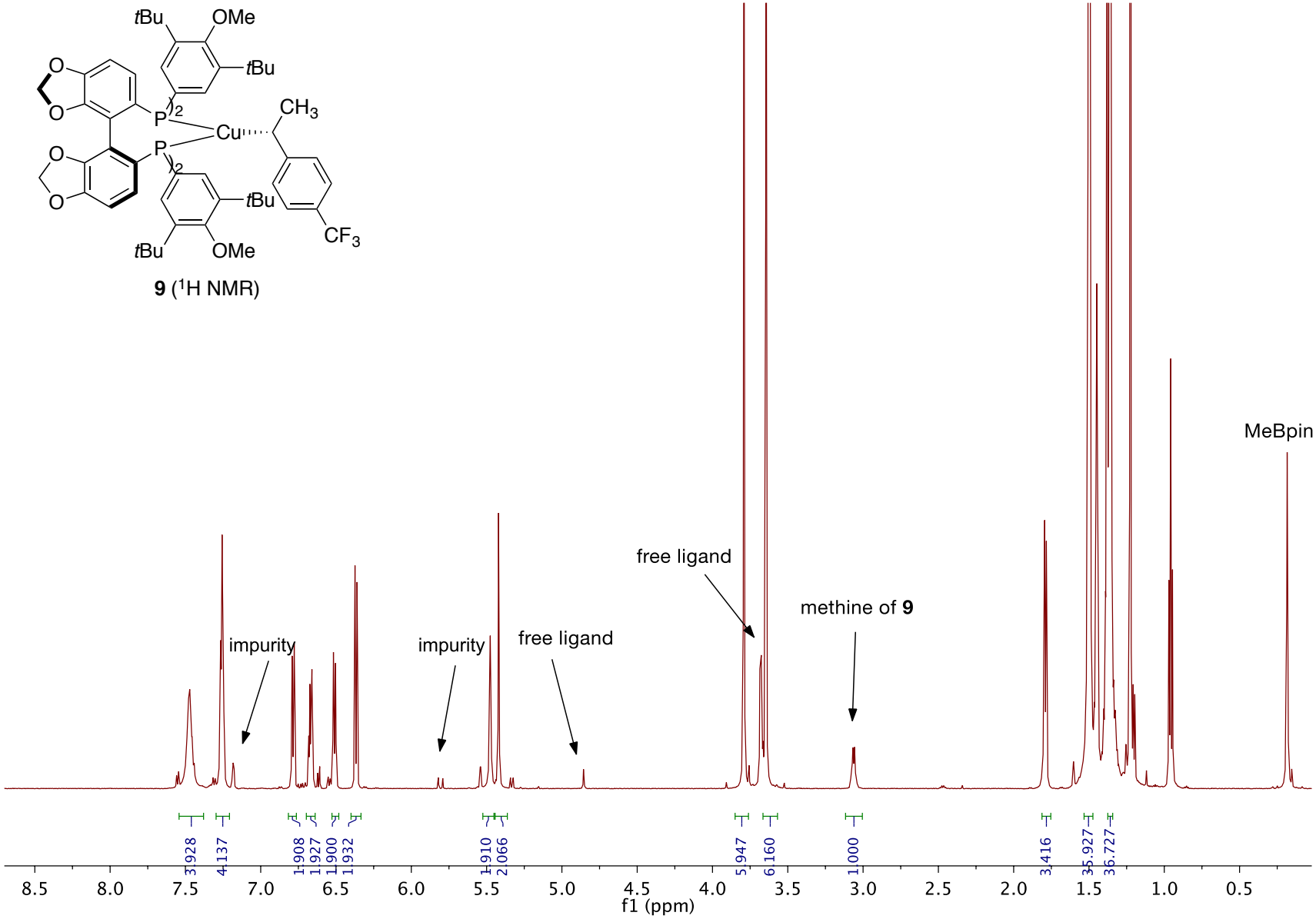

tBu
OMe
tBu
CH3
Cu
P
P
tBu
tBu
OMe
F
5 (31P NMR)
5
5'
DTBM-SEGPHOS
0.053
1.000
0.100
−1 −2 −3 −4 −5 −6 −7 −8 −9 −10 −11 −12 −13 −14 −15 −16 −17
f1 (ppm)

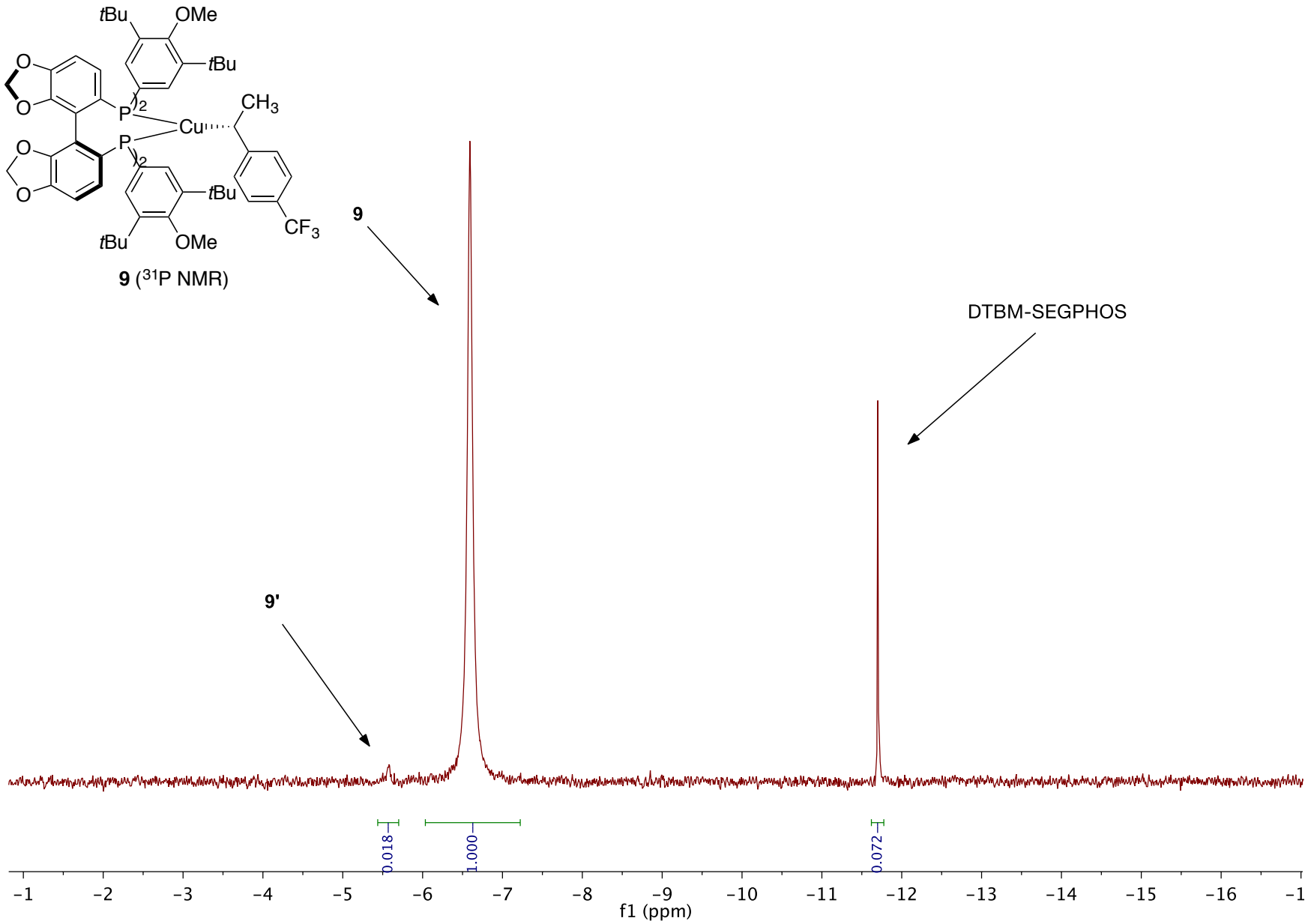

tBu
OMe
tBu
O
O
P
2
CH3
Cu
O
O
P
2
tBu
tBu
OMe
F

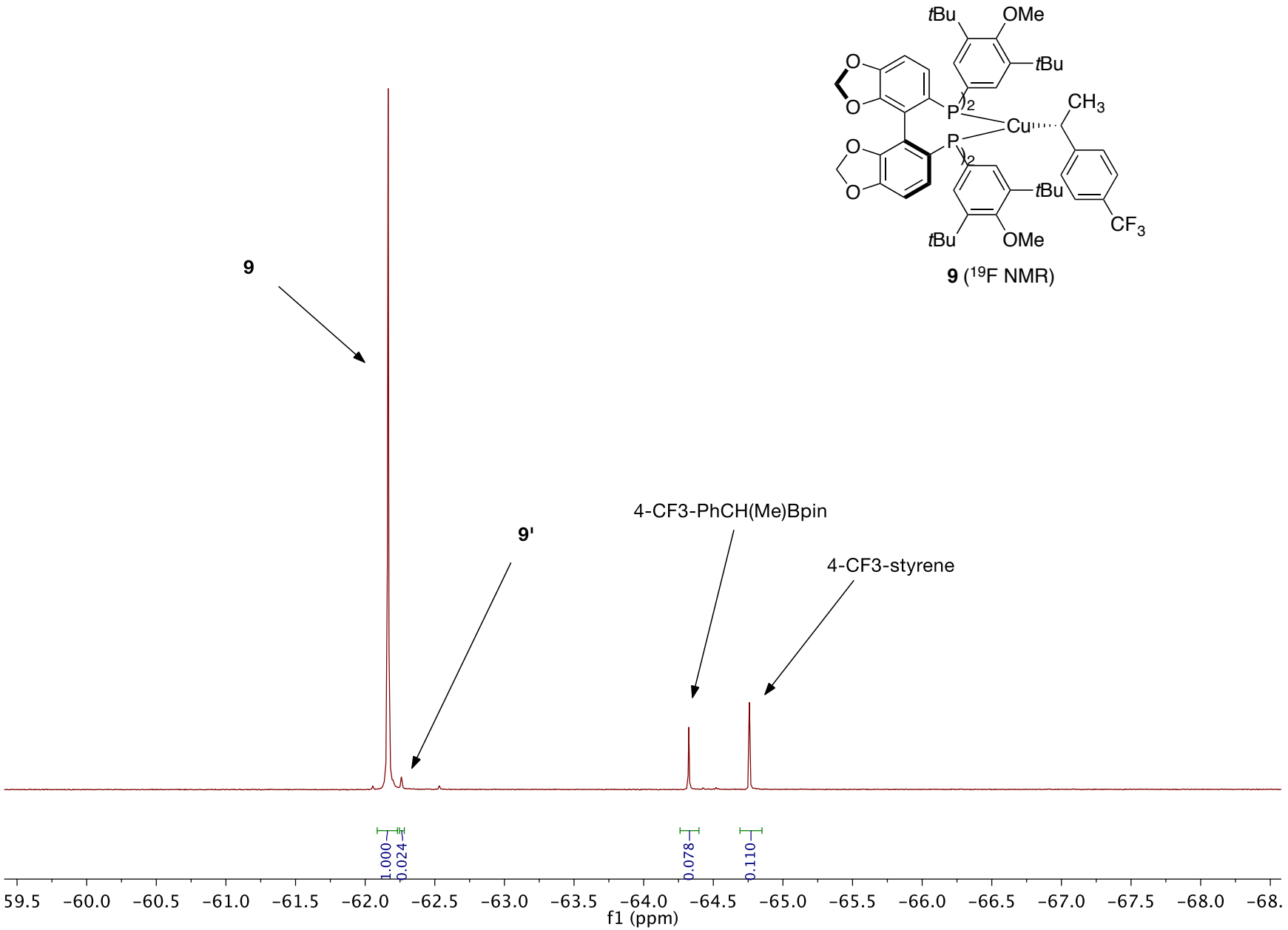
5 (^{19}F NMR)


