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SUPPLEMENTARY INFORMATION

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A Gold-Catalyzed Enantioselective Cope Rearrangement of Achiral 1,5-Dienes

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1. General Information

All reagents were reagent grade quality and used as received from Aldrich unless otherwise noted. Anhydrous THF (Stabilized, 99.9%, Acros Organics) and 1,2-Dichloroethane (99.8+%, extra pure) were purchased from Fisher Scientific and used as received. Phosphorous ligands were purchased from Strem Chemicals, Inc. and used without further purification. All glassware was flame dried under vacuum unless otherwise indicated. Anhydrous CH_2Cl_2, diethyl ether, and pentanes were passed through a column of alumina.[1] Column chromatography was performed using SilaFlash P60 40-63 μm (230-400 mesh). All NMR spectra were recorded on either a Bruker Avance 600 MHz or 400 MHz spectrometer at STP. All deuterated solvents were used as received from Cambridge Isotope Laboratories, Inc. ^{1}H, ^{13}C, and ^{31}P NMR chemical shifts are reported in parts per million (ppm) relative to residual solvent resonances ($CDCl_3$ or CD_2Cl_2) or an external standard (H_3PO_4, 85%, 0 ppm). GC-MS data was obtained using an Agilent G2570A GC/MSD system containing a 6850 GC equipped with an HP-5MS column (length 30 m,; I.D. 0.250 mm) connected to an Agilent 5983N MSD. Enantiomeric excess (*e.e.*'s) were determined on a HP-6890 GC using an Agilent β-Cyclosil column (length 30 m, I.D. 0.250 mm) or using a Berger Instruments SFC equipped with a Chiralpak AD-H column (length 250 mm, I.D. 4.6 mm). High resolution mass spectra (HRMS) were obtained from the University of Illinois Mass Spectrometry lab (Dr. Furong Sun).

[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics*, **1996**, *15*, 1518.

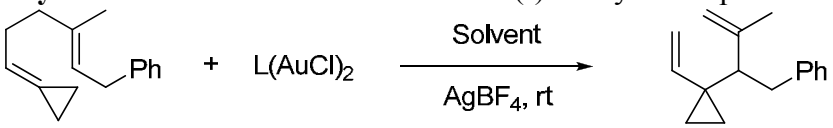
2. Catalyst Optimization Results

A. General Reaction Parameter Screening

Reaction conditions: 5 mol% Au(I) catalyst, 10.5 mol% Ag salt, 18 h.

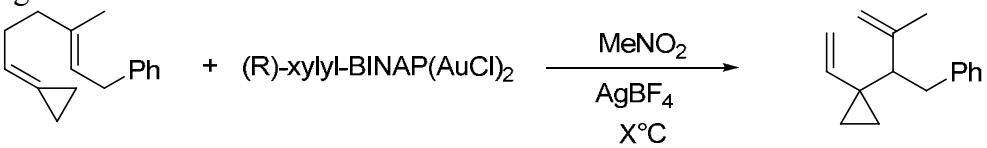
Enantioselectivities determined by chiral GC.

Supplementary Table 1. Solvent effects on the Au(I) catalyzed Cope rearrangement.



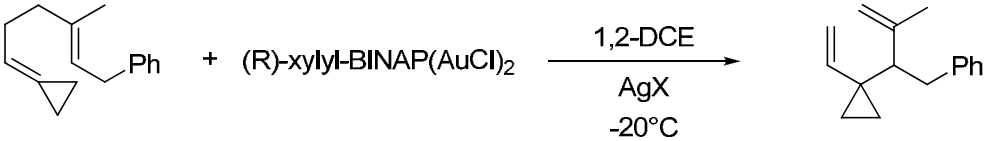
Ligand	Solvent	*e.e.* (%)
(R)-BINAP	DCM	15
(R)-BINAP	$MeNO_2$	19
(R)-xylyl-BINAP	$MeNO_2$	20
(R)-xylyl-BINAP	1,2-DCE	24
(R)-xylyl-BINAP	Toluene	15
(R)-xylyl-BINAP	Et_2O	0

Supplementary Table 2. Temperature effects on the Au(I) catalyzed Cope rearrangement.



Temperature (°C)	*e.e.* (%)
R.T.	20
0	22
-5	24
-20	25

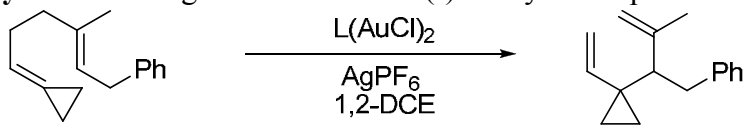
Supplementary Table 3. Counter-ion effects on Au(I) catalyzed Cope rearrangement.



X^-	*e.e.* (%)
BF_4	25
OTf	37[a]
PF_6	34
SbF_6	32
NTf_2	32

[a] Reaction only proceeded to 50% completion (GC-MS).

Supplementary Table 4. Ligand effects on Au(I) catalyzed Cope rearrangement.



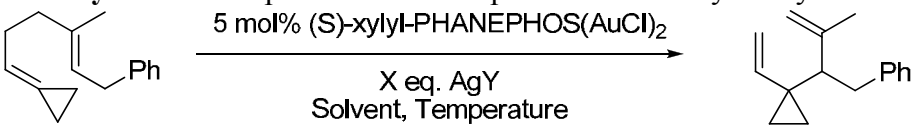
Entry	Ligand	T (°C)	*e.e.* (%)
1	(R)-xylyl-BINAP	0	28
2	(R)-xylyl-BINAP	-20	34
3	(R)-xylyl-MeO-BIPHEP	-20	19
4	(R)-SEGPHOS	-20	16
5	(R)-DIFLUORPHOS	-20	9
6	(R)-xyl-SDP	-20	5
7	(R)-DTBM-SEGPHOS$(AuCl)_2$	-20	25
8	(R,R)-Me-DuPHOS	0	2
9	(R)-SYNPHOS	0	15
10	(S)-3,5-xylyl-PHANEPHOS (**4**)	-20	79
11	(S)-SIPHOS-PE	0	7
12	Ag-(R)-(**5**)	rt	-

B. Optimization for (S)-3,5-xylyl-PHANEPHOS$(AuCl)_2$ (4).

Reactions Conditions: 5 mol% **4**, 18 h.

Enantioselectivities determined by chiral GC.

Supplementary Table 5. Optimization of Cope Reaction catalyzed by **4**.



X	Y^-	T (°C)	Solvent	*e.e.* (%)
1[a]	PF_6	-20	1,2-DCE	58

2.1	PF_6	-20	1,2-DCE	79
4	PF_6	-20	1,2-DCE	82
4	PF_6	-20	DCM	77
4	PF_6	-20	$MeNO_2$	81
4[a]	PF_6	-50	DCM	66
4	BF_4	-20	1,2-DCE	81
4	OTf	-20	1,2-DCE	74
4	SbF_6	-20	1,2-DCE	83
4	NTf_2	-20	1.2-DCE	82
4	SbF_6	-35	DCM:1,2-DCE 1:9	87

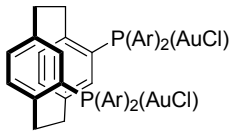
[a] Reaction did not go to completion.

3. Representative Experimental Procedures.

A. Preparation of Gold(I) Catalysts

Bis(phosphine) gold(I) catalysts were prepared by a modification to a procedure previously reported.[2] Spectroscopic data for the Au(I) complexes used in the optimization study have been reported previously.[3,4,5,6] To a solution of (S)-3,5-xylyl-PHANEPHOS (0.094 g, 0.136 mmol, 1.00 eq.) in CH_2Cl_2 (4 mL) at rt under air was added $Me_2S{\cdot}AuCl$ (0.080 g, 0.272 mmol, 2.00 eq.). The reaction was stirred for 2 h at rt, then concentrated and dried under vacuum overnight to provide the product compound as a white solid (0.128 g, 82%). X-ray quality crystals were obtained by layering a solution of **4**, in benzene, with pentanes and storing at 4°C.

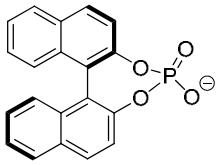
[2] Kleinbeck, F.; Toste, F. D. *J. Am. Chem. Soc.* **2009**, *131*, 9178.
[3] Johansson, M. J.; Gorin, D. J.; Stabe, S. T.; Toste, F. D. *J. Am. Chem. Soc.* **2005**, *127*, 18002.
[4] Melhado, A. D.; Luparia, M.; Toste, F. D. *J. Am. Chem. Soc.* **2007**, *129*, 12638.
[5] Pradal, A.; Chao, M-C.; Vitale, M. R.; Toullec, P. Y.; Michelet, V. *Tetrahedron*, **2011**, *67*, 4371.
[6] Hamilton, G. L.; Kang, E. J.; Mba, M.; Toste, F. D. *Science*, **2007**, *317*, 496.



Ar = 3,5-xylyl

4

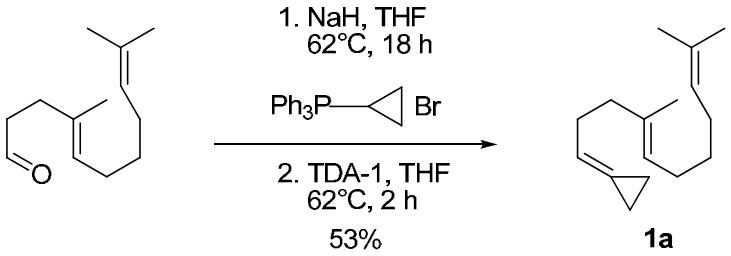
(S)-3,5-xylyl-PHANEPHOS(AuCl)$_2$ (4): **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.28-7.19 (m, 8H), 7.10-7.05 (m, 6H), 6.82-6.80 (m, 2H), 6.74-6.72 (m, 2H), 3.76-3.69 (m, 2H), 3.30 (t, *J* = 12 Hz, 2H), 3.07 (t, *J* = 12 Hz, 2H), 2.80-2.78 (m, 2H), 2.43 (s, 12H), 2.21 (s, 12H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 145.0, 144.9, 140.7, 140.6, 139.9, 139.8, 139.2, 139.1, 137.5, 135.9, 135.8, 135.0, 134.9, 133.8, 133.7, 133.6, 133.5, 132.8, 132.4, 131.7, 131.6, 128.2, 127.8, 127.4, 34.9, 34.8, 34.4, 22.0, 21.5; **^{31}P-NMR** (162 MHz, CD_2Cl_2) δ 31.5.



Ag-(R)-5

B. Synthesis of 1,5-Dienes

General Procedure for Wittig cyclopropylidination[7]



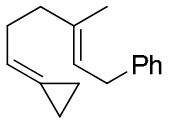
1a

To a Schlenk flask loaded with a suspension of dry NaH (0.075 g, 3.15 mmol, 1.30 eq.) in THF (13 mL) under N_2 atmosphere was added cyclopropyltriphenylphosphonium bromide (1.21 g, 3.15 mmol, 1.30 eq.) at rt. The reaction flask was then equipped with a

[7] Stafford, J. A.; McMurry, J. E. *Tetrahedron Lett*. **1988**, *29*, 2531.

condenser and heated to 62°C for 18 h. To the resulting orange suspension was then added (E)-4,10-dimethylundeca-4,9-dienal[8] (0.469 g, 2.42 mmol, 1.00 eq.) and tris[2-(2-methoxyethoxy)ethyl]amine (TDA-1) (0.077 mL, 0.242 mmol, 0.10 eq.) in THF (4 mL). The reaction was stirred for 2 h at 62°C before cooling to rt and quenching with saturated aqueous $NaHCO_3$. The reaction was diluted with deionized H_2O and Et_2O before separating the layers. The aqueous layer was extracted with Et_2O (2x) and the combined organic layers were then washed with brine (2x). The organic layer was then dried over $MgSO_4$, filtered, and concentrated *in vacuo*. Purification by silica gel chromatography (Hexanes) provided the product compound as a colorless oil (0.283 g, 53%). A small amount of CH_2Cl_2 was used to load the material onto the column.

(E)-(4,10-dimethylundeca-4,9-dienylidene)cyclopropane (1a): **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 5.75-5.72 (m, 1H), 5.16-5.10 (m, 2H), 2.29-2.25 (m, 2H), 2.12-2.09 (m, 2H), 1.99-1.94 (m, 4H), 1.68 (s, 3H), 1.60 (s, 3H), 1.59 (s, 3H), 1.37-1.32 (m, 2H), 1.02-1.00 (m, 4H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 135.4, 131.8, 125.2, 125.2, 121.5, 118.5, 39.9, 31.0, 30.6, 28.1, 28.0, 26.0, 17.9, 16.2, 2.5, 2.1. HRMS (EI+) calculated for $C_{16}H_{26}$ 218.20345, found 218.20366.

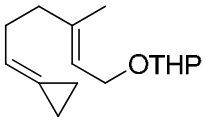


1b

(E)-(6-cyclopropylidene-3-methylhex-2-enyl)benzene (1b): Prepared using the same general procedure as for (**1a**) from (E)-4-methyl-6-phenylhex-4-enal.[9] Purified by silica gel chromatography (Hexanes). 34% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.27-7.24 (m, 2H),

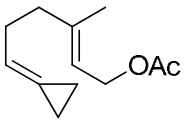
[8] Sokol, J. G.; Korapala, C. S.; White, P. S.; Becker, J. J.; Gagné, M. R. *Angew. Chem. Int. Ed.* **2011**, *50*, 5658.
[9] Zhao, J-F.; Loh, T-P. *Angew. Chem. Int. Ed.* **2009**, *48*, 7232.

7.17-7.14 (m, 3H), 5.75-5.73 (m, 1H), 5.36-5.32 (m, 1H), 3.35 (d, J = 7.8 Hz, 1H), 2.34-2.30 (m, 2H), 2.19-2.17 (m, 2H), 1.73 (s, 3H), 1.00 (s, 4H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 142.5, 136.6, 128.8, 126.1, 123.7, 121.7, 118.4, 39.9, 34.7, 30.9, 16.4, 2.5, 2.2. HRMS (EI+) calculated for $C_{16}H_{20}$ 212.15650, found 212.15613.



1g

(E)-2-(6-cyclopropylidene-3-methylhex-2-enyloxy)tetrahydro-2H-pyran (1g): Prepared using the same general procedure as for (**1a**) from (E)-4-methyl-6-(tetrahydro-2H-pyran-2-yloxy)hex-4-enal.[10] Purified by silica gel chromatography (10:1 Hexanes:Et_2O). 45% **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.75-5.72 (m, 1H), 5.39-5.36 (m 1H), 4.62-4.61 (m, 1H), 4.23 (dd, J = 11.9 Hz, 6.4 Hz, 1H), 4.02 (dd, J = 11.9 Hz, 7.4 Hz, 1H), 3.91-3.87 (m, 1H), 3.52-3.49 (m, 1H), 2.33-2.29 (m, 2H), 2.18-2.16 (m, 3H), 1.86-1.81 (m, 1H), 1.74-1.69 (m, 1H), 1.69 (s, 3H), 1.60-1.56 (m, 3H), 1.55-1.51 (m, 2H), 1.01 (bs, 4H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 140.1, 121.3, 120.6, 117.6, 97.8, 63.6, 62.3, 39.2, 30.7, 30.1, 25.5, 19.6, 16.4, 2.2, 1.8.

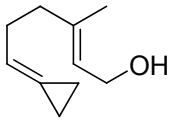


1h

(E)-6-cyclopropylidene-3-methylhex-2-enyl acetate (1h): Prepared using the same general procedure as for (**1a**) from (E)-3-methyl-6-oxohex-2-enyl acetate.[11] Purified by an silica gel chromatography using 9:1 Hexanes:EtOAc in an initial column, followed by a second silica gel column utilizing 15:1 Hexanes:EtOAc as the eluant. 22% **^{1}H-NMR**

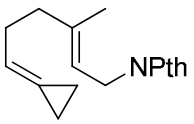
[10] Koh, J. H.; Gagné, M. R. *Angew. Chem. Int. Ed.* **2004**, *43*, 3459.
[11] Surendra, K. Qiu, W.; Corey, E. J. *J. Am. Chem. Soc.* **2011**, *133*, 9724.

(600 MHz, $CDCl_3$) δ 5.74-5.72 (m, 1H), 5.37-5.34 (m, 1H), 4.58 (d, J = 7.1 Hz, 2H), 2.33-2.29 (m, 2H), 2.19-2.16 (m, 2H), 2.05 (s, 3H), 1.71 (s, 3H), 1.01 (bs, 4H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 171.2, 142.2, 121.6, 118.3, 117.4, 61.4, 39.1, 30.0, 21.1, 16.5, 2.2, 1.8.



1i

(E)-6-cyclopropylidene-3-methylhex-2-en-1-ol (1i): Prepared by removal of the tetrahydropyran protecting group from **1g**. To a small vial loaded with **1g** (0.250 g, 1.06 mmol, 1 eq.) was added MeOH (2.5 mL). *p*-Toluenesulfonic acid monohydrate was then added (0.010 g, 0.053 mmol, 5 mol%) and the reaction was stirred for 30 minutes at room temperature. The reaction mixture was then concentrated *in vacuo* and purified by silica gel chromatography (5:1 Hexanes:EtOAc) to give 0.1136 of the product compound. 71% **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.75-5.72 (m, 1H), 5.44-5.41 (m, 1H), 4.15 (d, J = 6.9 Hz, 2H), 2.32-2.29 (m, 2H), 2.17-2.15 (m, 2H), 1.69 (s, 3H), 1.21 (bs, 1H), 1.01 (bs, 4H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 139.7, 123.4, 121.5, 117.5, 59.4, 39.1, 30.1, 16.2, 2.2, 1.81.

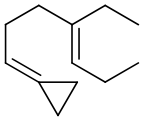


1j

(E)-2-(6-cyclopropylidene-3-methylhex-2-enyl)isoindoline-1,3-dione (1j): Prepared by a Mitsunobu reaction of compound **1i**. To a small flask was added THF (4 mL), **1i** (0.050 g, 0.328 mmol, 1eq.), phthalimide (0.063 g, 0.426 mmol, 1.3 eq.), then triphenylphosphine (0.112 g, 0.426 mmol, 1.3 eq.). The reaction flaks was then wrapped

in aluminum foil and diisopropyl azodicarboxylate (0.084 mL, 0.426 mmol, 1.3 eq.) was then added dropwise. The reaction was stirred for 4.5 h at room temperature before being poured into 16 mL H_2O. The layers were separated and the aqueous layer was extracted twice each with Et_2O and Hexanes. The combined organics were washed with two times with brine, dried over $MgSO_4$, filtered and concentrated *in vacuo*. The product compound was purified by silica gel chromatography (10:1 Hexanes:Et_2O) to give 0.0597 of product as a colorless oil which solidified upon placing in the freezer. 65% **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.84-7.82 (m, 2H), 7.71-7.69 (m, 2H), 5.69-5.67 (m, 1H), 5.29-5.26 (m, 1H), 4.27 (d, J = 7.1 Hz, 2H), 2.29-2.25 (m, 2H), 2.13-2.11 (m, 2H), 1.83 (s, 3H), 0.97 (bs, 4H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 168.1, 140.4, 133.8, 132.3, 123.1, 121.5, 118.0, 117.4, 39.0, 35.8, 30.0, 16.4, 2.2, 1.8.

Alkylidenecyclopropanes **1c**, **1d**, **1e**, and **1k** were prepared from aldehydes synthesized using a published ruthenium-catalyzed coupling procedure.[12]

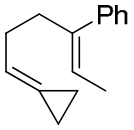


1c

(E)-(4-ethylhept-4-enylidene)cyclopropane (1c): Prepared using the same general procedure as for (**1a**). Purified by silica gel chromatography (Hexanes). 56% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 5.76-5.73 (m, 1H), 5.10 (t, J = 7.2 Hz, 1H), 2.26 (q, J = 7.7 Hz, 2H), 2.11 (t, J = 7.2 Hz, 2H), 2.04 (q, J = 7.6 Hz, 2H), 2.00 (m, 2H), 1.01 (bs, 4H), 0.96 (t, J = 7.6 Hz, 3H), 0.93 (t, J = 7.7 Hz, 3H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 140.7,

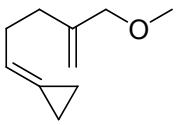
[12] Dérien, S.; Jan, D.; Dixneuf, P. H. *Tetrahedron* **1996**, *52*, 5511.

126.6, 121.4, 118.6, 36.7, 31.2, 23.5, 21.3, 15.1, 13.7, 2.5, 2.2. HRMS (EI+) calculated for $C_{12}H_{20}$ 164.15650, found 164.15546.



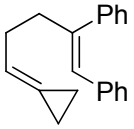
1d

(Z)-(6-cyclopropylidenehex-2-en-3-yl)benzene (1d): Prepared using the same general procedure as for (**1a**). Purified by silica gel chromatography (Hexanes). 25% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.35-7.33 (m, 2H), 7.25-7.23 (m, 1H), 7.17-7.15 (m, 1H), 5.74-5.71 (m, 1H), 5.60-5.56 (m, 1H), 2.49 (t, *J* = 7.8 Hz, 2H), 2.22 (q, *J* = 7.8 Hz, 2H), 1.60 (d, *J* = 7.2 Hz, 3H), 1.01-0.95 (m, 4H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 142.0, 141.6, 129.1, 128.5, 126.9, 121.8, 121.7, 118.2, 39.4, 31.2, 15.0, 2.5, 2.2. HRMS (EI+) calculated for $C_{15}H_{18}$ 198.14085, found 198.13973.



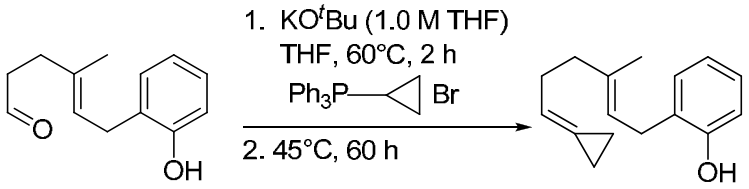
1e

(4-(methoxymethyl)pent-4-enylidene)cyclopropane (1e): Prepared using the same general procedure as for (**1a**). Purified by silica gel chromatography (5:1 Pentanes:Et_2O). 31% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 5.76-5.74 (m, 1H), 4.97 (s, 1H), 4.89 (s, 1H), 3.83 (s, 2H), 3.27 (s, 3H), 2.35-2.31 (m, 2H), 2.17 (t, *J* = 7.8 Hz, 2H), 1.01 (bs, 4H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 146.7, 121.9, 118.1, 111.4, 75.9, 58.2, 33.2, 30.5, 2.5, 2.2. HRMS (EI+) calculated for $C_{10}H_{15}O$ ($[M^+ - H^+]$) 151.11230, found 151.11278.



1k

(Z)-(5-cyclopropylidenepent-1-ene-1,2-diyl)dibenzene (1k): Prepared using the same general procedure as for (**1a**). Purified by silica gel chromatography (Hexanes). 39% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.31-7.28 (m, 2H), 7.27-7.24 (m, 1H), 7.16-7.14 (m, 2H), 7.08-7.02 (m, 3H), 6.92-6.90 (m, 2H), 6.47 (s, 1H), 5.79 (tt, J = 6.6 Hz, 2.4 Hz, 1H), 2.64 (ddd, J = 9.0 Hz, 6.6 Hz, 1.2 Hz, 2H), 2.31-2.27 (m, 2H), 1.03-0.98 (m, 4H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 143.7, 141.9, 138.2, 129.5, 129.2, 129.0, 128.3, 127.4, 126.9, 126.6, 122.1, 117.9, 40.8, 30.8, 2.5, 2.3. HRMS (EI+) calculated for $C_{20}H_{20}$ 260.15650, found 260.15682.



1f

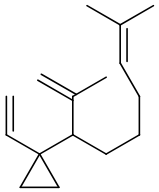
(E)-2-(6-cyclopropylidene-3-methylhex-2-enyl)phenol (1f): The general procedure for the Wittig reaction did not work to synthesize **1f** as decomposition of the aldehyde was observed. Instead a procedure employing KO^{t}Bu to activate the phosphonium salt was utilized.[13] To a Schlenk flask loaded with cyclopropyltriphenylphosphonium bromide (1.00 g, 2.61 mmol, 1.33 eq.) and THF (20 mL) under N_2 atmosphere was slowly added KO^{t}Bu (1.0 M in THF, 5.22 mL, 5.22 mmol, 2.66 eq.) at rt. The reaction changed from yellow upon initial addition of the KO^{t}Bu and was orange by the end of the addition. The reaction was then heated to 60°C for 2 h. The aldehyde, (E)-6-(2-hydroxyphenyl)-4-methylhex-4-enal,[14] dissolved in THF (2.5 mL), was then added and the reaction was heated at 45°C for 60 h. After allowing the reaction to cool to rt, H_2O was added then

[13] Maercker, A.; Daub, V. E. E. *Tetrahedron*, **1994**, *50*, 2439.
[14] Koh, J. H.; Mascarenhas, C.; Gagné, M. R. *Tetrahedron*, **2004**, *60*, 7405.

saturated aqueous NH_4Cl. The layers were separated and the aqueous layer extracted with Et_2O (2x). The combined organic layers were washed with brine (1x), dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The product compound was then purified by silica gel chromatography using 5:1 Pentanes:Et_2O. Compound **1f** was obtained as a colorless oil (0.075g, 17%). **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.09-7.07 (m, 2H), 6.89 (dt, J = 7.8 Hz, 1.2 Hz, 1H), 6.78-6.76 (m, 1H), 5.73-5.70 (m, 1H), 5.33-5.31 (m, 1H), 5.11-5.09 (m, 1H), 3.35 (d, J = 7.2 Hz, 2H), 2.35-2.31 (m, 2H), 2.21-2.19 (m, 2H), 1.76 (s, 3H), 1.02-0.99 (m, 4H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 154.9, 138.6, 130.4, 127.9, 127.6, 122.3, 122.1, 121.1, 118.1, 116.0, 39.8, 30.7, 30.0, 16.4, 2.6, 2.2. HRMS (EI+) calculated for $C_{16}H_{20}O$ 228.15142, found 228.15209.

C. General Procedure for Au(I) Catalyzed Cope Rearrangement

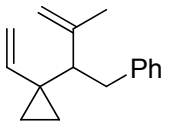
To a vial loaded with silver hexafluoroantimonate (3.2 mg, 0.0092 mmol, 0.2 eq.) would be added a 1:9 CH_2Cl_2:1,2-DCE solution (1 mL). Au(I) catalyst **4** (2.6 mg, 0.0023 mmol, 0.05 eq.) was then added and the reaction stirred at rt for 15 min. The reaction was then placed into a NesLab Cryobath CB-80 maintained at -35°C and stirred for 10 min before addition of **1a** (10 mg, 0.046 mmol, 1 eq.). The reaction would then be stirred for 18 h at -35°C before concentrating the reaction *in vacuo*. The product was then isolated by a pipette column.



2a

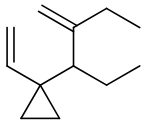
1-(2,8-dimethylnona-1,7-dien-3-yl)-1-vinylcyclopropane (2a): Silica gel column (Hexanes). Product isolated as a colorless oil (9.4 mg, 94%). **^{1}H-NMR** (600 MHz,

$CDCl_3$) δ 6.09 (dd, *J* = 15.6 Hz, 10.5 Hz, 1H), 5.12-5.09 (m, 1H), 4.85-4.80 (m, 2H), 4.80 (bs, 1H), 4.66 (bs, 1H), 1.97-1.92 (m, 2H), 1.71 (s, 3H), 1.68 (s, 3H), 1.52-1.47 (m, 2H), 1.33-1.28 (m, 2H), 0.64-0.58 (m, 3H), 0.54-0.51 (m, 1H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 147.1, 141.5, 131.5, 124.9, 111.3, 111.1, 52.7, 30.3, 28.4, 28.3, 25.9, 25.6, 22.2, 17.9, 14.6, 12.9. HRMS (EI+) calculated for $C_{16}H_{26}$ 218.20345, found 218.20224.