5
4-F-PhCH(Me)Bpin
4-F-styrene
5'
−100 −102 −104 −106 −108 −110 −112 −114 −116 −118 −120 −122 −124 −126 −128 −130 −132 −134 −136 −138 −140 −142 −144
f1 (ppm)


tBu
OMe
tBu
O
O
P
2
Cu
CH3
O
O
P
2
tBu
F
tBu
OMe
5 (1H COSY)
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
f2 (ppm)
1.4
1.5
1.6
1.7
1.8
1.9
2.0
2.1
2.2
2.3
2.4
2.5
2.6
2.7
2.8
2.9
3.0
3.1
f1 (ppm)

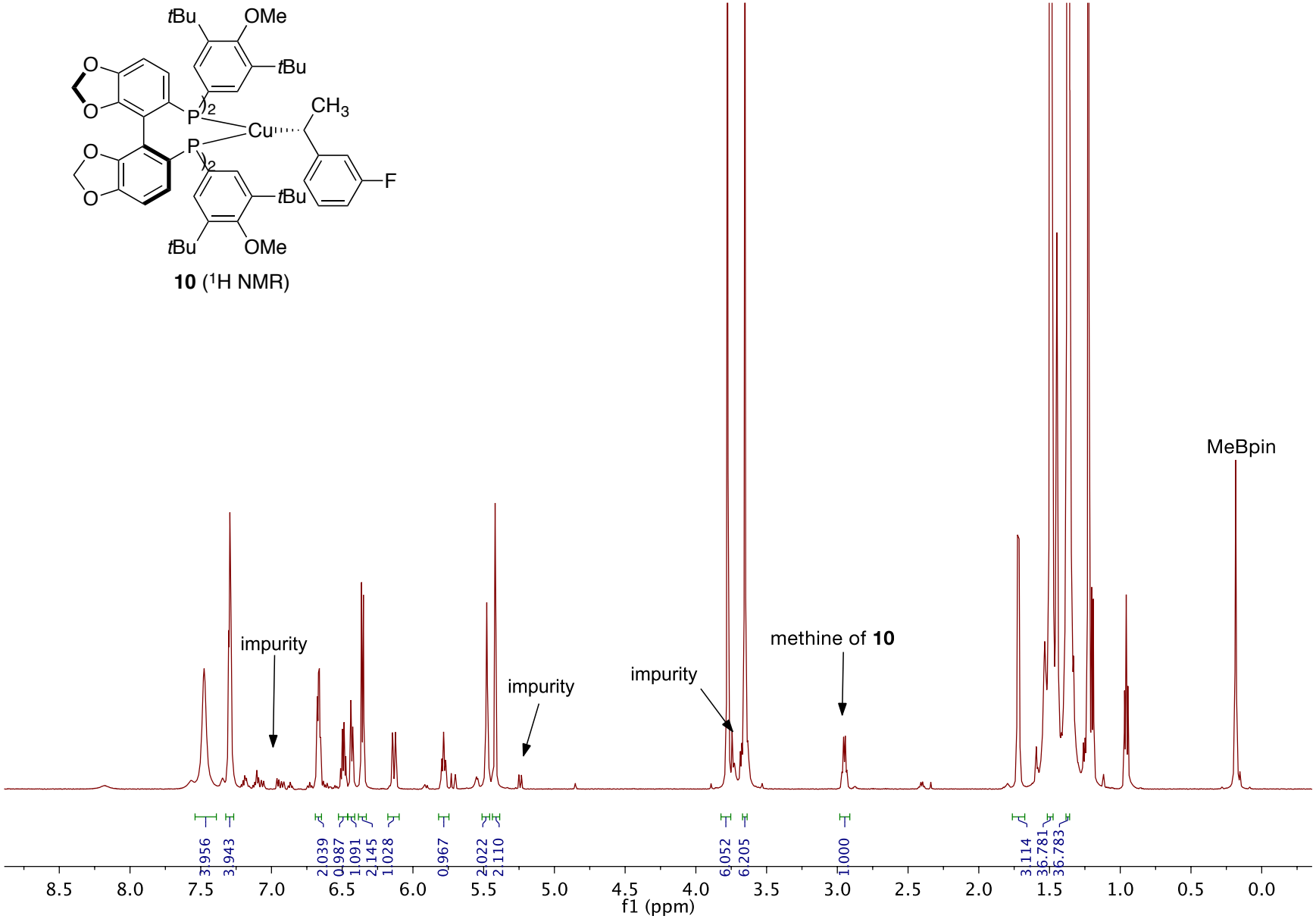

tBu
OMe
tBu
O
O
P
2
CH3
Cu
O
O
P
2
tBu
tBu
OMe
CF3
9 (1H NMR)
impurity
impurity
free ligand
free ligand
methine of 9
MeBpin
3.928
4.137
1.908
1.927
1.900
1.932
1.910
2.066
5.947
6.160
1.000
3.416
35.927
36.727
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

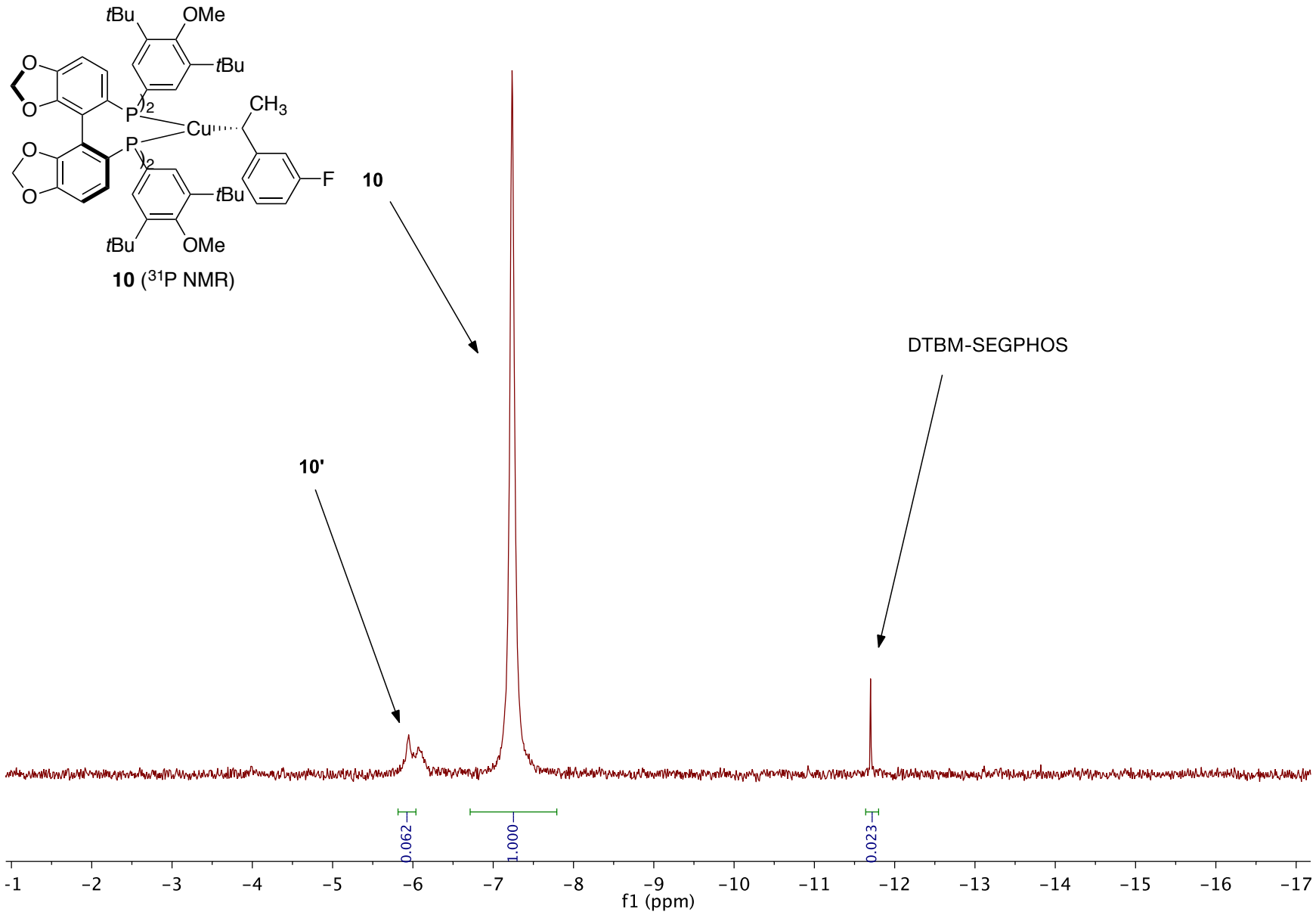

tBu
OMe
tBu
O
O
P
2
Cu
CH3
O
O
P
2
tBu
tBu
OMe
CF3
9 (31P NMR)
9
9'
DTBM-SEGPHOS
0.018
1.000
0.072
−1
−2
−3
−4
−5
−6
−7
−8
−9
−10
−11
−12
−13
−14
−15
−16
−1
f1 (ppm)