2b

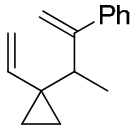
(3-methyl-2-(1-vinylcyclopropyl)but-3-enyl)benzene (2b): Silica gel column (Hexanes). Product isolated as a colorless oil (89%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.25-7.23 (m, 2H), 7.17-7.14 (m, 3H), 6.13 (dd, *J* = 17.1 Hz, 10.5 Hz, 1H), 4.94-4.88 (m, 2H), 4.82 (bs, 1H), 4.70 (bs, 1H), 2.90 (dd, *J* = 13.8 Hz, 6.0 Hz, 1H), 2.85 (dd, *J* = 13.8 Hz, 8.7 Hz, 1H) 1.92 (dd, *J* = 8.7 Hz, 6.0 Hz, 1H), 1.76 (s, 3H), 0.66-0.64 (m, 2H), 0.60-0.58 (m, 1H), 0.33-0.30 (m, 1H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 146.3, 141.6, 140.9, 129.1, 128.1, 125.7, 112.0, 111.8, 54.2, 37.3, 25.3, 23.3, 14.1, 13.9. HRMS (EI+) calculated for $C_{16}H_{20}$ 212.15650, found 212.15739.



2c

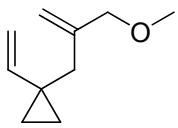
1-(4-methylenehexan-3-yl)-1-vinylcyclopropane (2c): Silica gel column (Hexanes). Product isolated as a colorless oil (87%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 6.02 (dd, *J* = 16.8 Hz, 10.8 Hz, 1H), 4.85-4.80 (m, 2H), 4.83 (bs, 1H), 4.70 (bs, 1H), 2.10-2.03 (m, 1H), 2.02-1.95 (m, 1H), 1.59-1.50 (m, 3H), 1.01 (t, *J* = 7.8 Hz, 3H), 0.86 (t, *J* = 7.2 Hz,

3H), 0.61-0.57 (m, 3H), 0.51-0.48 (m, 1H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 151.9, 141.9, 110.0, 108.3, 53.0, 28.7, 25.4, 24.1, 14.4, 12.8, 12.6, 12.3.



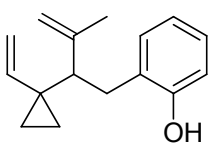
2d

(3-(1-vinylcyclopropyl)but-1-en-2-yl)benzene (2d): Silica gel column (Hexanes). Product isolated as a colorless oil (90%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.31-7.29 (m, 4H), 7.27-7.25 (m, 1H), 6.00 (dd, J = 17.1 Hz, 10.8 Hz), 5.21 (bs, 1H), 5.11 (bs, 1H), 4.90 (d, J = 10.8 Hz, 1H), 4.84 (d, J = 17.1 Hz, 1H), 2.45 (q, J = 7.2 Hz, 1 H), 1.19 (d, J = 7.2 Hz, 3H), 0.61-0.58 (m, 1H), 0.48-0.38 (m, 3H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 152.1, 144.0, 141.1, 128.1, 127.1, 127.0, 113.0, 111.5, 43.4, 25.7, 17.3, 14.2, 13.5. HRMS (EI+) calculated for $C_{15}H_{18}$ 198.14085, found 198.14154.



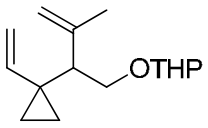
2e

1-(2-(methoxymethyl)allyl)-1-vinylcyclopropane (2e): Silica gel column (10:1 Pentanes:Et_2O). Product isolated as a colorless oil (98%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.62 (dd, J = 17.4 Hz, 10.8 Hz, 1H), 5.07 (bs, 1H), 5.03 (bs, 1H), 4.89 (d, J = 17.4 Hz, 1H), 4.86 (d, J = 10.8 Hz, 1H), 3.86 (s, 2H), 3.30 (s, 3H), 2.20 (s, 2H), 0.68-0.63 (m, 4H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 143.9, 143.6, 113.6, 110.8, 75.9, 57.9, 39.6, 20.3, 14.7. HRMS (EI+) calculated for $C_{10}H_{15}O$ ($[M^+ - H^+]$) 151.11230, found 151.11209.



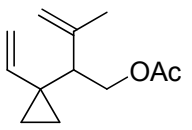
2f

2-(3-methyl-2-(1-vinylcyclopropyl)but-3-enyl)phenol (2f): Silica gel column (10:1 Pentanes:Et_2O). Product isolated as a colorless oil (71%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.08-7.05 (m, 2H), 6.83 (td, *J* = 7.2 Hz, 1.2 Hz, 1H), 6.75-6.74 (m, 1H), 6.16 (dd, *J* = 17.1 Hz, 10.8 Hz, 1H), 4.96 (dd, *J* = 10.8 Hz, 1.8 Hz, 1H), 4.94 (dd, *J* = 17.1 Hz, 1.8 Hz, 1H), 2.88 (dd *J* = 14.4 Hz, 7.8 Hz, 1H), 2.85 (dd, *J* = 14.4 Hz, 7.2 Hz, 1H), 1.95 (pt, *J* = 7.8 Hz, 7.2 Hz, 1H), 1.80 (s, 3H), 0.67-0.59 (m, 3H), 0.33-0.30 (m, 1H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 153.8, 147.2, 140.9, 131.0, 127.5, 127.3, 120.7, 115.5, 112.1, 111.7, 52.4, 31.8, 24.9, 23.6, 14.5, 13.5. HRMS (EI+) calculated for $C_{16}H_{20}O$ 228.15142, found 228.15274.



2g

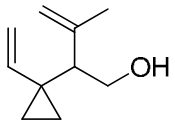
2-(3-methyl-2-(1-vinylcyclopropyl)but-3-enyloxy)tetrahydro-2H-pyran (2g): Silica gel column (10:1 Hexanes:Et_2O). Product isolated as a colorless oil, in a 1:1 mixture of diasteromers (60%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 6.01 (dd, *J* = 7.2 Hz, 6.5 Hz, 1H), 4.87-4.73 (m, 4H), 4.56 (bs, 1H), 3.95-3.91 (m, 1H), 3.85-3.83 (m, 1H), 3.54-3.47 (m, 2H), 1.86 (bs, 1H), 1.78 (bs, 4H), 1.55 (bs, 1H), 1.53-1.47 (m, 4H), 0.67-0.64 (m, 4H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 145.0, 140.8, 111.7, 111.5, 99.3, 68.6, 62.2, 51.9, 30.9, 25.5, 23.4, 23.1, 19.5, 13.9, 13.4.



2h

3-methyl-2-(1-vinylcyclopropyl)but-3-enyl acetate (2h): Silica gel column (10:1 Hexanes:Et_2O). Product isolated as a colorless oil (70%). **^{1}H-NMR** (600 MHz, $CDCl_3$)

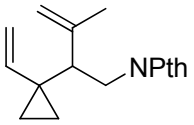
δ 5.94 (dd J = 16.9 Hz, 10.8 Hz, 1H), 4.90 (m, 2H), 4.87 (dd, J = 8.4 Hz, 1.4 Hz, 1H), 4.73 (bs, 1H), 4.26 (d, J = 7.2 Hz, 2H), 2.03 (s, 3H), 1.94 (t, J = 7.2 Hz, 1H), 1.79 (s, 3H), 0.72-0.65 (m, 3H), 0.63-0.60 (m, 1H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 171.1, 143.7, 139.8, 112.3, 112.0, 64.8, 50.6, 23.0, 21.0, 13.6, 13.1.



2i

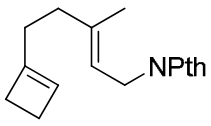
3-methyl-2-(1-vinylcyclopropyl)but-3-en-1-ol (2i): Silica gel column (10:1 Hexanes:EtOAc). Product isolated as a colorless oil (35%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 5.97 (dd, J = 17.4 Hz, 10.3 Hz, 1H), 4.98 (bs, 1H), 4.90 (pd, J = 1.8 Hz, 1H), 4.87 (pd, J = 2.9 Hz, 1H), 4.80 (bs, 1H), 3.77-3.75 (m, 2H), 1.90 (t, J = 7.2 Hz, 1H), 1.81 (s, 3H), 1.54 (bs, 1H), 0.73-0.70 (m, 1H), 0.67-0.62 (m, 2H), 0.61-0.58 (m, 1H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 144.4, 140.4, 112.0, 112.0, 62.9, 54.1, 31.6, 23.1, 13.0, 12.9

Conversion of 2i to 2h: Dissolved alcohol **2i** (13 mg, 0.085 mmol, 1 eq.) in pyridine (0.12 mL) and cooled to 0°C. Added a single small crystal of 4-(dimethylamino)pyridine (DMAP) then acetic anhydride (0.0126 mL, 0.133 mmol, 1.5 eq.). The reaction was stirred briefly at 0° then allowed to warm to room temperature and stirred for 2 h. The reaction was then diluted with hexanes and quenched with ice/H_2O. The layers were separated and the aqueous layer was washed with hexanes (2x). The combined organic layers were then washed with 10% HCl (2x) and saturated $NaHCO_3$ (2x) before drying over $MgSO_4$. The product was then concentrated *in vacuo* to give the product as a colorless oil (7.6 mg, 46%). ^{1}H and ^{13}C NMR spectra matched that of compound **2h**.



2j

2-(3-methyl-2-(1-vinylcyclopropyl)but-3-enyl)isoindoline-1,3-dione (2j): Silica gel column (10:1 Hexanes:Et2O). Product isolated as a pale green oil, as an intractable mixture with **3j** (45%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.84-7.81 (m, 2H), 7.71-7.69 (m, 2H), 6.08 (dd, *J* = 17.1 Hz, 10.5 Hz, 1H), 4.96 (dd, *J* = 17.1 Hz, 1.3 Hz, 1H), 4.93 (dd, *J* = 17.1 Hz, 1.3 Hz, 1H), 3.97 (dd, *J* = 13.8 Hz, 9.5 Hz, 1H), 3.79 (dd *J* = 13.8 Hz, 6.1 Hz, 1H), 2.39 (dd, *J* = 9.5 Hz, 6.1 Hz, 1H), 1.78 (s, 3H), 0.71-0.68 (m, 1H), 0.67-0.62 (m, 3H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 168.4. 144.0, 140.0, 133.8, 132.0, 123.1, 112.8, 112.3, 49.5, 39.3, 23.4, 22.5, 13.8, 12.3.

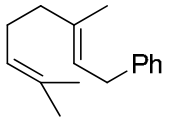


3j

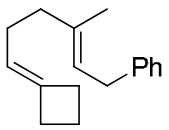
(E)-2-(5-cyclobutenyl-3-methylpent-2-enyl)isoindoline-1,3-dione (3j): Silica gel column (10:1 Hexanes:Et2O). Product isolated as a pale green oil, as an intractable mixture with **2j** (23%). **^{1}H-NMR** (600 MHz, $CDCl_3$) δ 7.84-7.81 (m, 2H), 7.71-7.69 (m, 2H), 5.62 (bs, 1H), 5.28 (t, *J* = 7.1 Hz, 1H), 4.27 (d, *J* = 7.1 Hz, 2H), 2.36 (bs, 2H), 2.26 (bs, 2H), 2.12-2.07 (m, 4H), 1.82 (s, 3H); **^{13}C-NMR** (150 MHz, $CDCl_3$) δ 168.1, 149.8, 140.4, 133.8, 132.3, 127.0, 123.1, 118.0, 36.6, 35.8, 31.1, 29.3, 26.5, 16.2.

D. Synthesis of control alkylidene substrates

Substrates prepared by Wittig reaction of phosphonium halide salt with (E)-4-methyl-6-phenylhex-4-enal.

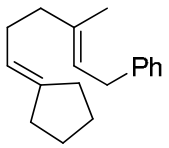


(E)-(3,7-dimethylocta-2,6-dienyl)benzene: Isopropyltriphenyphosphonium iodide (0.717 g, 1.66 mmol, 1.2 eq.) was suspended in dry THF (12 mL) and cooled to 0°C. *n*-BuLi (1.6 M, 1.04 mL, 1.66 mmol, 1.2 eq.) was added dropwise and the reaction was then stirred for 10 minutes at 0°C before adding the aldehyde (0.260 g, 1.38 mmol, 1 eq.) dissolved in THF (1 mL). The reaction was stirred 2h at 0°C before quenching at that temperature with saturated aqueous NH_4Cl. Added H_2O and Et_2O and separated the layers. The aqueous layer was extracted 2 times with Et_2O and the combined organics were then washed 2 times with brine before drying over $MgSO_4$, filtering, and concentrating *in vacuo*. The product was then purified by silica gel chromatography (Hexanes) to give 0.130 g of the product as a colorless oil. 44% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.27-7.25 (m, 2H), 7.18-7.14 (m, 3H), 5.34 (t, J = 7.0 Hz, 1H), 5.13-5.10 (m, 1H), 3.35 (d, J = 7.4 Hz, 2H), 2.14-2.10 (m, 2H), 2.07-2.04 (m, 2H), 1.72 (s, 3H), 1.68 (s, 3H), 1.60 (s, 3H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 142.3, 136.5, 131.7, 128.6, 128.6, 125.9, 124.6, 123.4, 40.0, 34.4, 26.9, 25.8, 17.7, 16.1.



(E)-(6-cyclobutylidene-3-methylhex-2-enyl)benzene: Added cyclobutyltriphenylphosphonium bromide (0.505 g, 1.27 mmol, 1.2 eq.) to a small flask and suspended in THF (25 mL). Added PhLi (2.0M, 0.70 mL, 1.40 mmol, 1.3 eq.) slowly at room temperature. Stirred 2h at room temperature then added aldehyde (0.200 g, 1.06 mmol, 1 eq.) in THF (1 mL) to the dark red solution. The reaction turned green

with the formation of a precipitate and stirred for 3h. The reaction was then quenched with H_2O and saturated aqueous NH_4Cl. Et_2O was added and the layers were separated before extracting the aqueous layer 2 times with Et_2O. The combined organic layers were washed 2 times with brine before drying over $MgSO_4$, filtering, and concentrating *in vacuo*. The product was then purified via silica gel chromatography (Hexanes) to give 0.154 g of the product as an intractable mixture with biphenyl. **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.28-7.25 (m, 2H), 7.19-7.15 (m, 3H), 5.34-5.31 (m, 1H), 5.04-5.01 (m, 1H), 3.35 (d, J = 7.3 Hz, 2H), 2.64-2.60 (m, 4H), 2.07-2.04 (m, 2H), 2.02-1.99 (m, 2H), 1.91 (p, J = 7.9 Hz, 2H), 1.71 (s, 3H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 142.3, 140.3, 136.5, 128.6, 128.6, 125.9, 123.4, 120.3, 40.0, 34.5, 31.2, 29.5, 26.8, 17.4, 16.1.

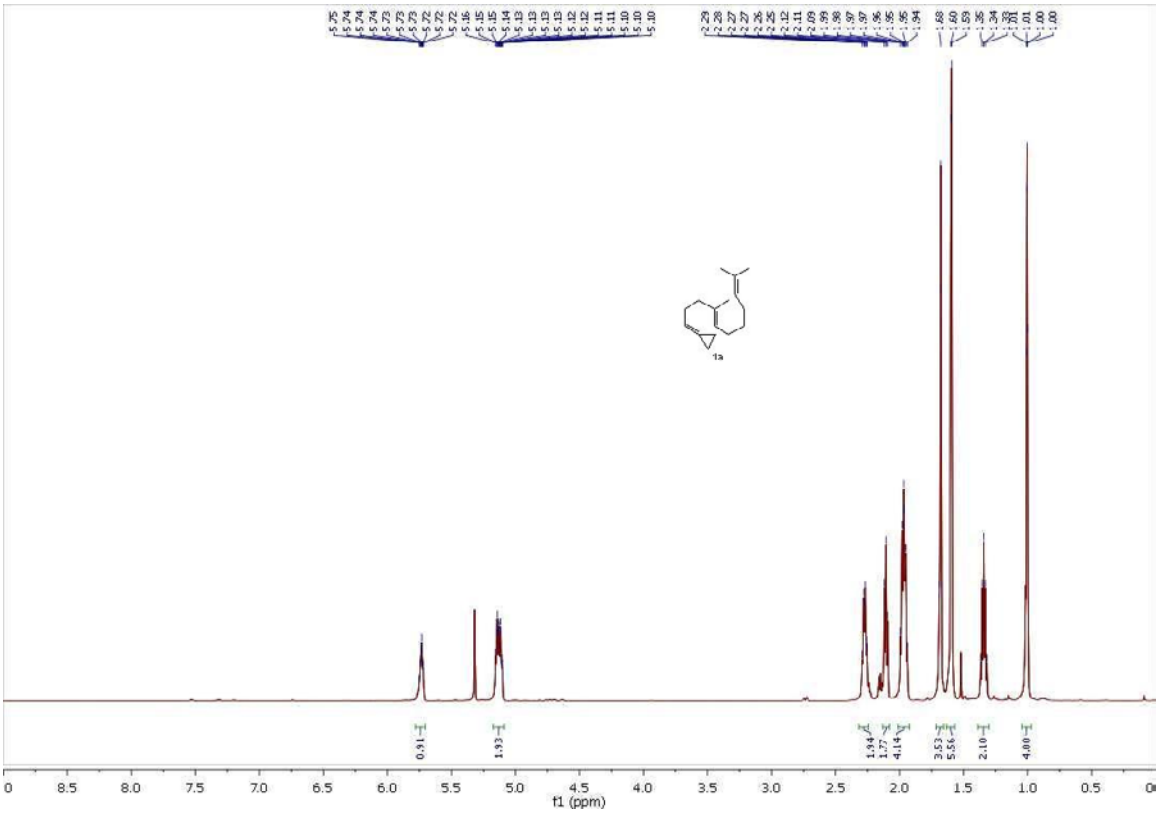


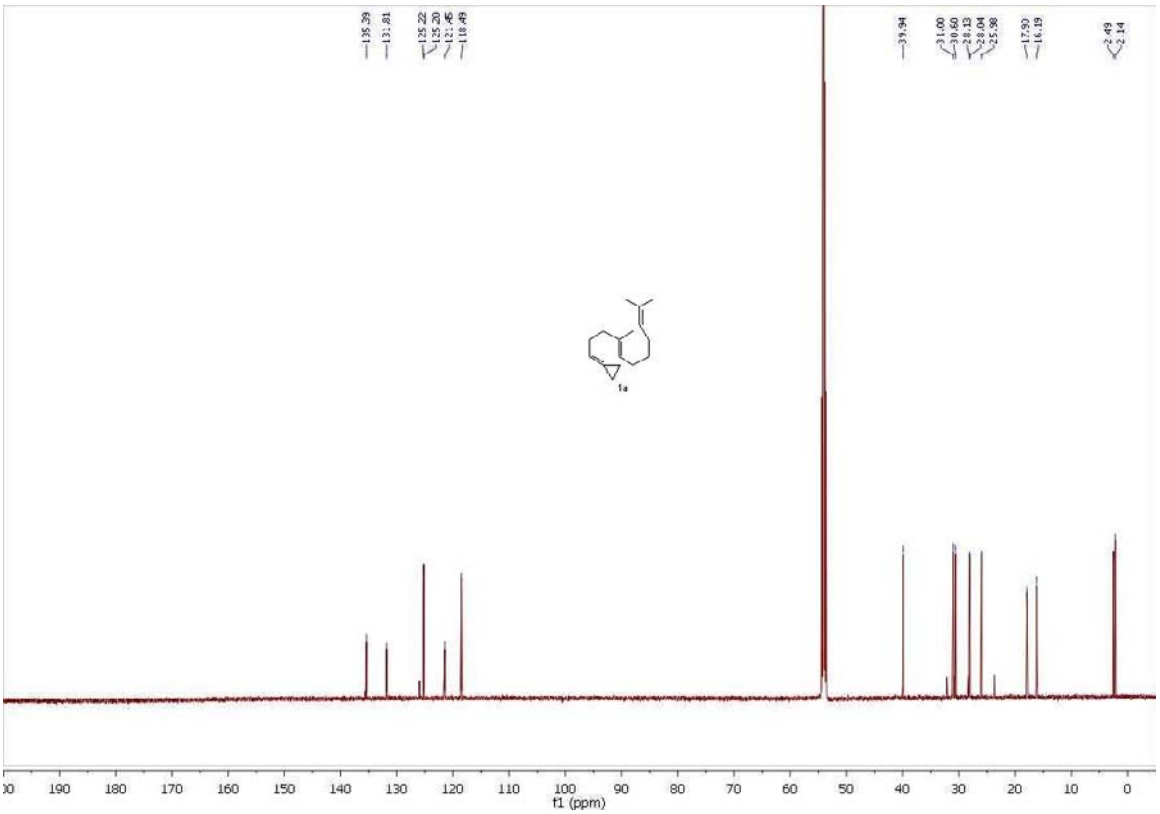
(E)-(6-cyclopentylidene-3-methylhex-2-enyl)benzene:

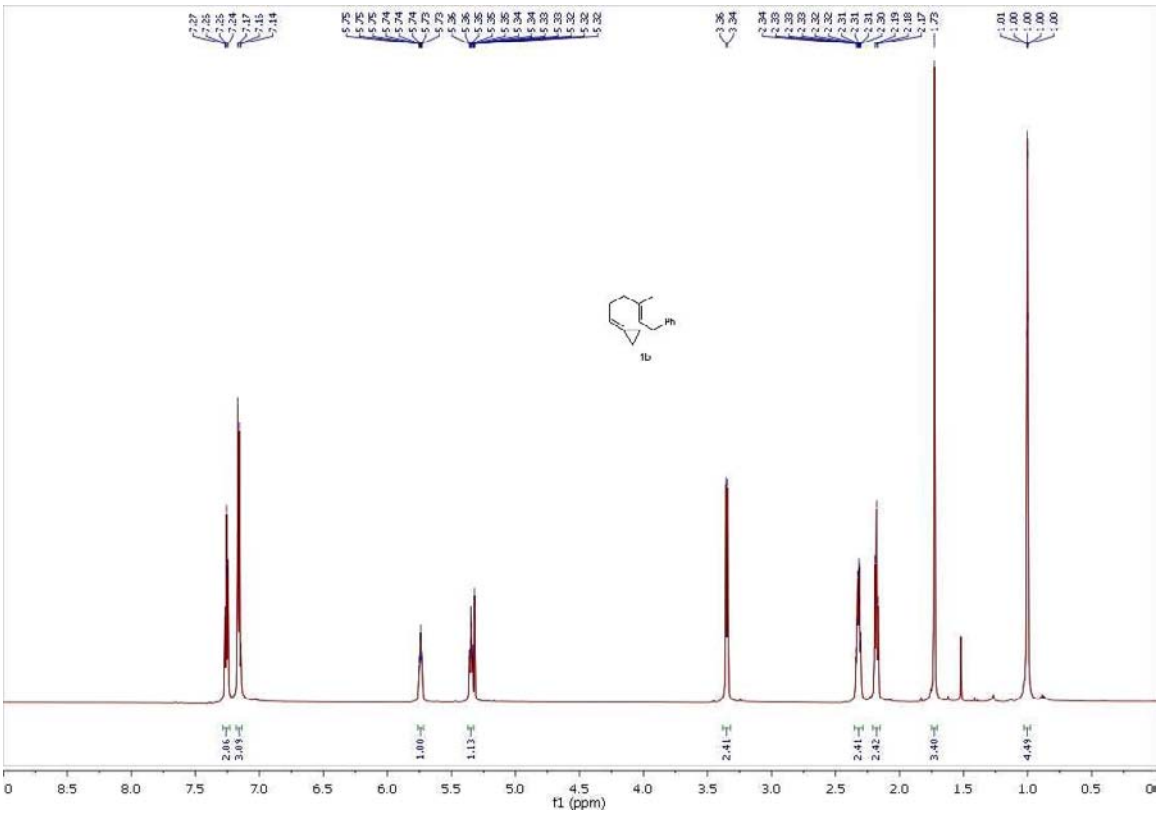
Cyclopentyltriphenylphosphonium bromide (0.522 g, 1.27 mmol, 1.2 eq.) was suspended in dry THF (12 mL) and cooled to 0°C. *n*-BuLi (1.6 M, 0.793 mL, 1.27 mmol, 1.2 eq.) was added dropwise and the reaction was then stirred for 30 minutes at 0°C before adding the aldehyde (0.200 g, 1.06 mmol, 1 eq.) dissolved in THF (1 mL). The reaction was stirred 1.5h at 0°C before quenching at that temperature with saturated aqueous NH_4Cl. Added H_2O and Et_2O and separated the layers. The aqueous layer was extracted 2 times with Et_2O and the combined organics were then washed 2 times with brine before drying over $MgSO_4$, filtering, and concentrating *in vacuo*. The product was then purified by silica gel chromatography (Hexanes) to give 0.130 g of the product as a colorless oil. 51% **^{1}H-NMR** (600 MHz, CD_2Cl_2) δ 7.27-7.25 (m, 2H), 7.19-7.14 (m, 3H), 5.33 (t, J =

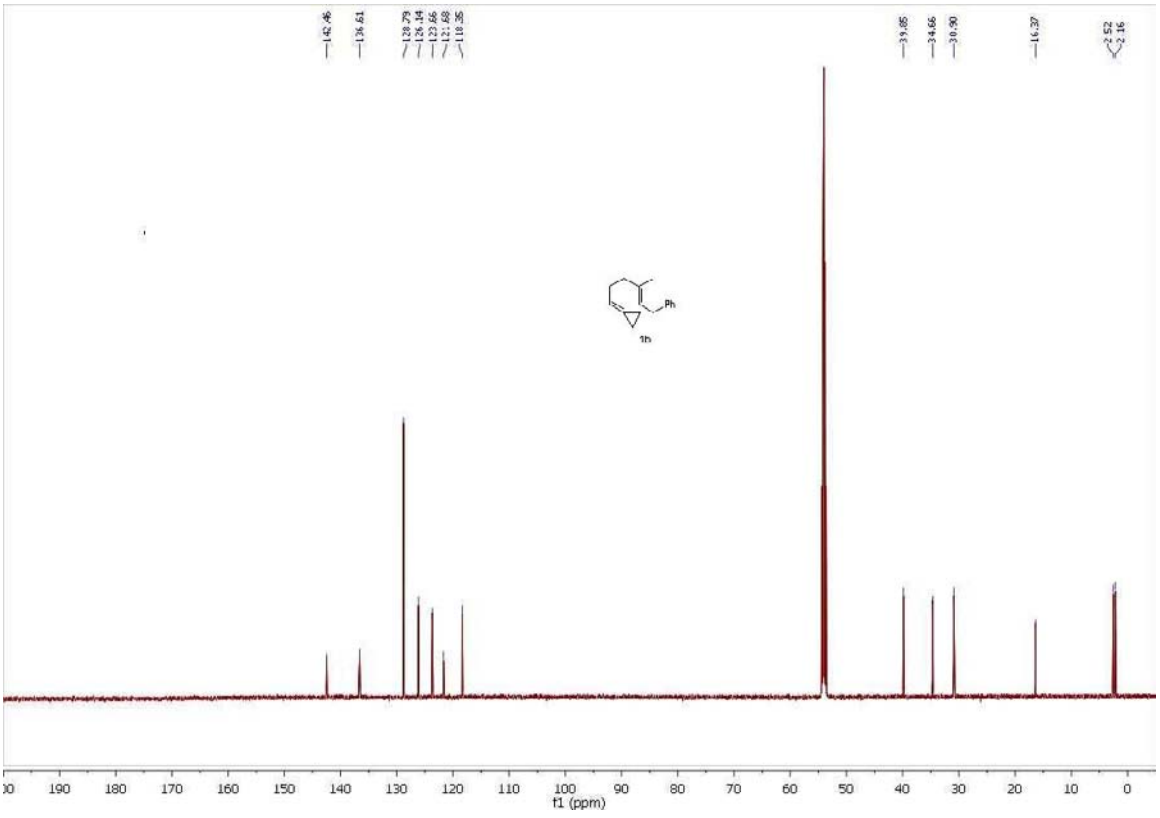
7.3 Hz, 1H), 5.23 (bs, 1H), 3.35 (d, J = 7.4, 2H), 2.19 (dt, J = 19.7 Hz, 7.2 Hz, 4H), 2.12-2.06 (m, 4H), 1.72 (s, 3H), 1.65 (p, J = 7.0 Hz, 2H), 1.58 (p, J = 6.8 Hz, 2H); **^{13}C-NMR** (150 MHz, CD_2Cl_2) δ 143.5, 142.3, 136.6, 128.6, 128.6, 125.9, 123.3, 120.0, 39.9, 34.5, 33.9, 28.8, 28.5, 26.8 26.7, 16.2.