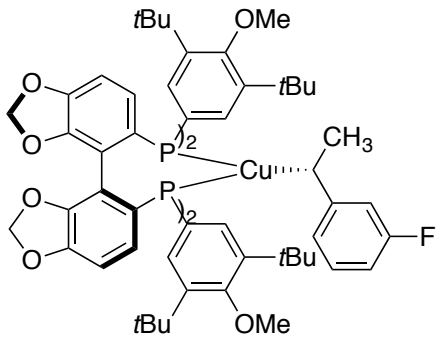

tBu
OMe
tBu
O
O
P
2
Cu
CH3
O
O
P
2
tBu
CF3
tBu
OMe
9 (19F NMR)
9
9'
4-CF3-PhCH(Me)Bpin
4-CF3-styrene
1.000
0.024
0.078
0.110
59.5
-60.0
-60.5
-61.0
-61.5
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
-65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
-68.
f1 (ppm)

tBu
OMe
tBu
O
O
P
2
CH3
Cu
O
O
P
2
F
tBu
tBu
OMe

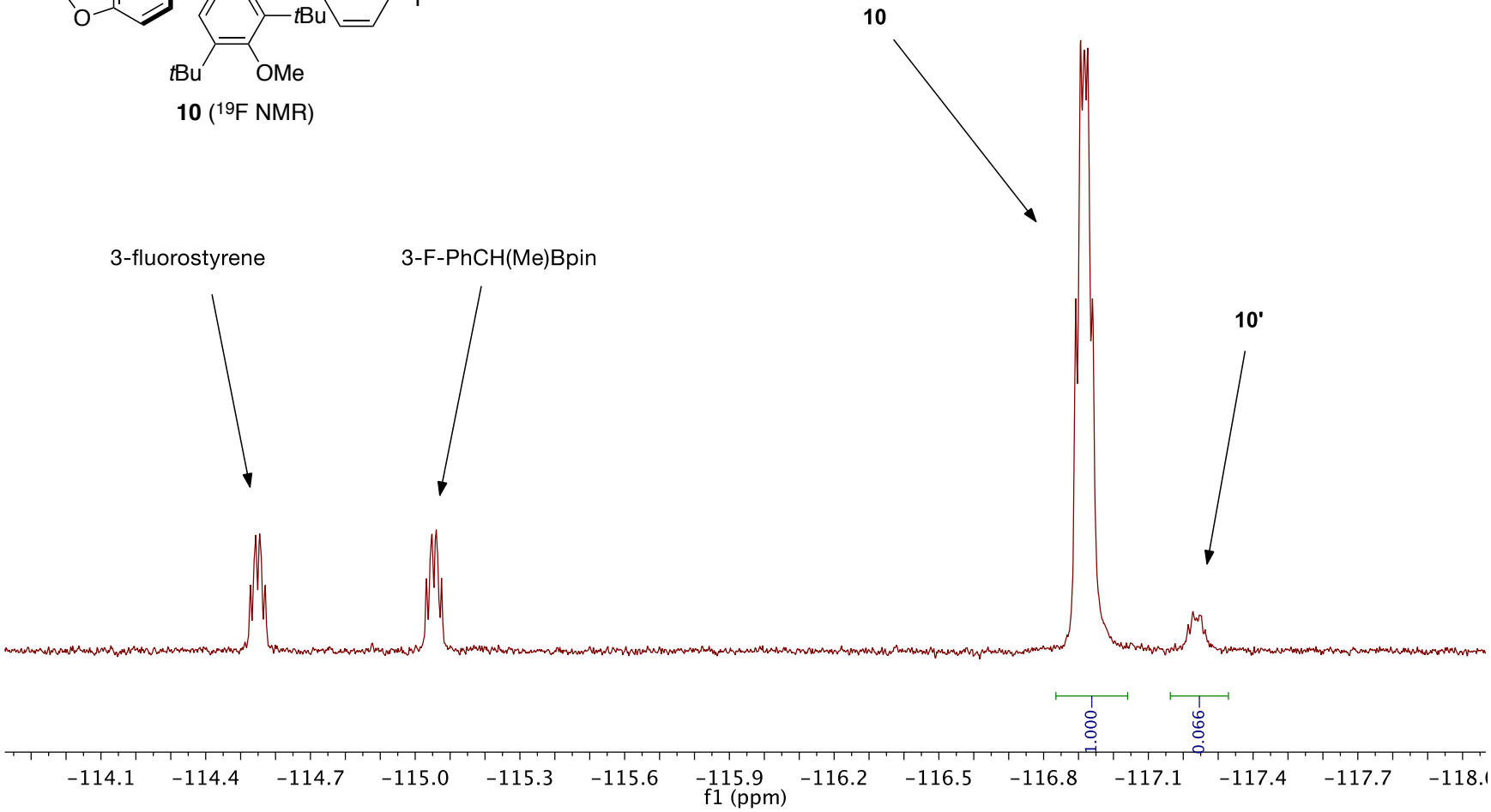
10 (^{1}H NMR)

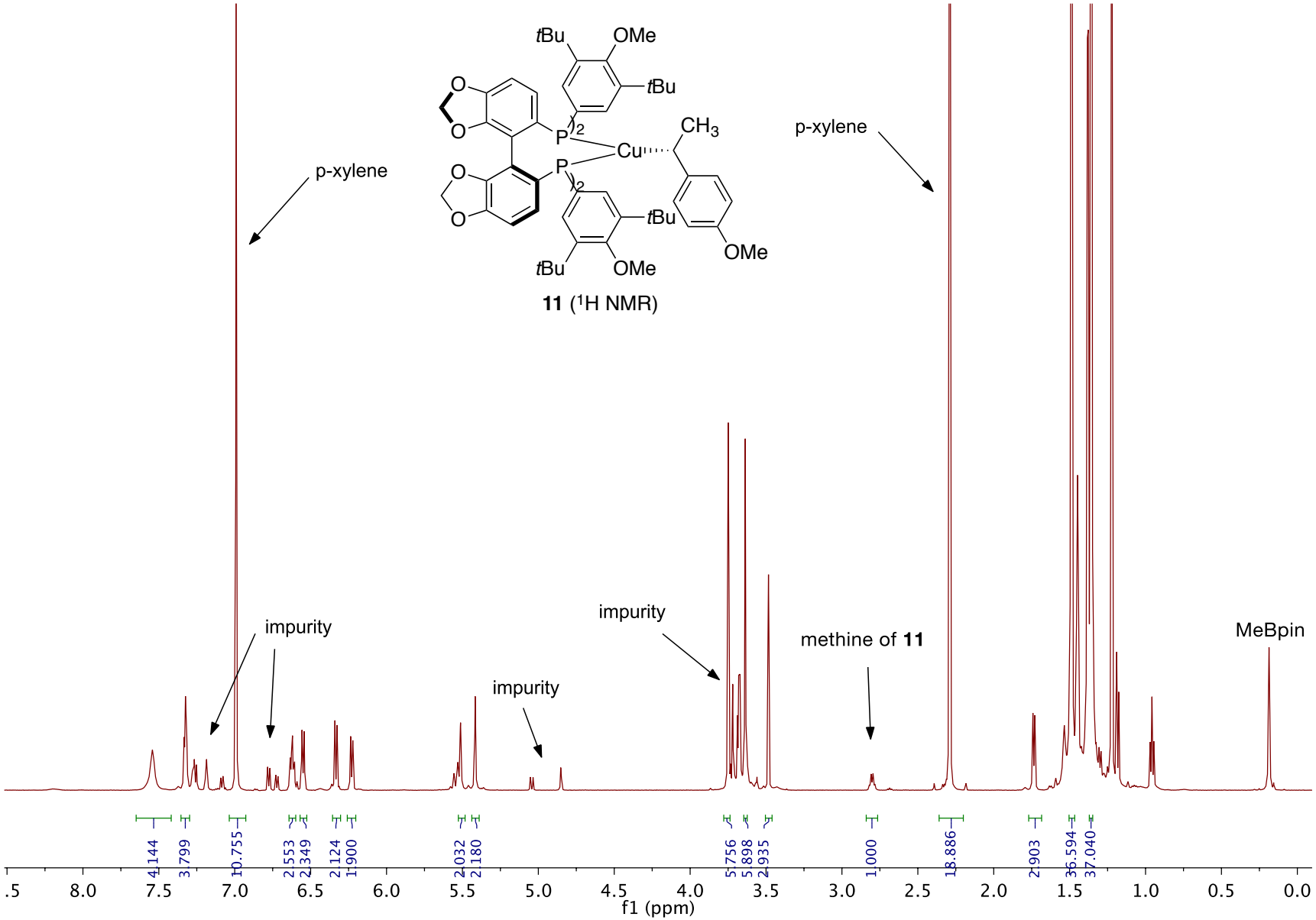

impurity
impurity
impurity
methine of 10
MeBpin
3.956
3.943
2.039
0.987
1.091
2.145
1.028
0.967
2.022
2.110
6.052
6.205
1.000
3.114
36.781
36.783
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

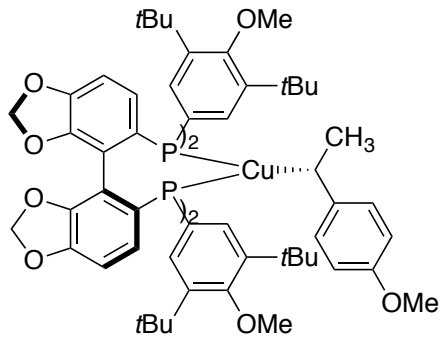

tBu
OMe
tBu
O
O
P
2
Cu
CH3
O
O
P
2
F
tBu
tBu
OMe
10 (31P NMR)
10
10'
DTBM-SEGPHOS
0.062
1.000
0.023
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
f1 (ppm)


tBu
OMe
tBu
O
O
P
2
Cu
CH3
O
O
P
2
F
tBu
tBu
OMe

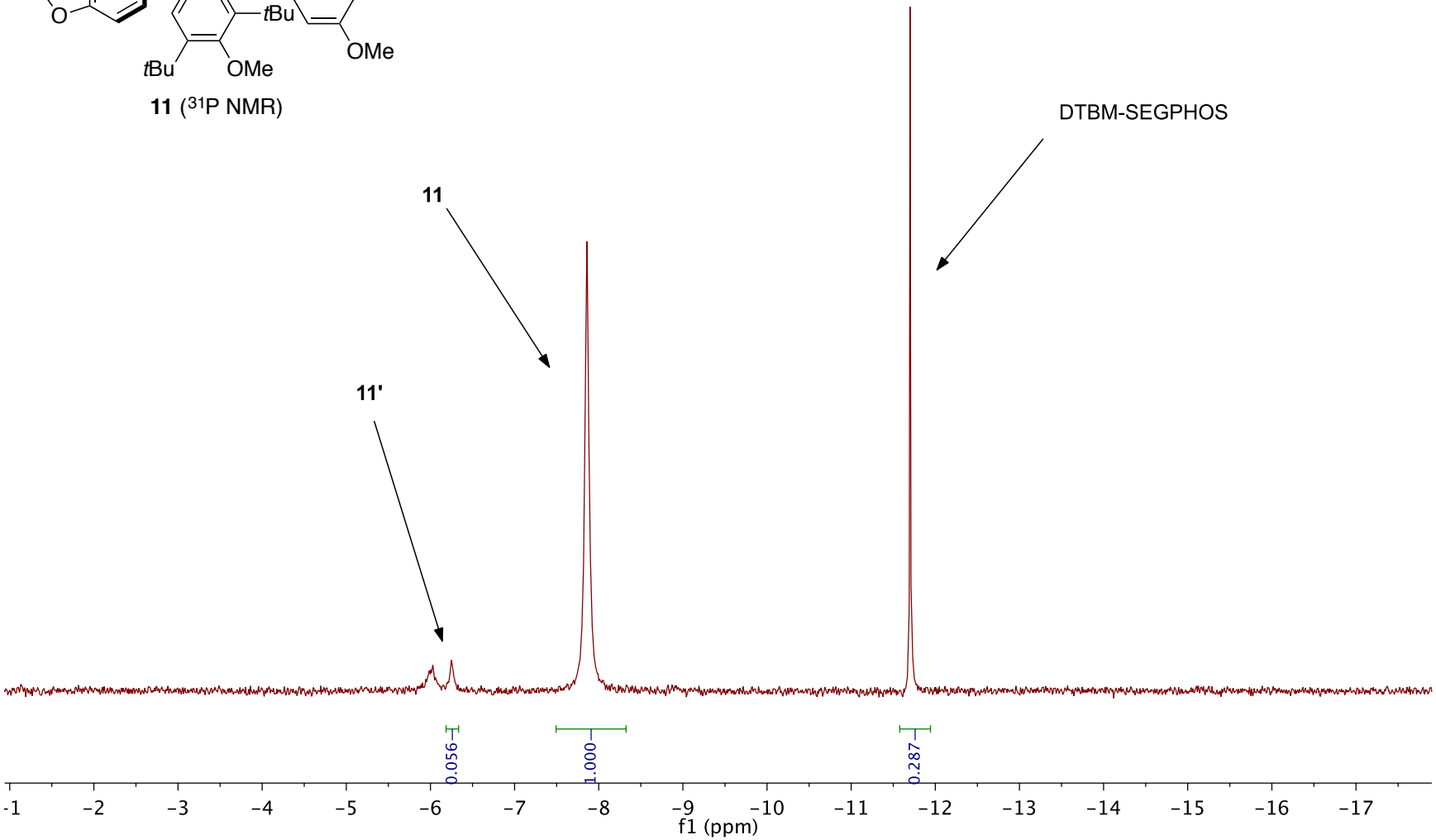
10 (^{19}F NMR)