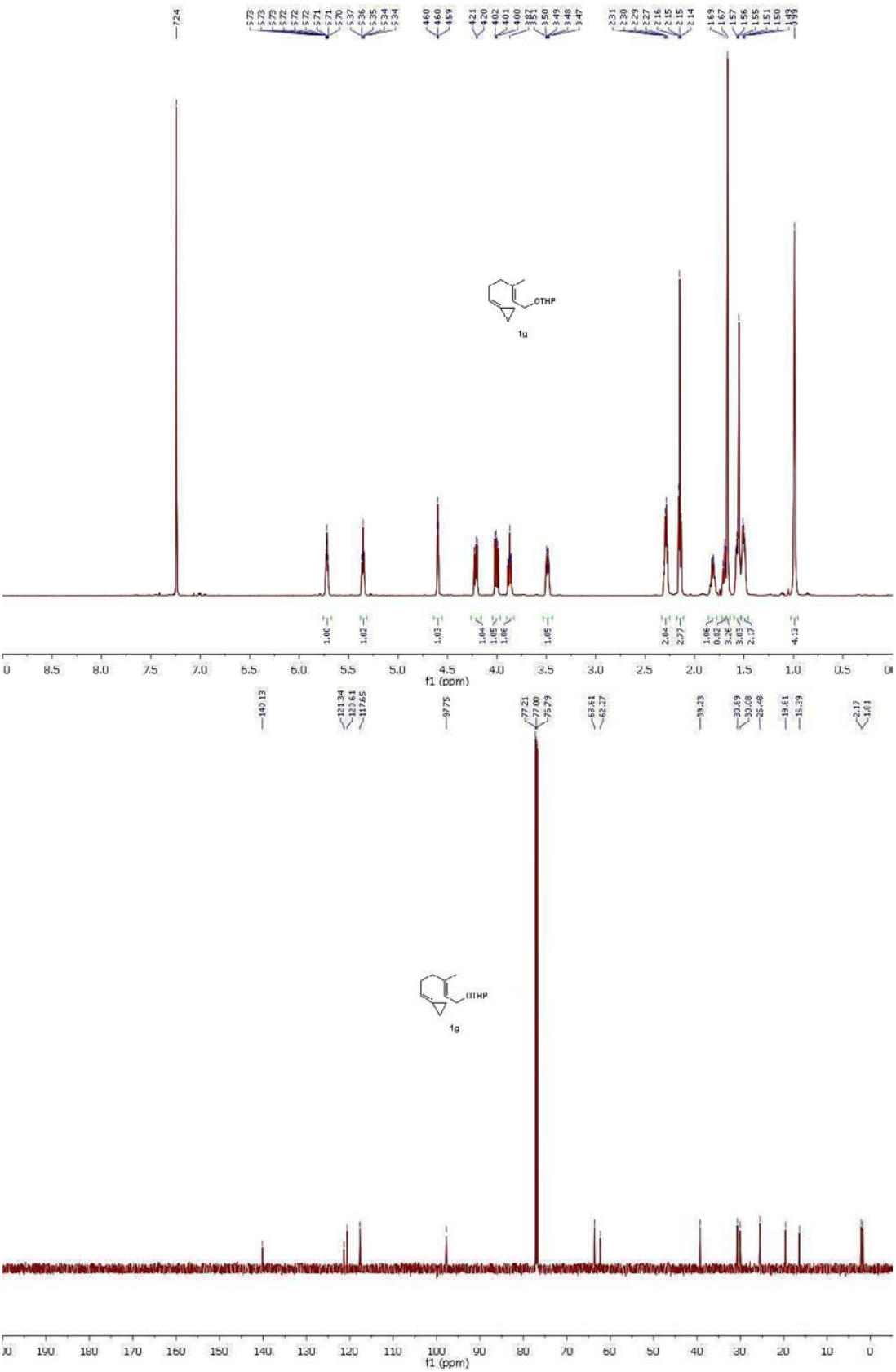
4. NMR Spectra. It should be noted that n-hexane is an impurity in the NMR spectra of many of the Cope rearranged product. In most cases the trace amount of hexanes could not be removed even with repeated trituration with the deuterated NMR solvent. This impurity comes with a multiplet at δ 1.35-1.25 ppm and what appears to be a triplet at δ 0.90 ppm. The n-hexane signals are most easily seen and proven to be an impurity by the HSQC included with the spectra of **2b**.

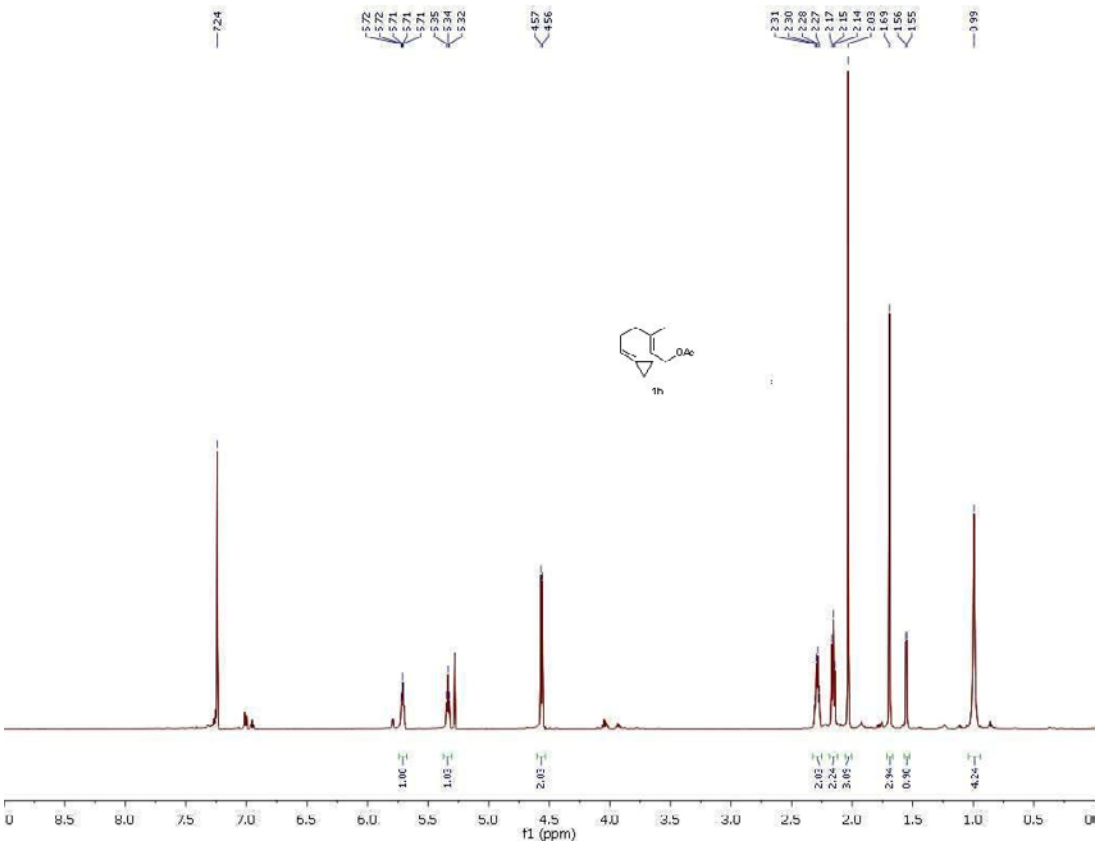


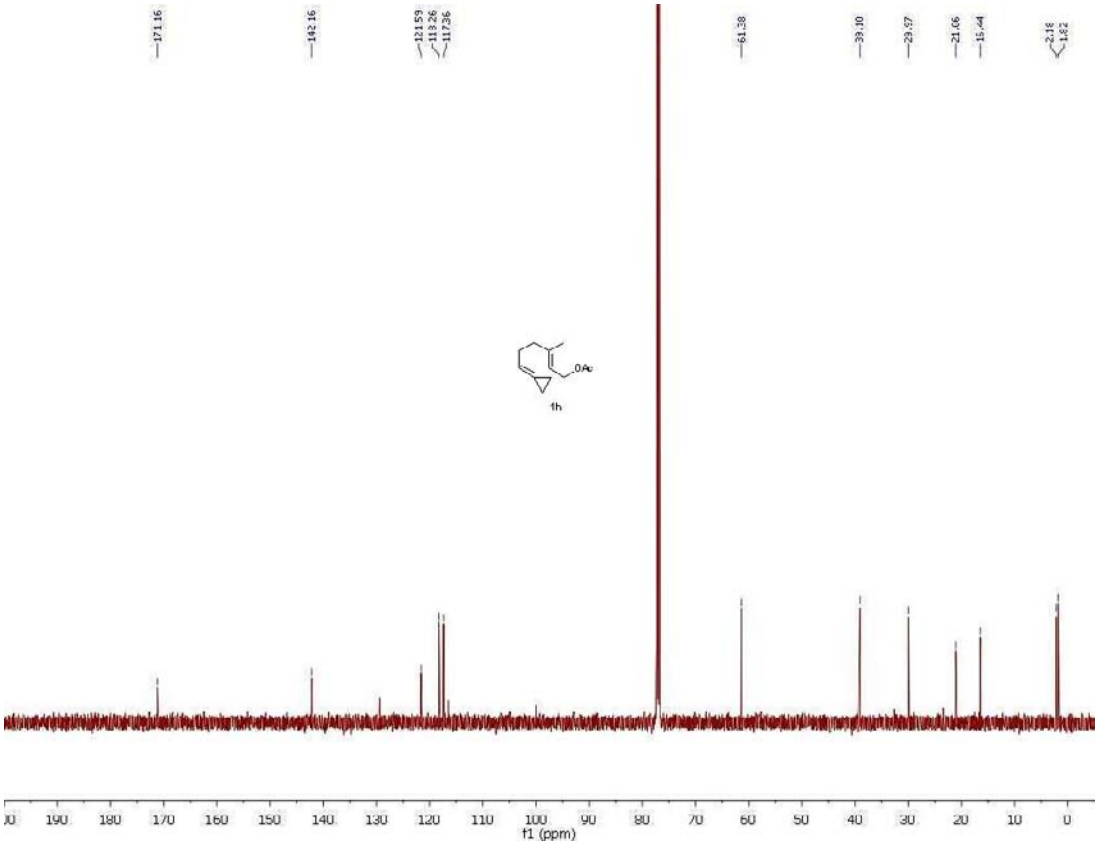


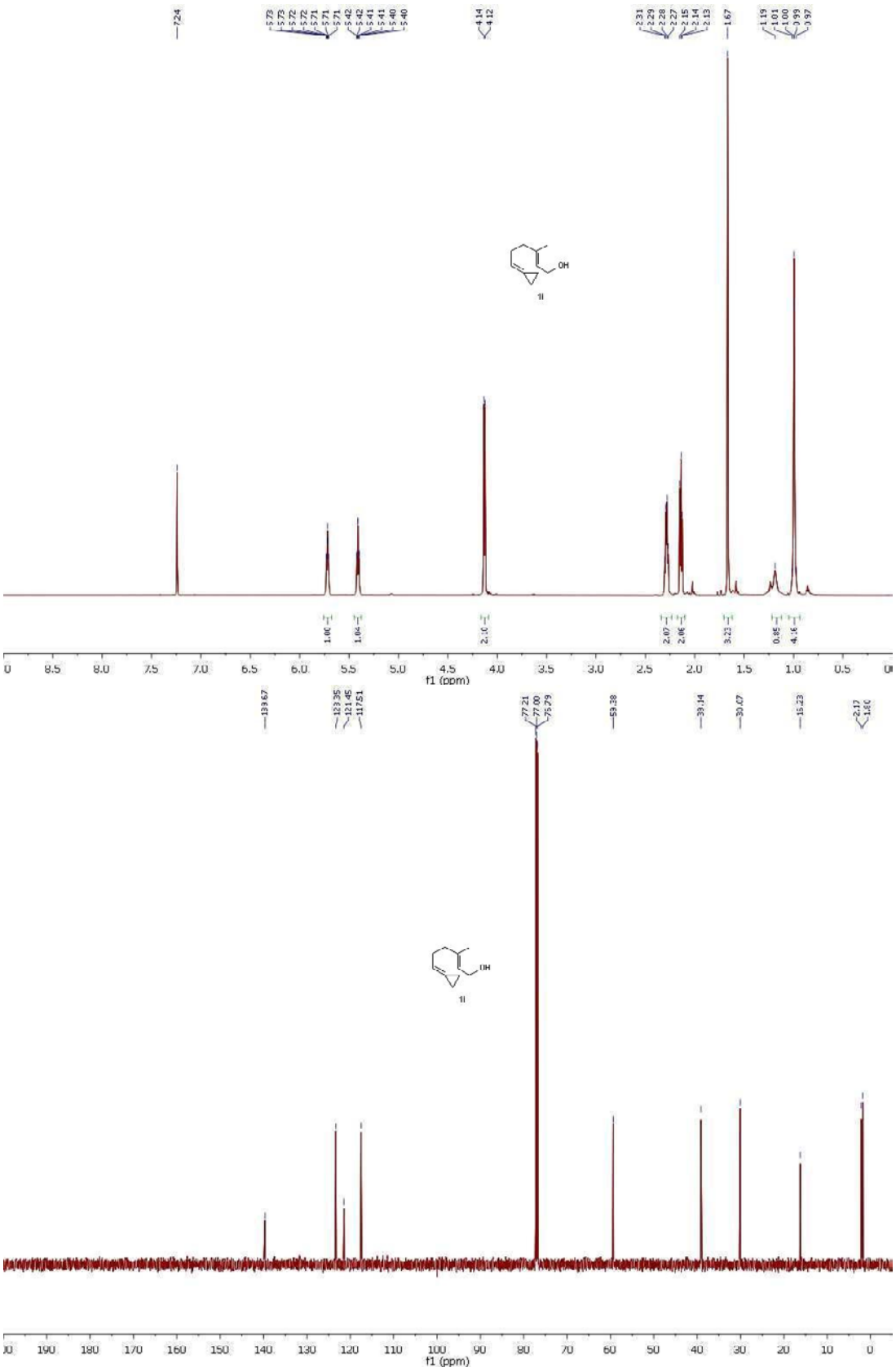


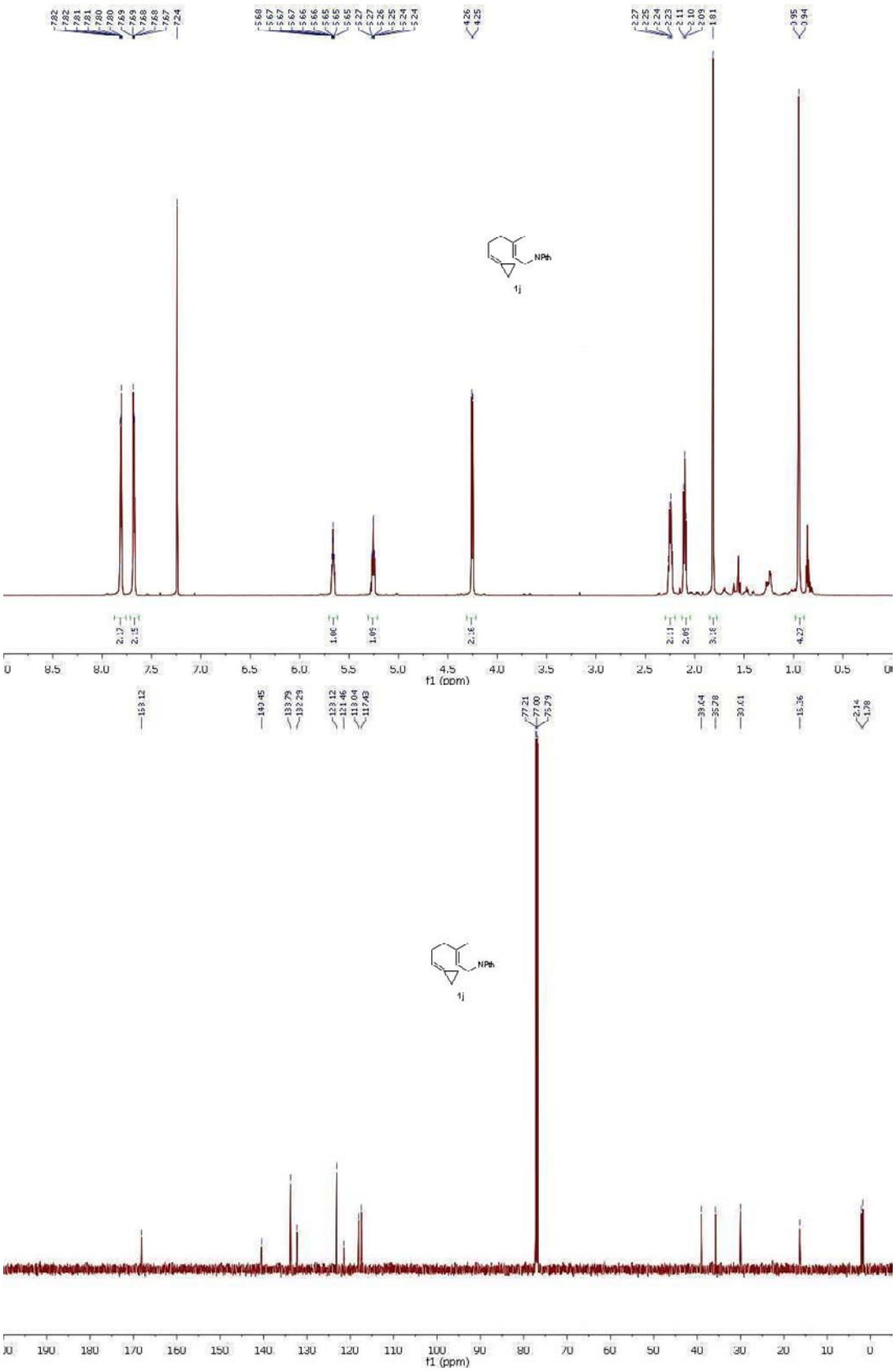


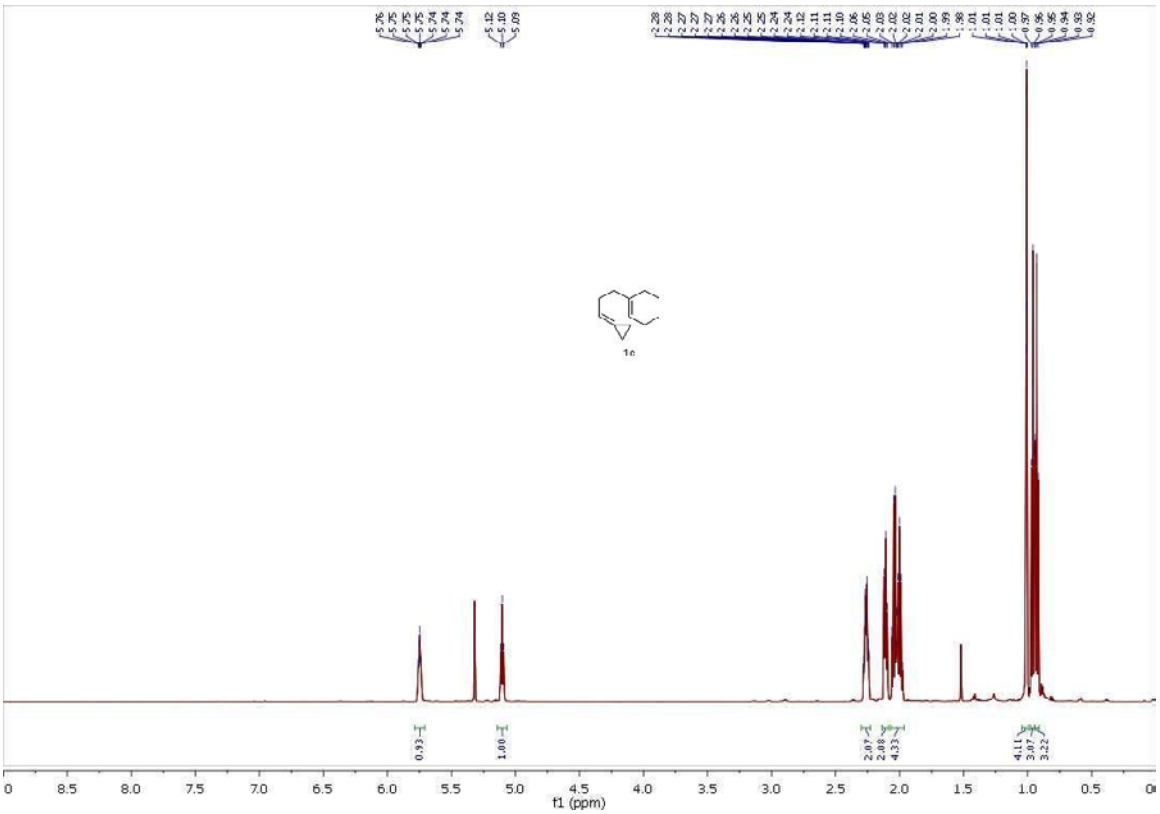