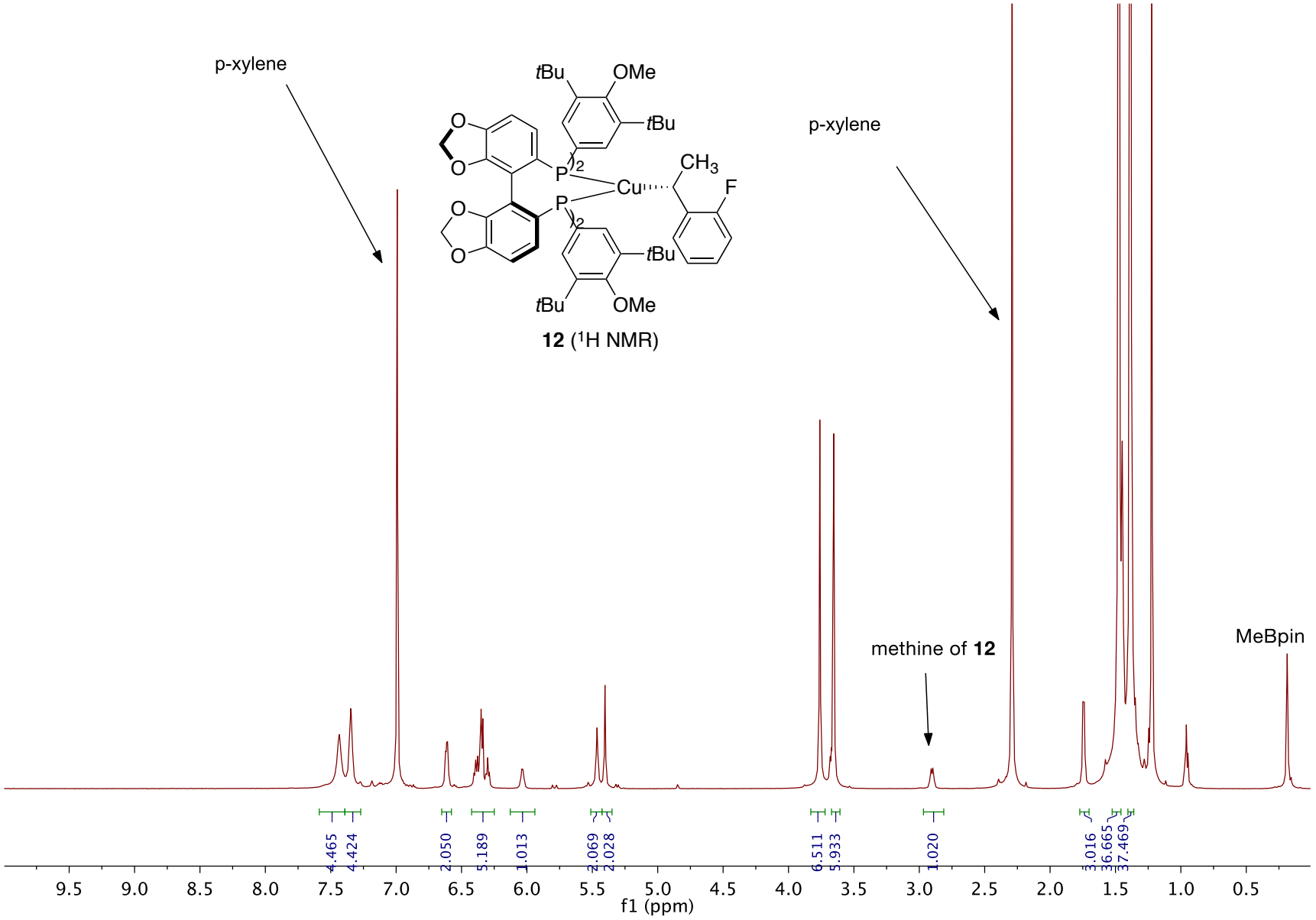

10
3-fluorostyrene
3-F-PhCH(Me)Bpin
10'
1.000
0.066
-114.1
-114.4
-114.7
-115.0
-115.3
-115.6
-115.9
-116.2
-116.5
-116.8
-117.1
-117.4
-117.7
f1 (ppm)

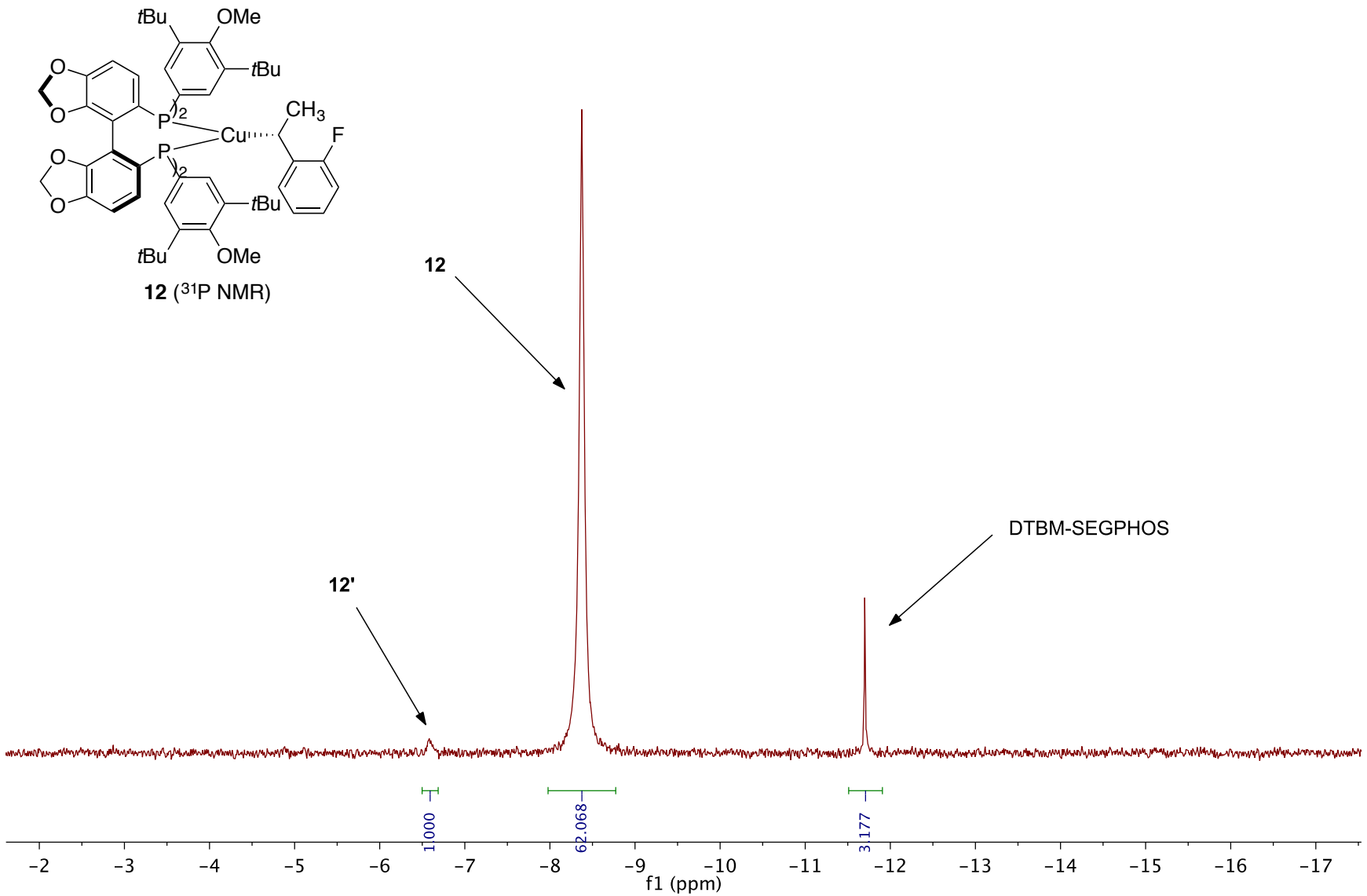

tBu
OMe
tBu
O
O
P
2
Cu
CH3
P
2
O
O
tBu
tBu
OMe
OMe
11 (1H NMR)
p-xylene
p-xylene
impurity
impurity
impurity
methine of 11
MeBpin
4.144
3.799
10.755
2.553
2.349
2.124
1.900
2.032
2.180
5.756
5.898
2.935
1.000
18.886
2.903
36.594
37.040
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

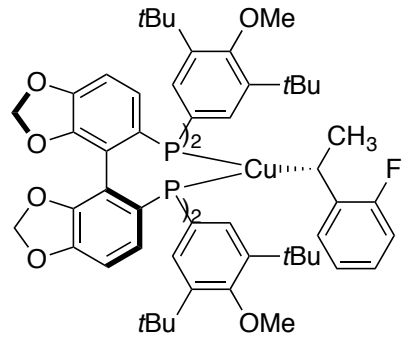

tBu
OMe
tBu
O
O
P
2
Cu
CH3
O
O
P
2
tBu
tBu
OMe
OMe

11 (^{31}P NMR)

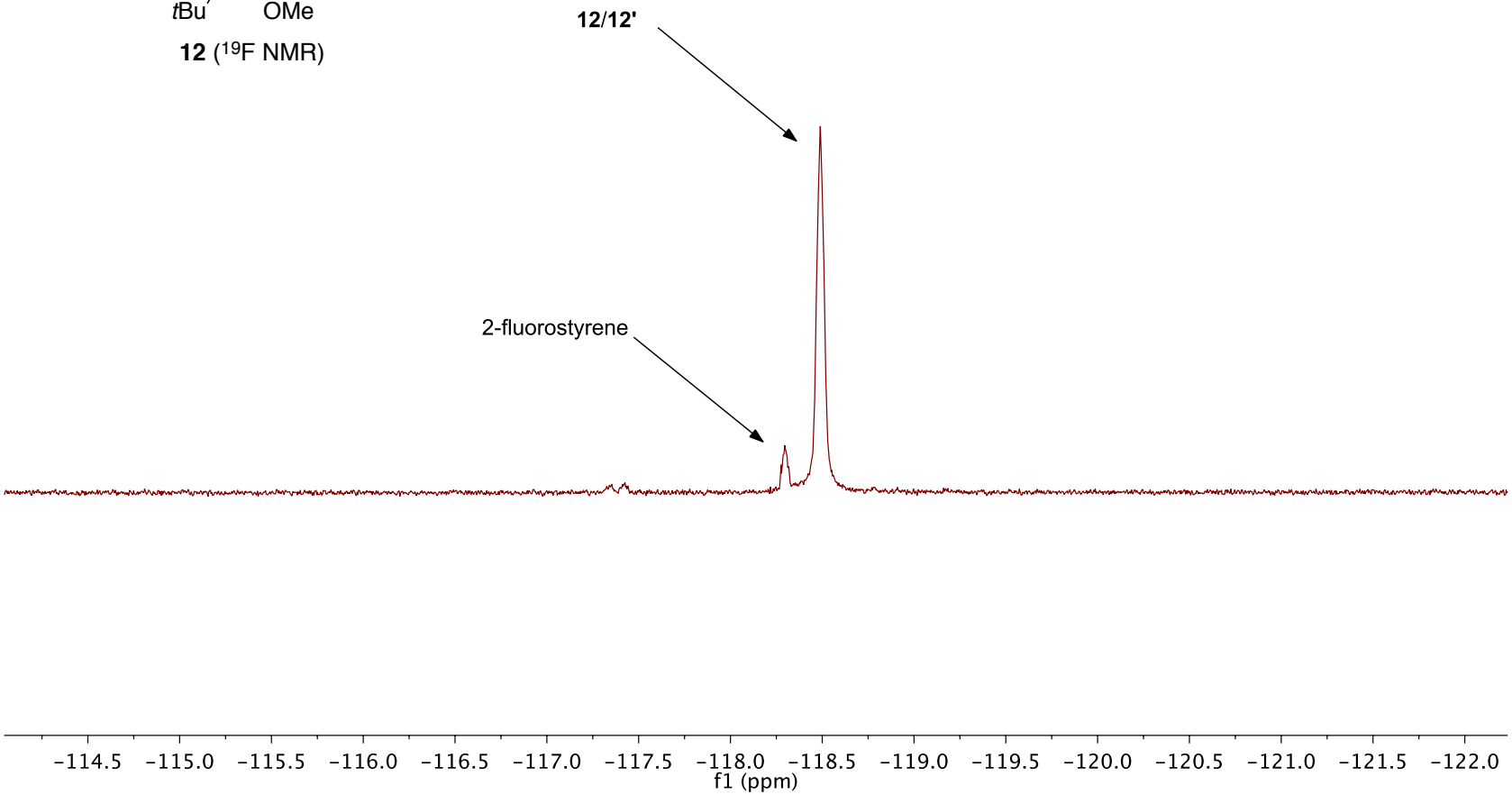

DTBM-SEGPHOS
11
11'
0.056
1.000
0.287
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
f1 (ppm)


p-xylene
tBu
OMe
tBu
O
O
P
2
Cu
CH3
F
O
O
P
2
tBu
tBu
OMe
12 (1H NMR)
p-xylene
methine of 12
MeBpin
4.465
4.424
2.050
5.189
1.013
2.069
2.028
6.511
5.933
1.020
3.016
36.665
37.469
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


tBu
OMe
tBu
O
O
P
2
Cu
CH3
F
O
O
P
2
tBu
tBu
OMe
12 (31P NMR)
12
12'
DTBM-SEGPHOS
1.000
62.068
3.177
−2
−3
−4
−5
−6
−7
−8
−9
−10
−11
−12
−13
−14
−15
−16
−17
f1 (ppm)

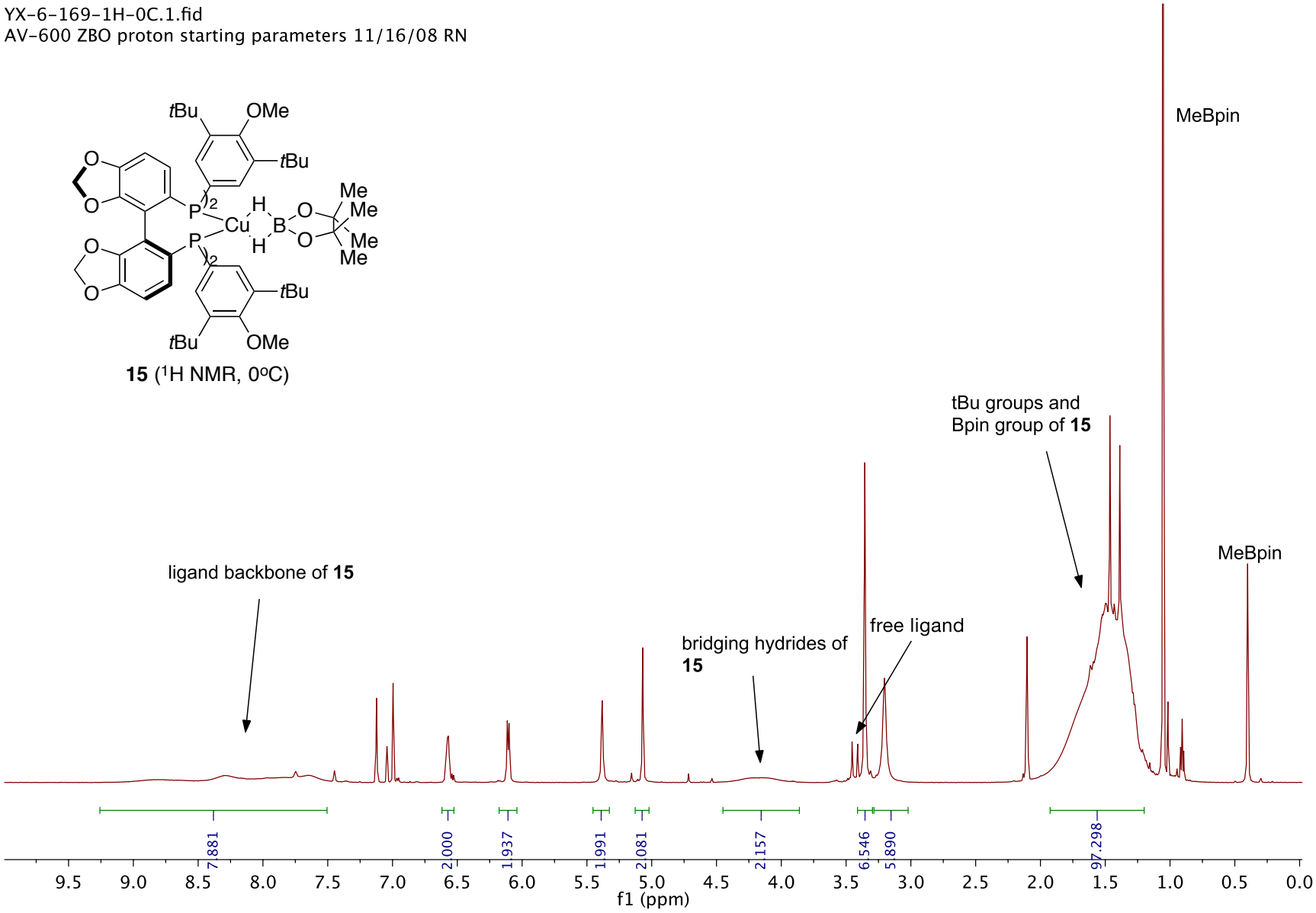

tBu
OMe
tBu
O
O
P
2
Cu
CH3
F
O
O
P
2
tBu
tBu
OMe

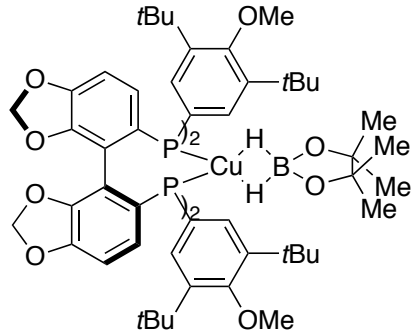
12 (^{19}F NMR)


12/12'
2-fluorostyrene
-114.5
-115.0
-115.5
-116.0
-116.5
-117.0
-117.5
-118.0
-118.5
-119.0
-119.5
-120.0
-120.5
-121.0
-121.5
-122.0
f1 (ppm)

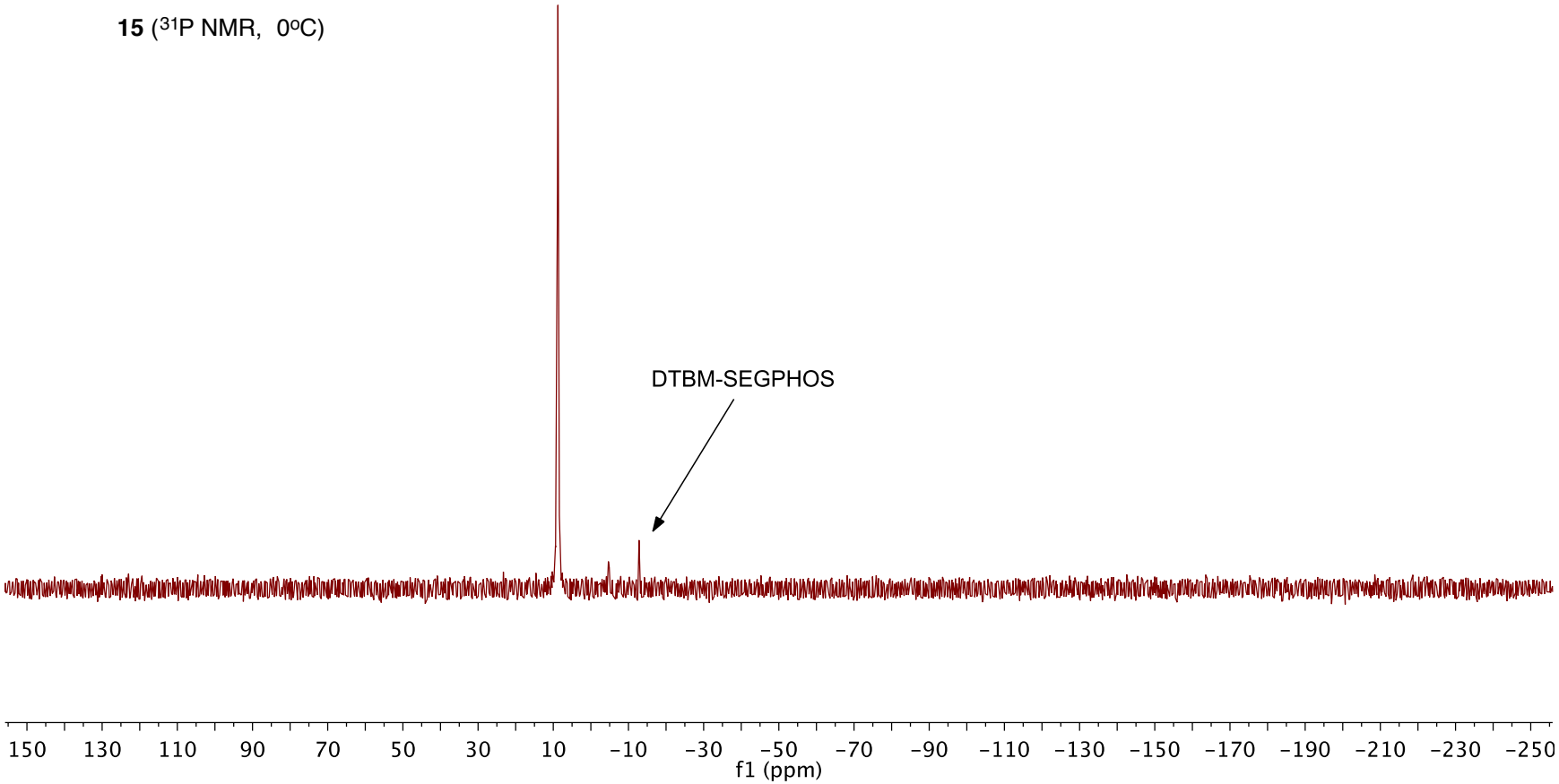
YX-6-169-1H-0C.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN