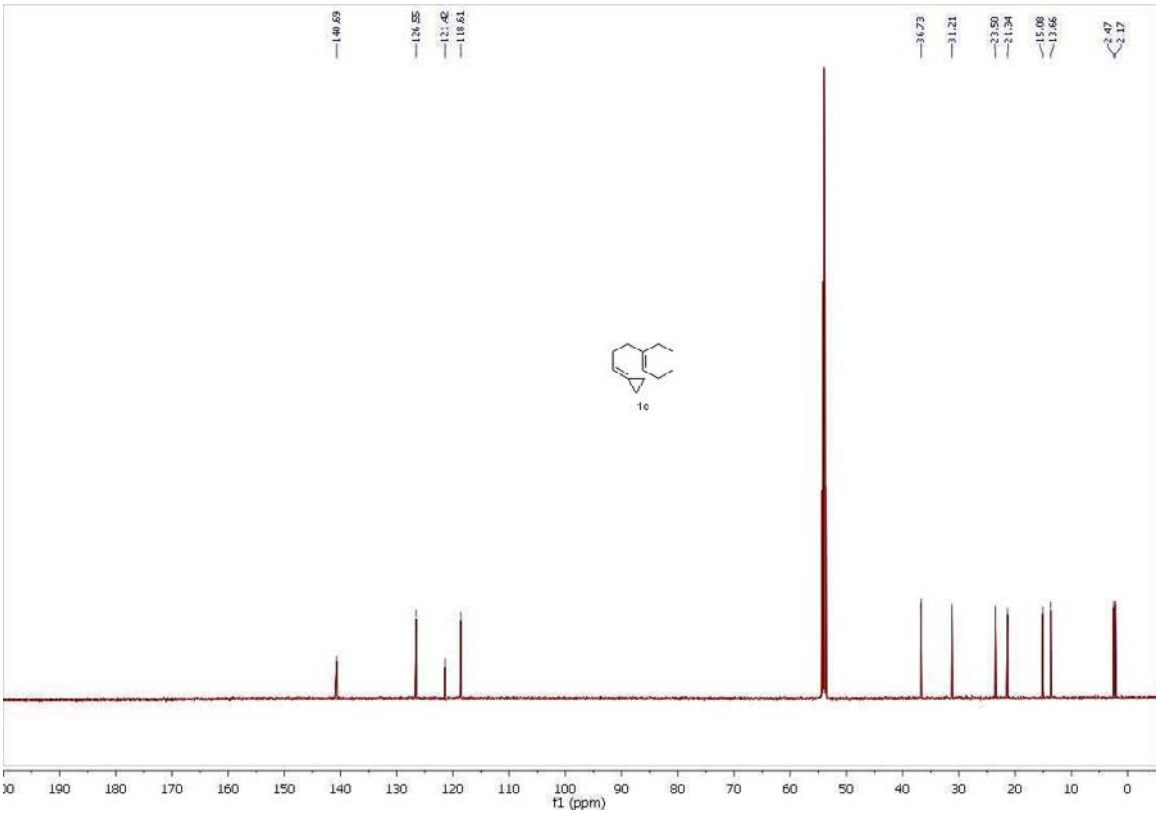


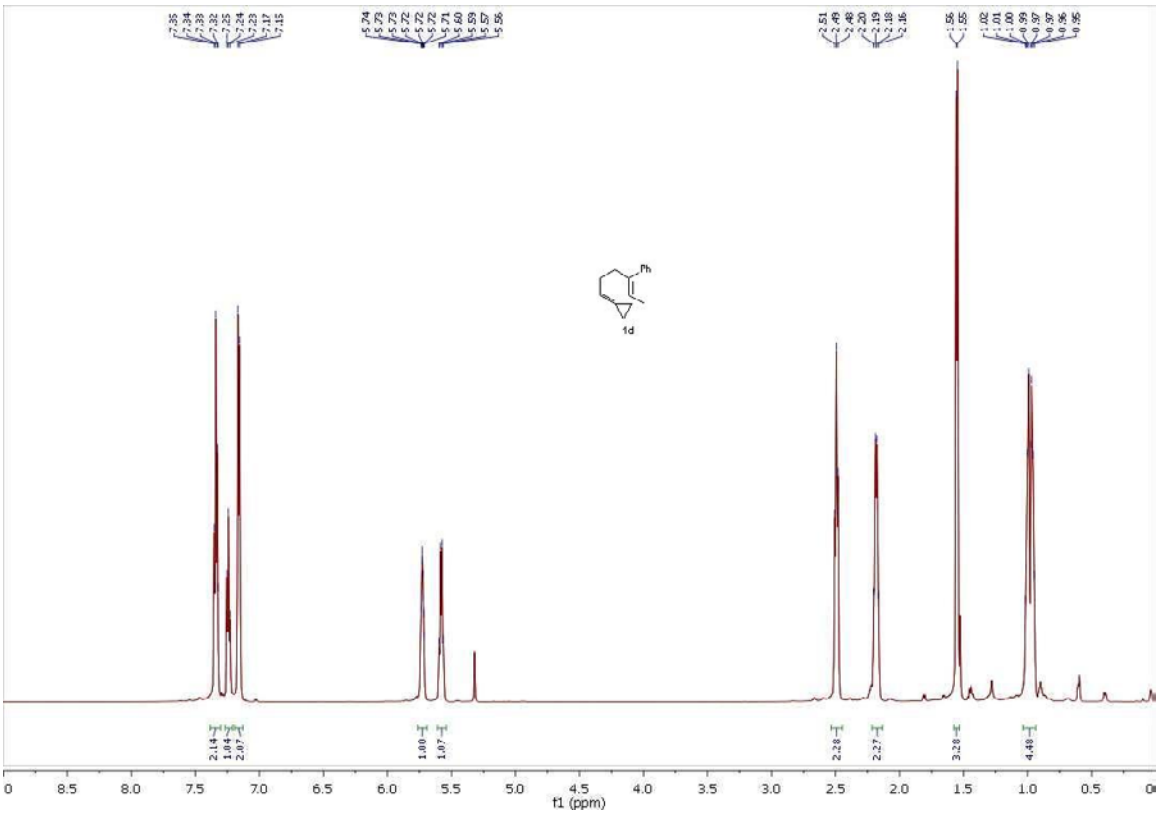


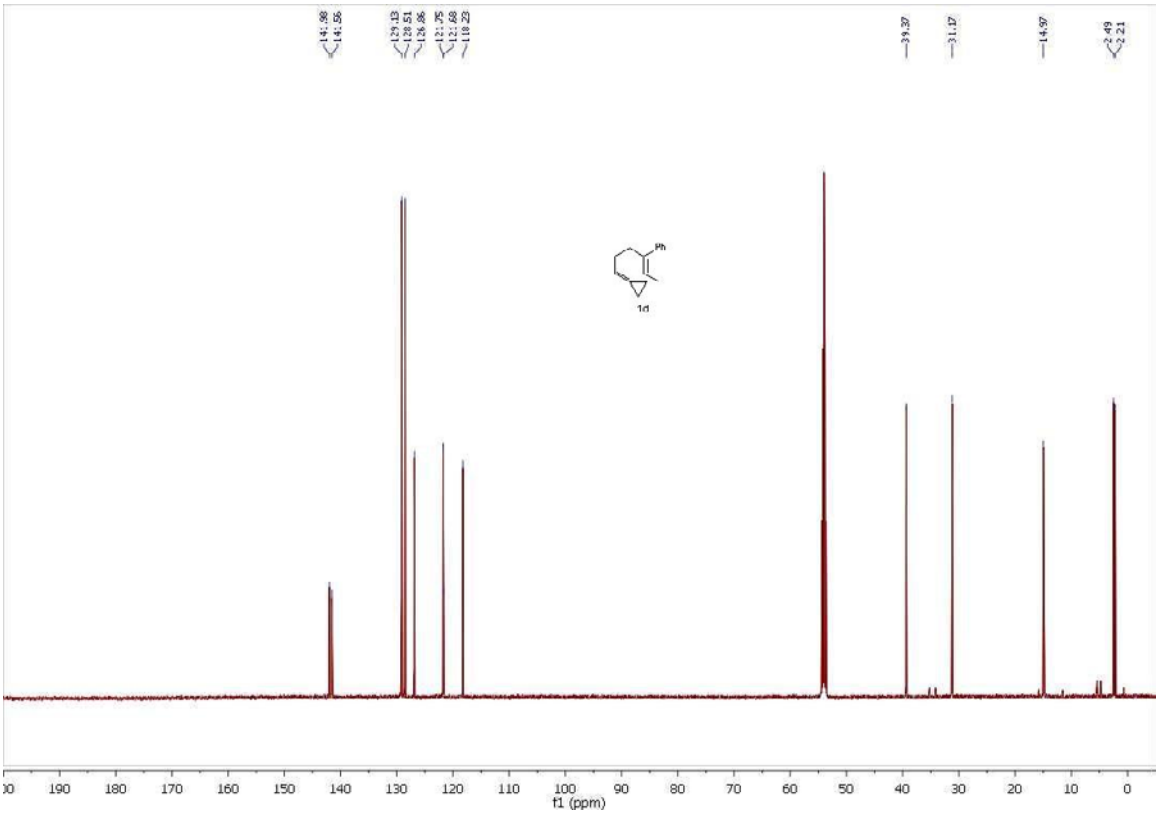


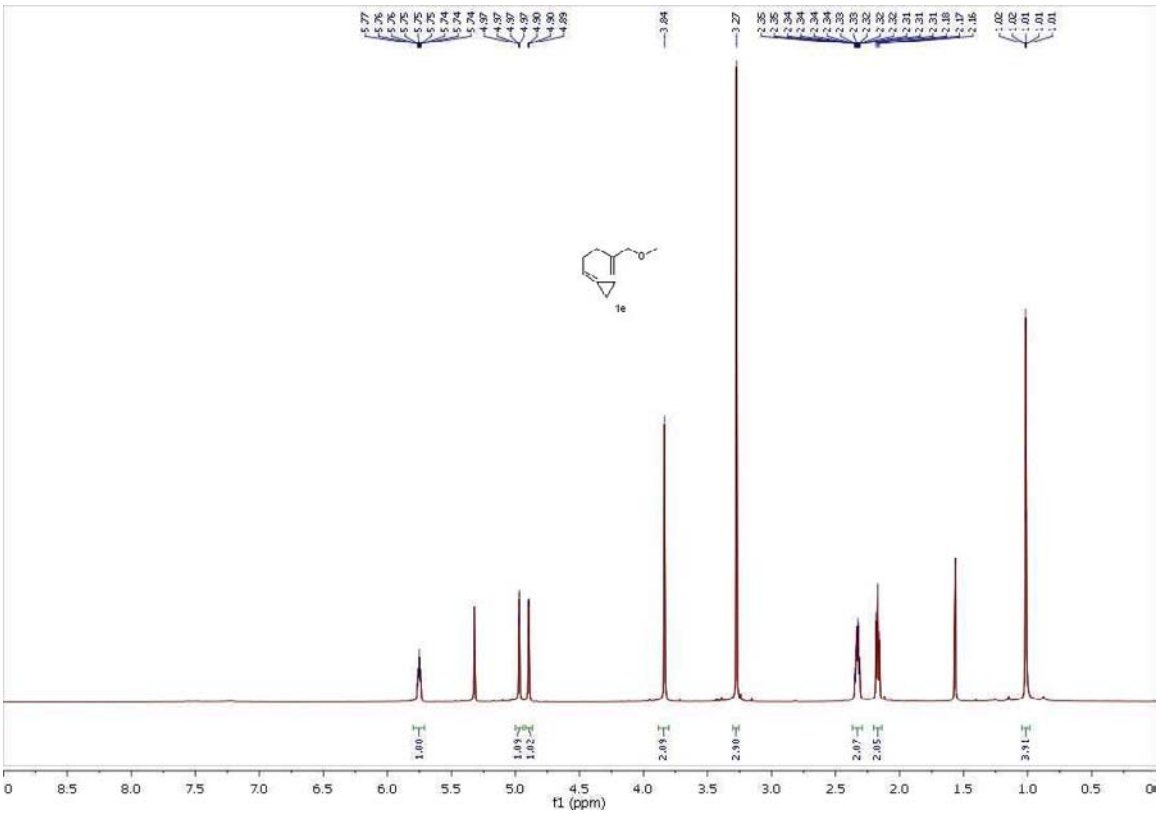


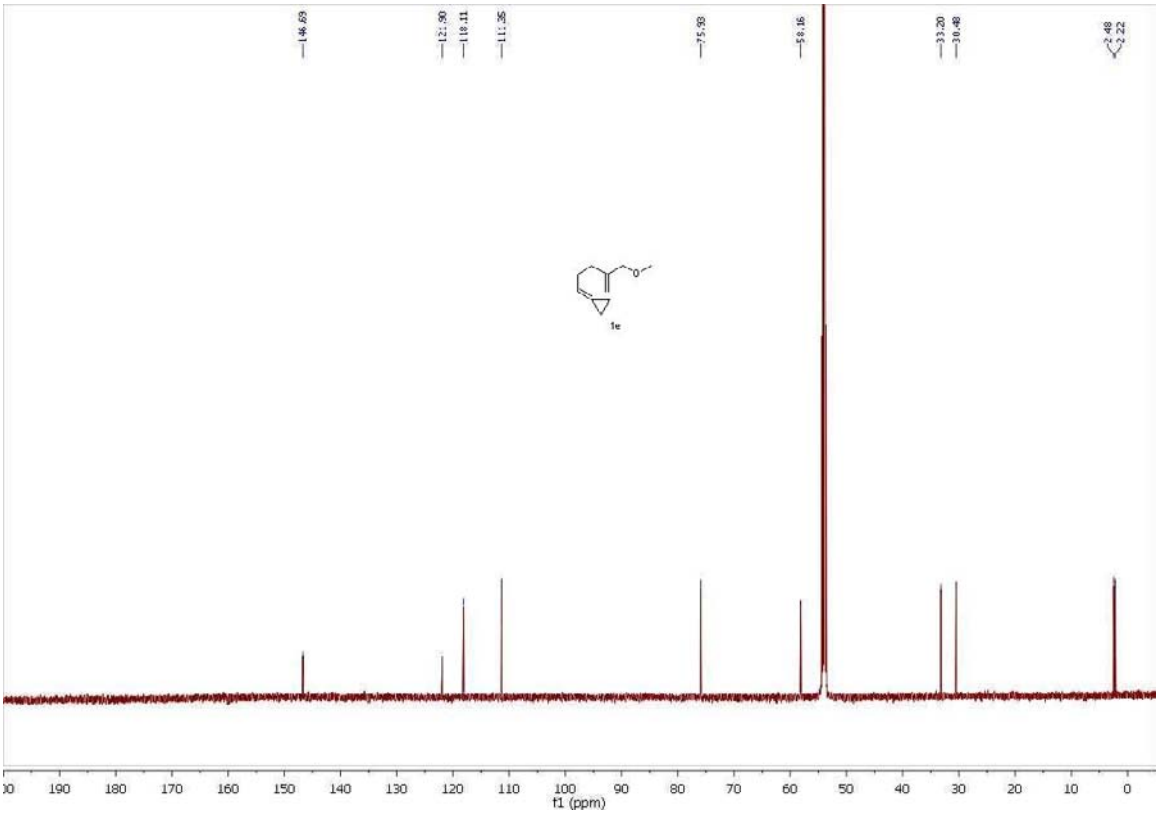


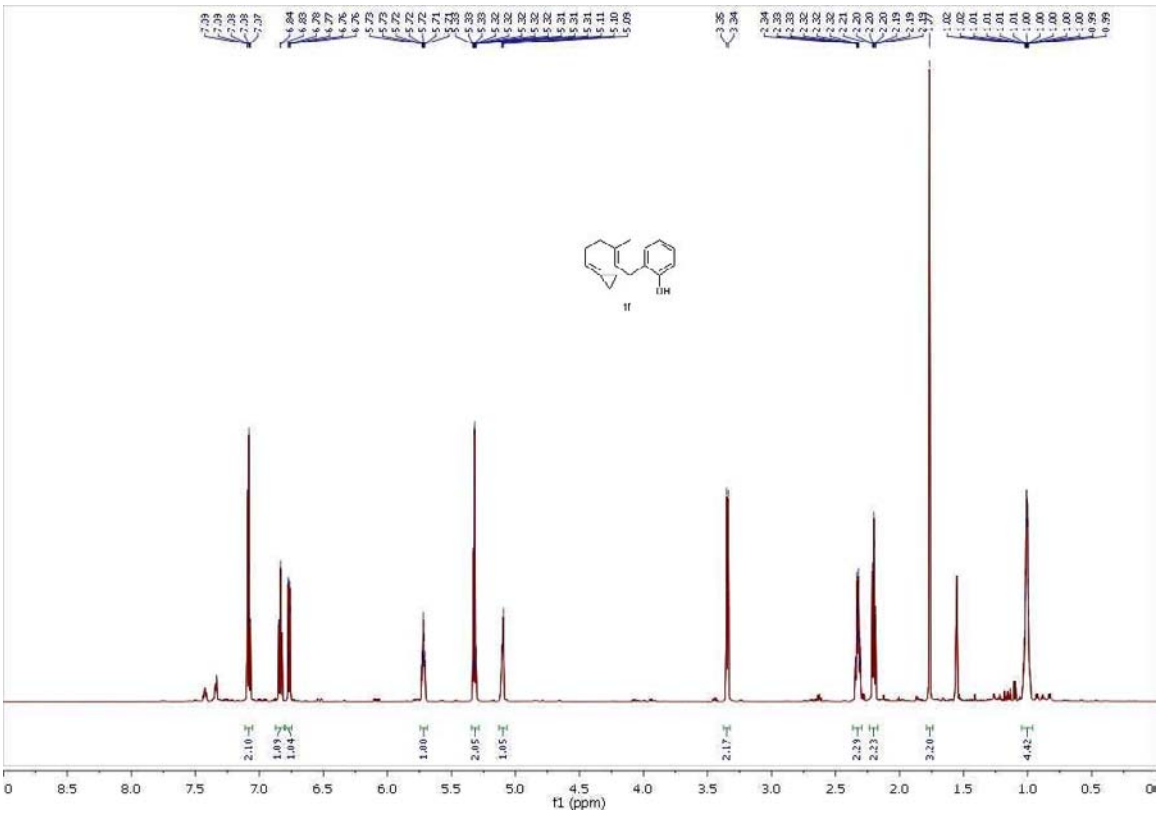