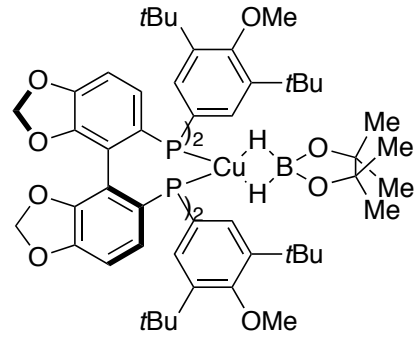
15 (^{1}H NMR, 0^{o}C)



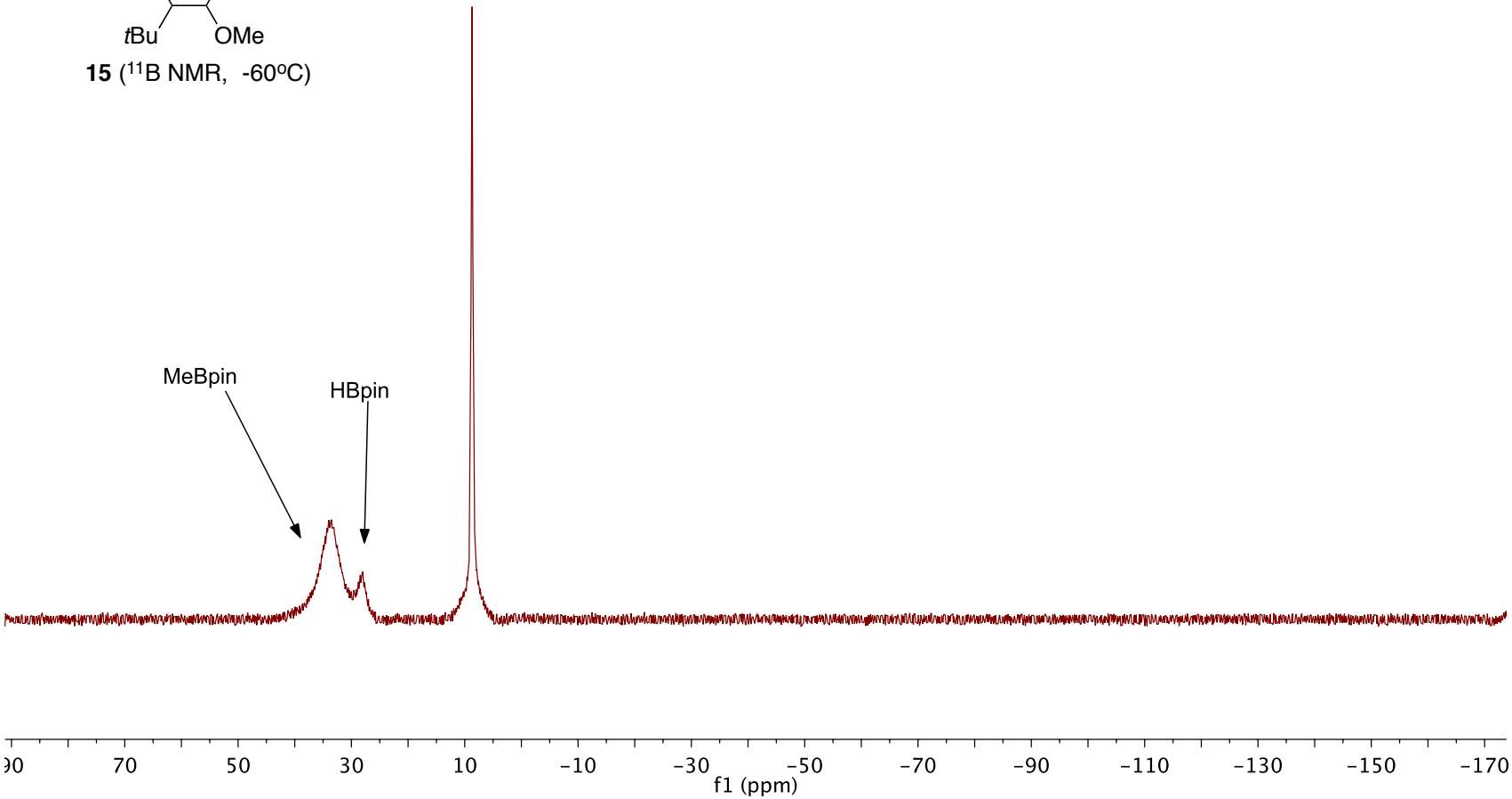


15 (^{31}P NMR, 0^{o}C)

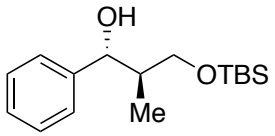




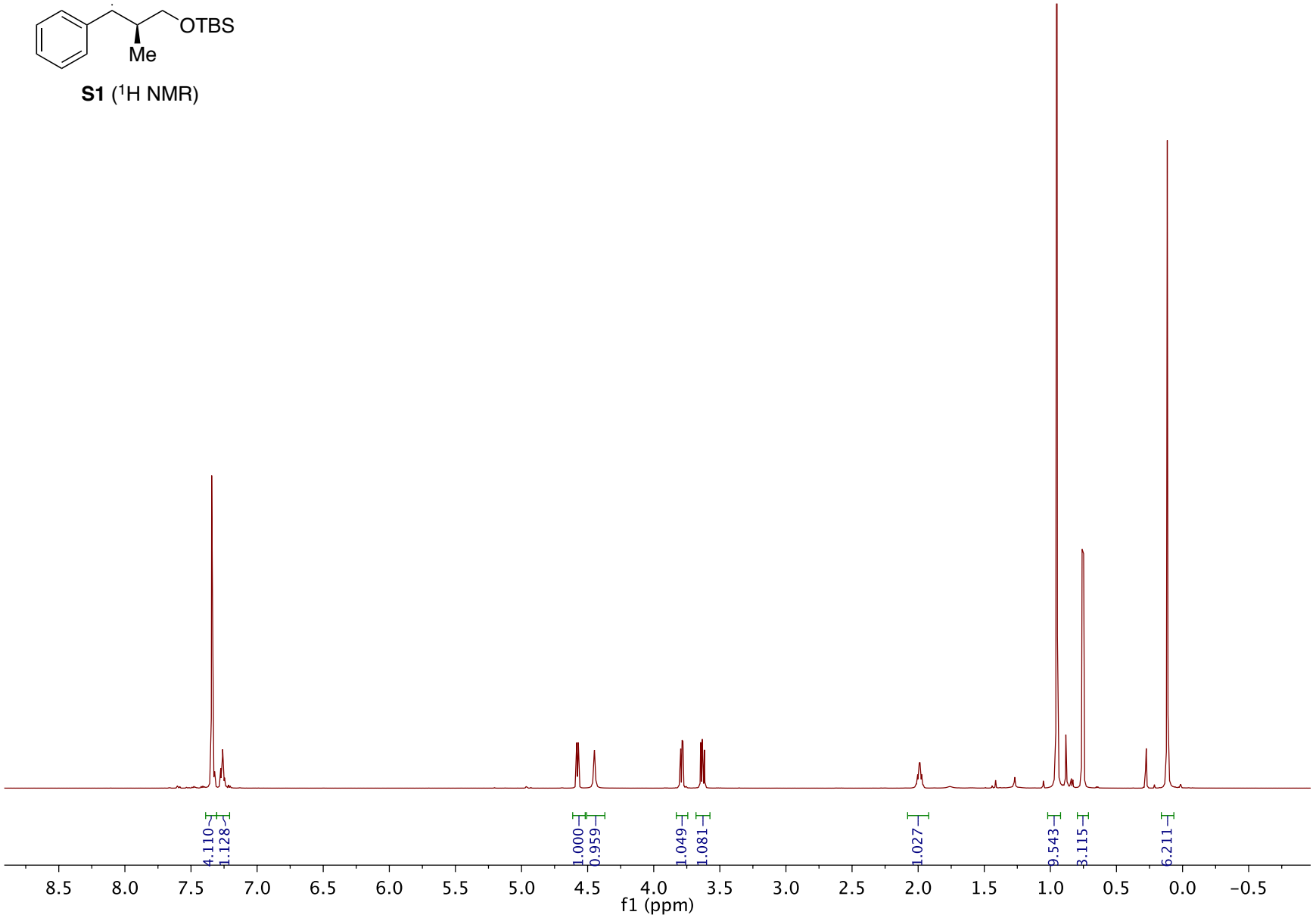
15 (^{11}B NMR, -60°C)



Note: Multiple baseline corrections were performed to remove the uneven baseline that results from boron in the borosilicate glass NMR tubes.

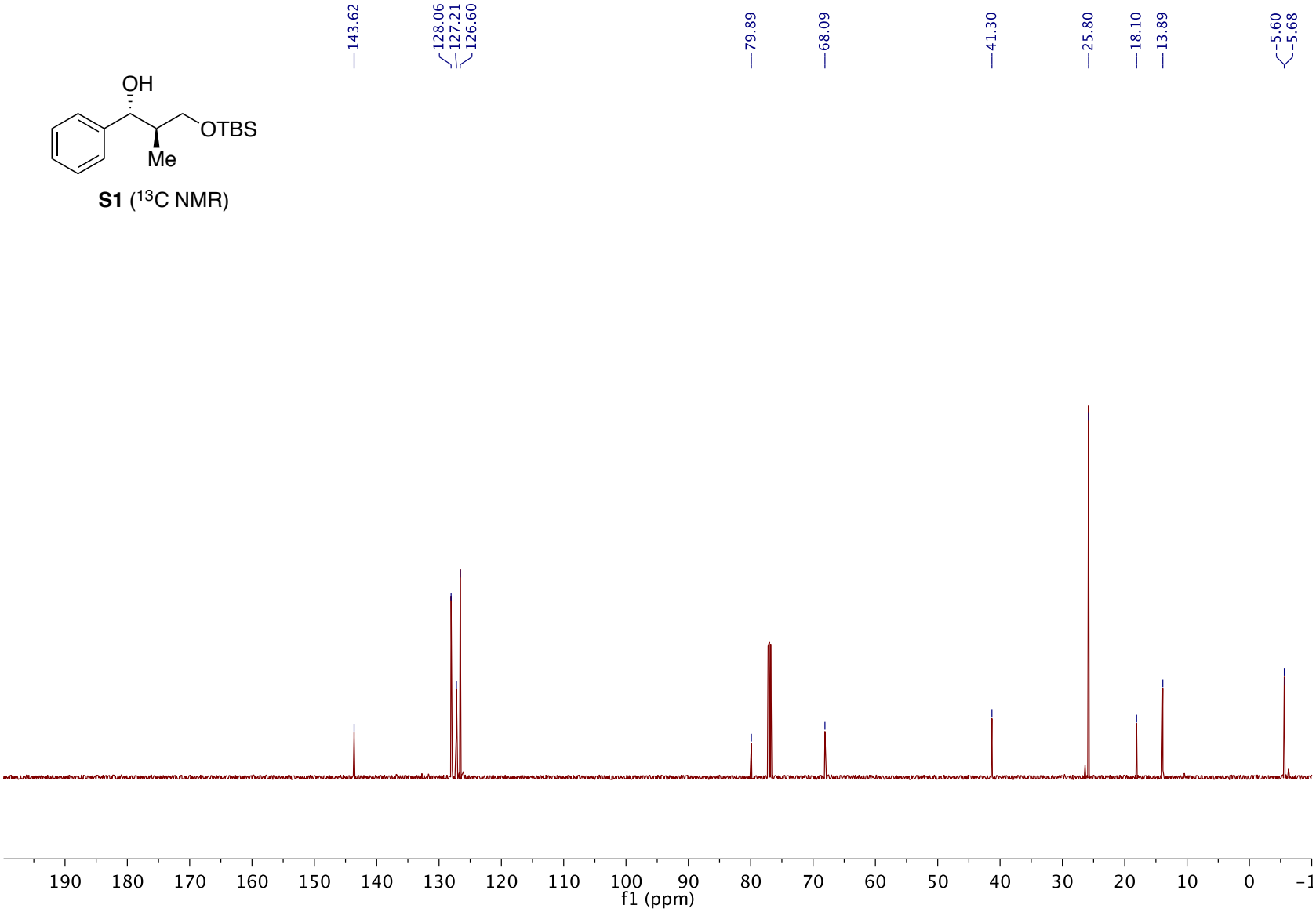

OH
OTBS
Me

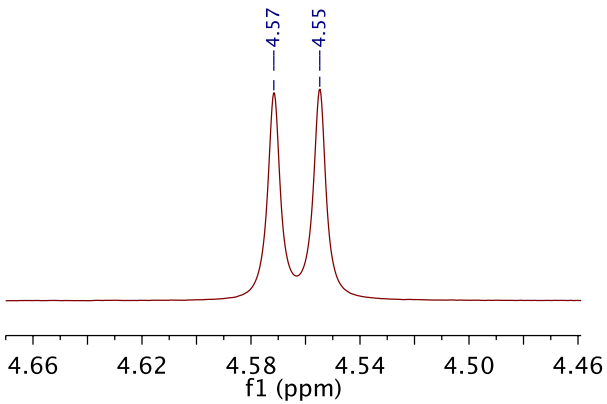
S1 (^{1}H NMR)

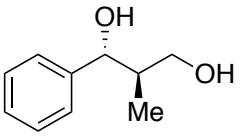

4.110
1.128
1.000
0.959
1.049
1.081
1.027
9.543
3.115
6.211
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

OH
OTBS
Me

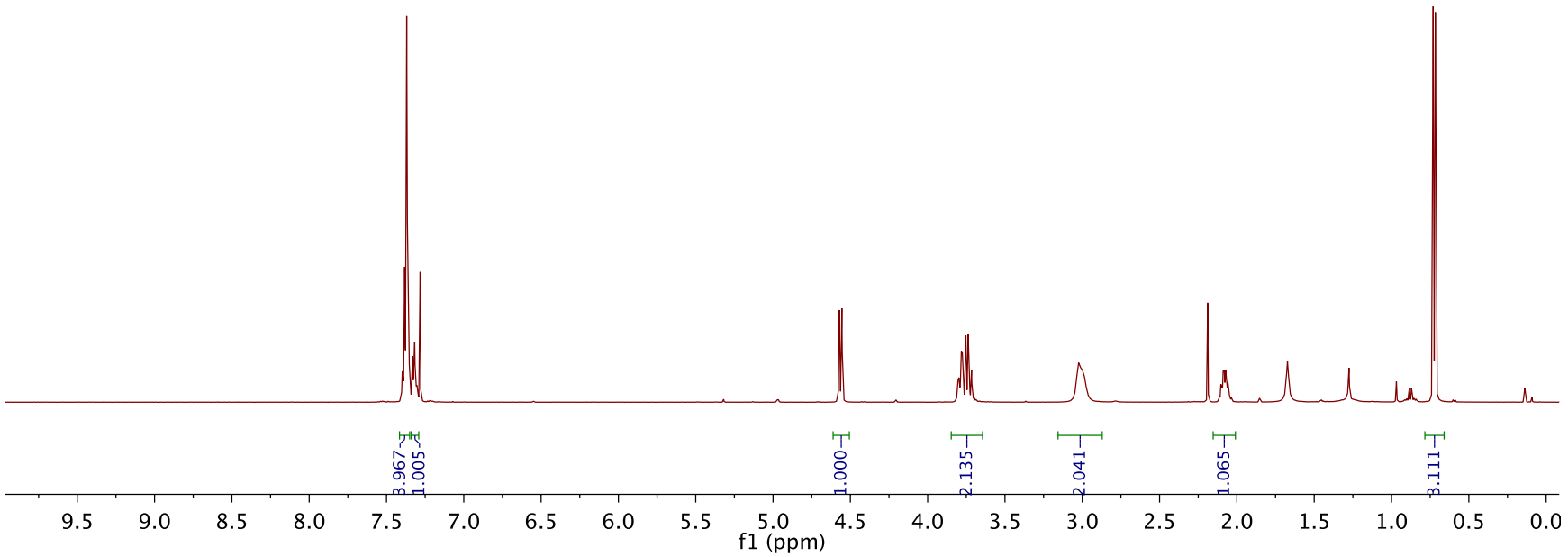
S1 (^{13}C NMR)

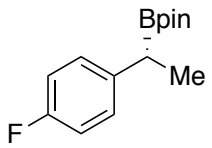

143.62
128.06
127.21
126.60
79.89
68.09
41.30
25.80
18.10
13.89
-5.60
-5.68
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


4.57
4.55
4.66
4.62
4.58
4.54
4.50
4.46
f1 (ppm)

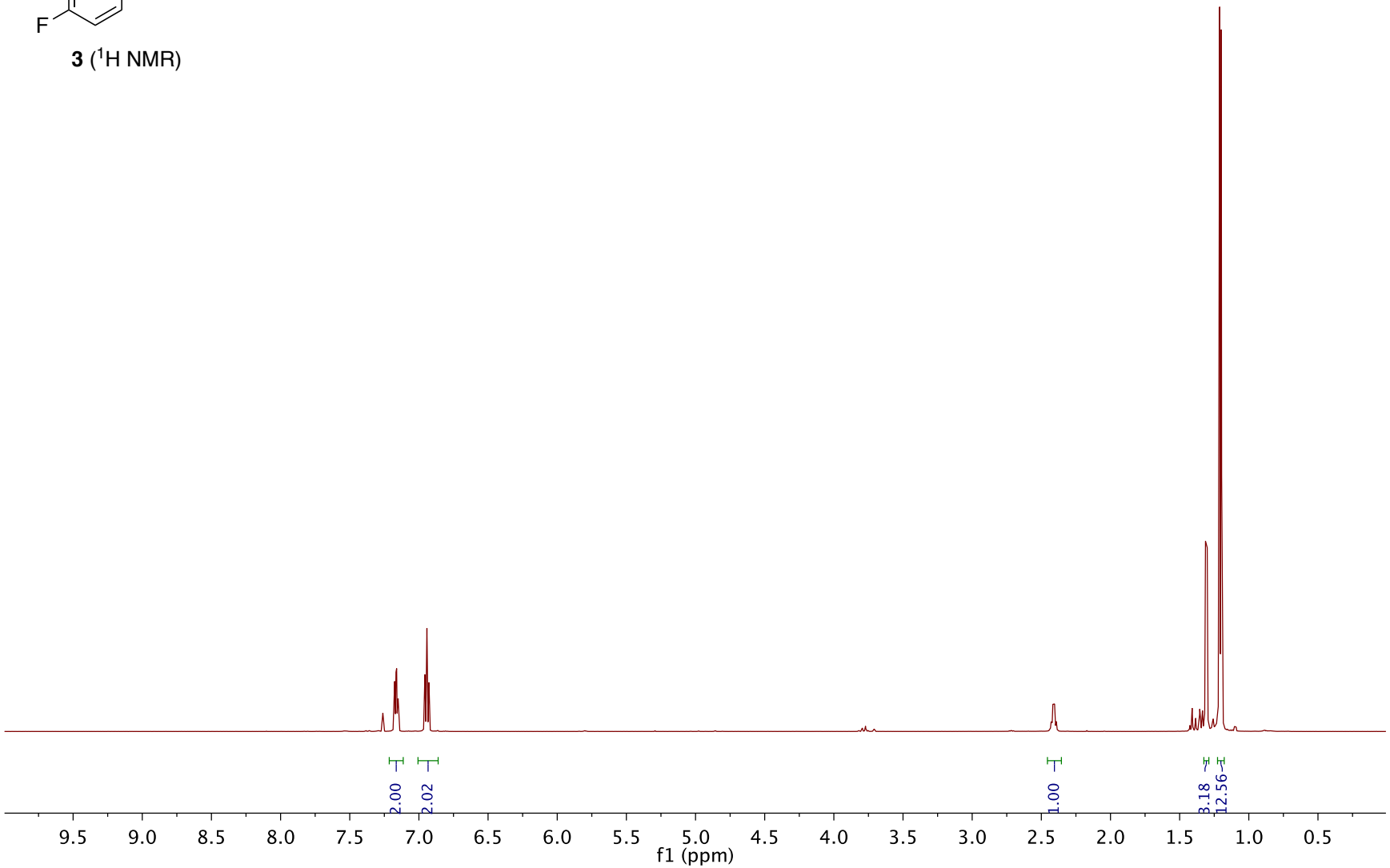

OH
OH
Me

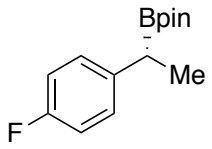
19-OH (^{1}H NMR)


3.967
1.005
1.000
2.135
2.041
1.065
3.111
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

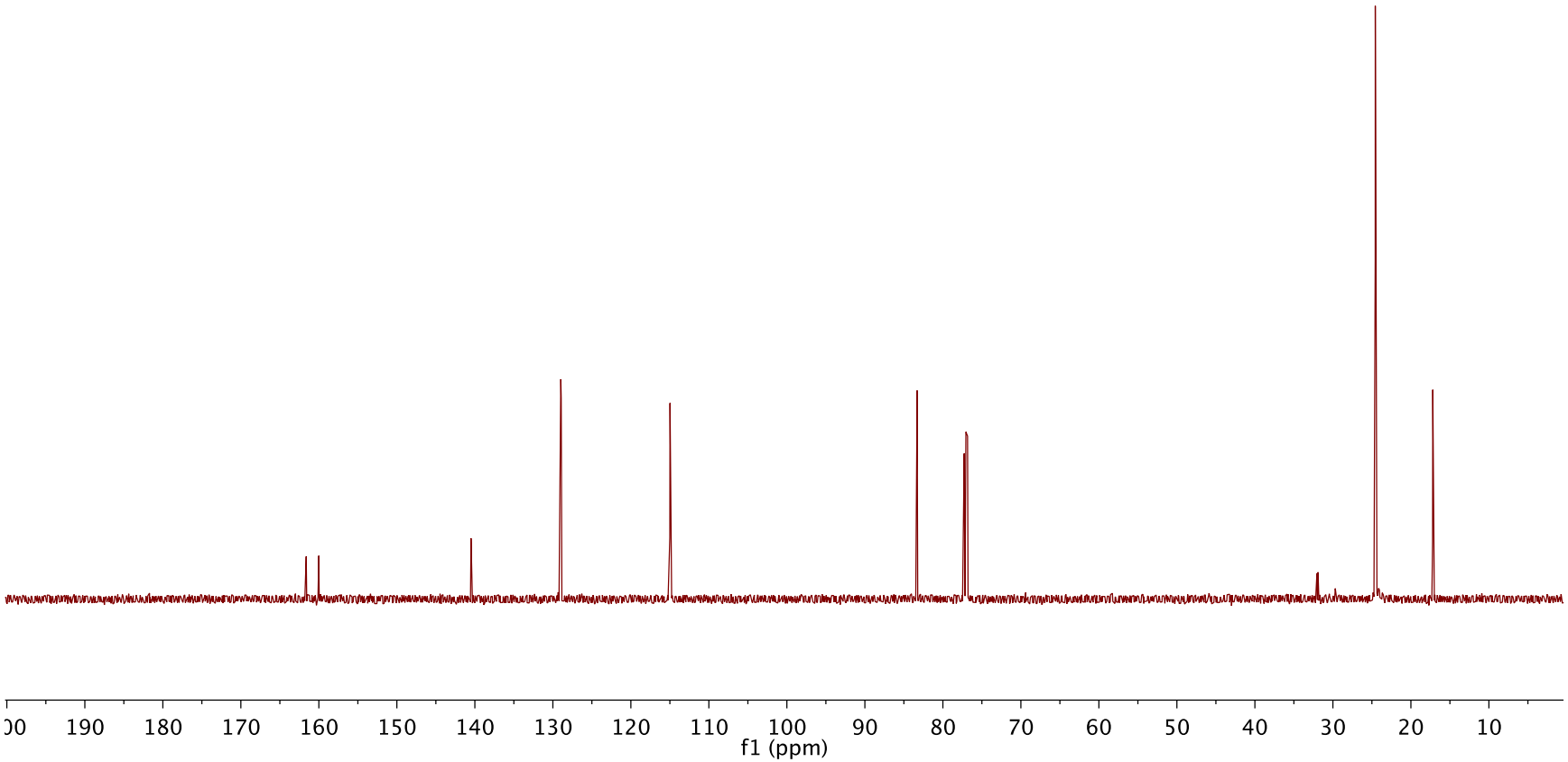

Bpin
Me
F

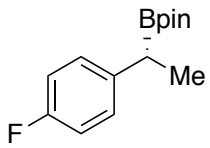
3 (^{1}H NMR)


2.00
2.02
1.00
3.18
12.56
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

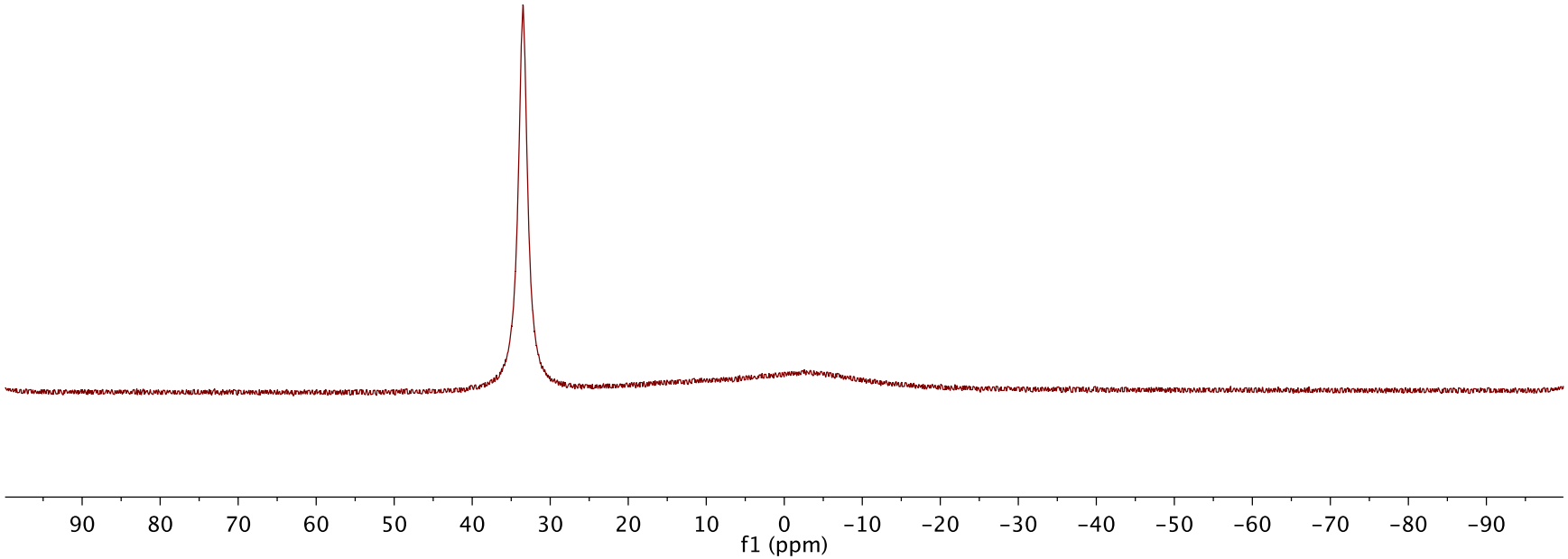

Bpin
Me
F

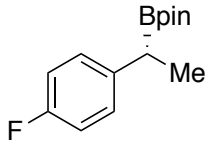
3 (^{13}C NMR)


00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

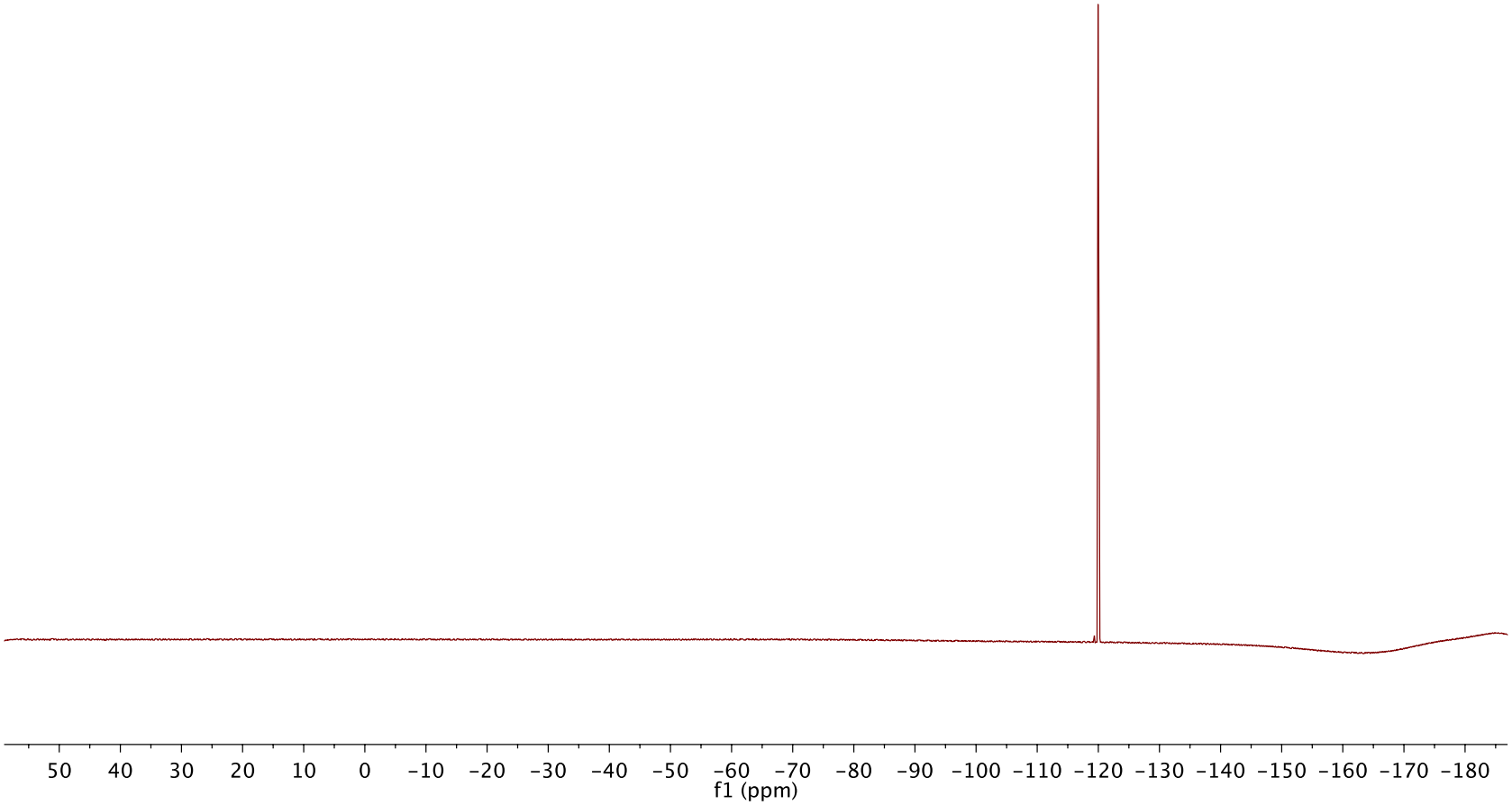


3 (^{11}B NMR)




Bpin
Me
F

3 (^{19}F NMR)


50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)