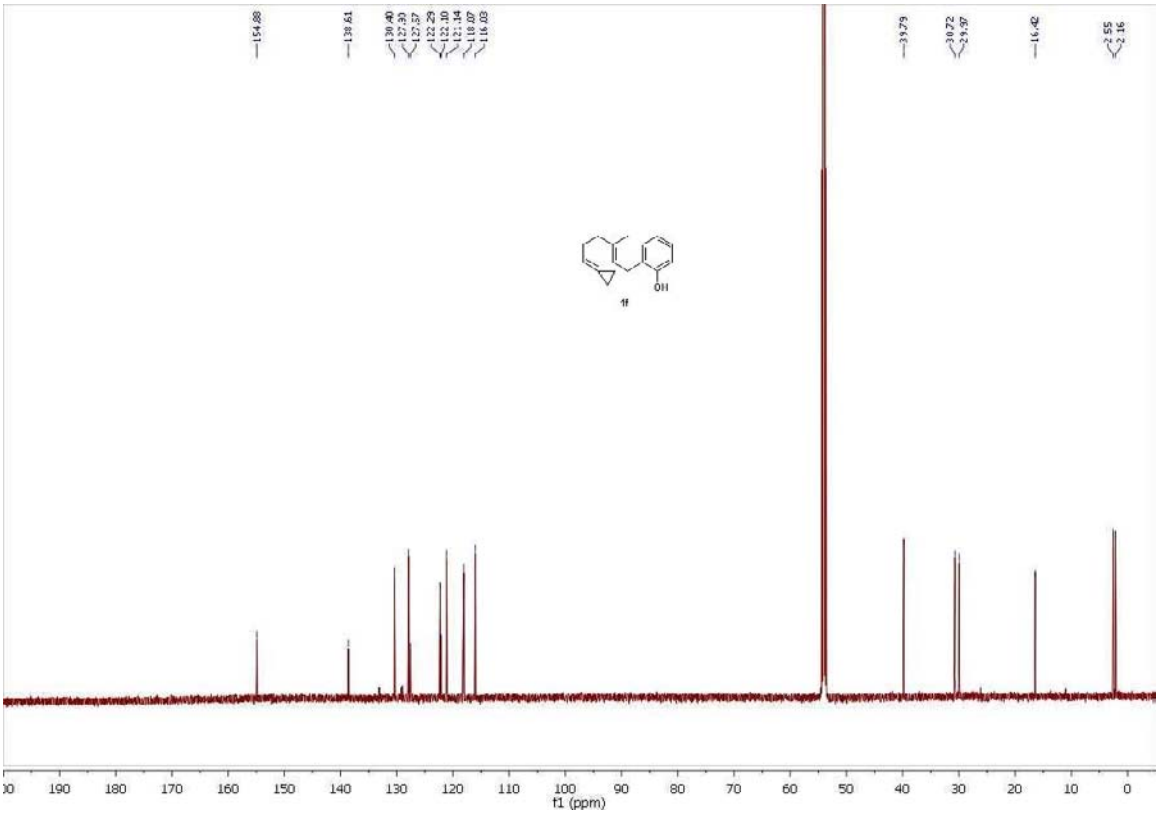


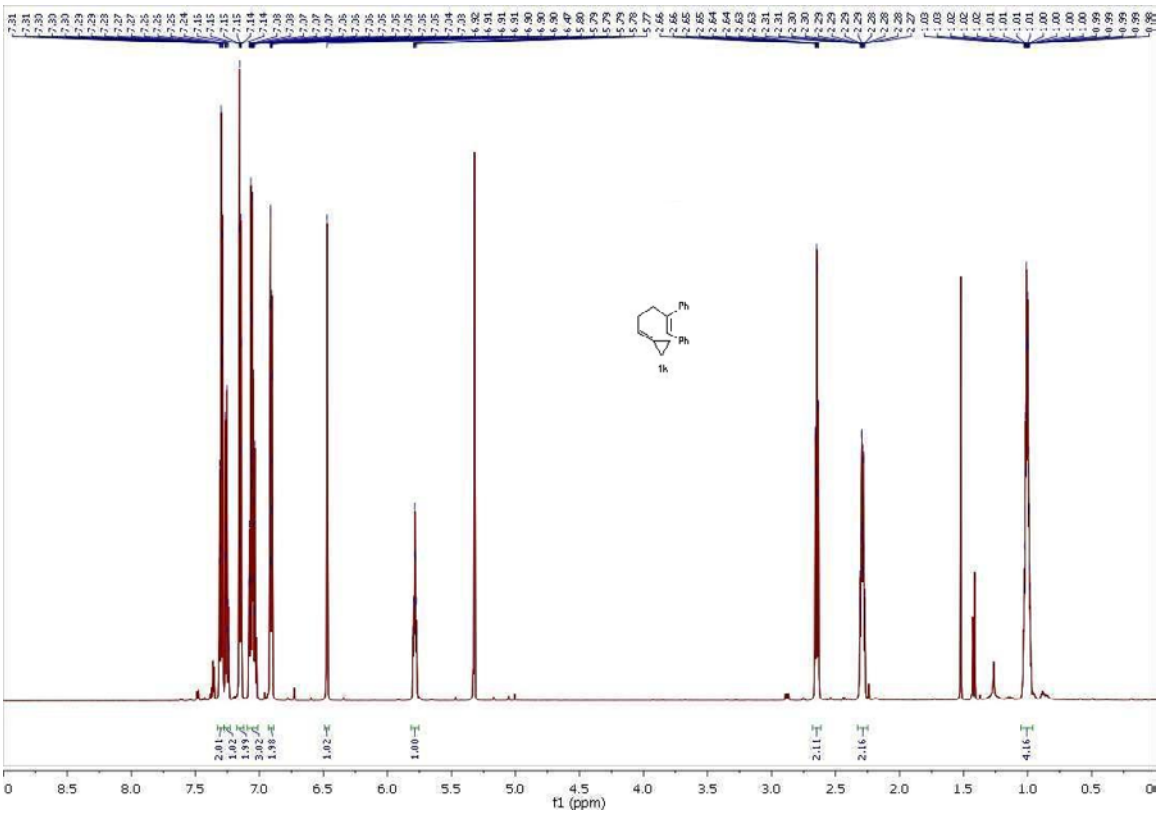


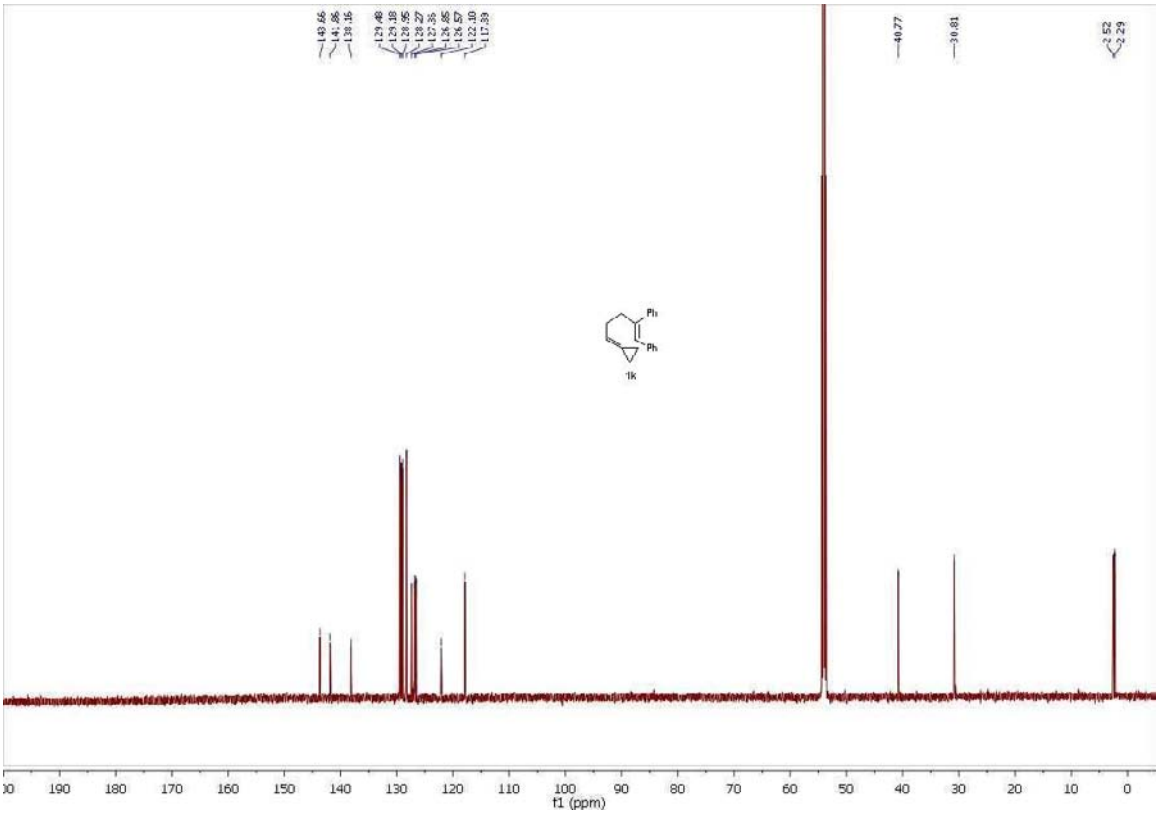


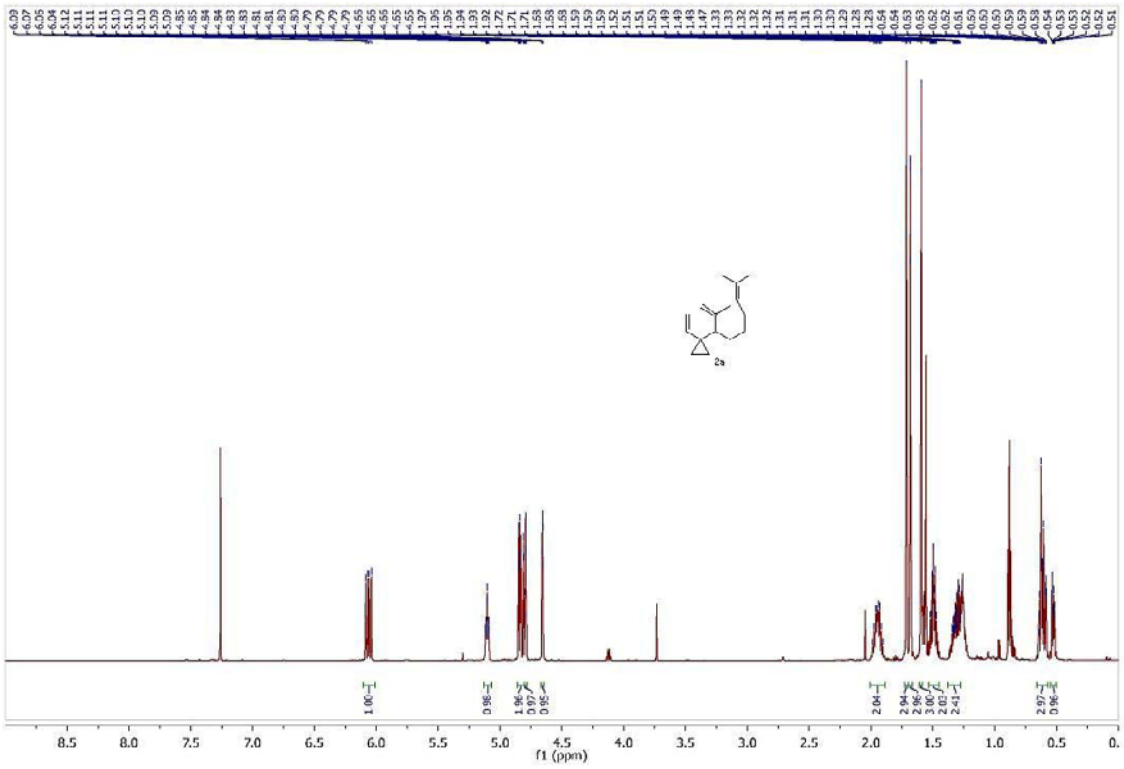


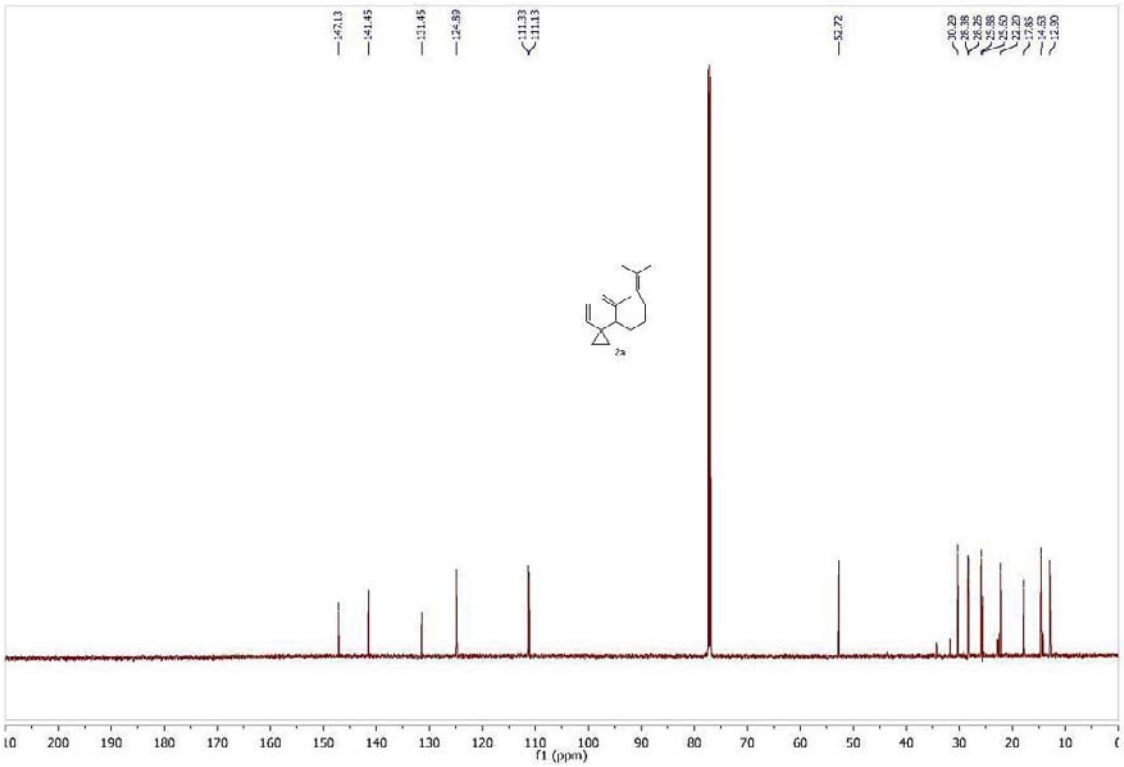


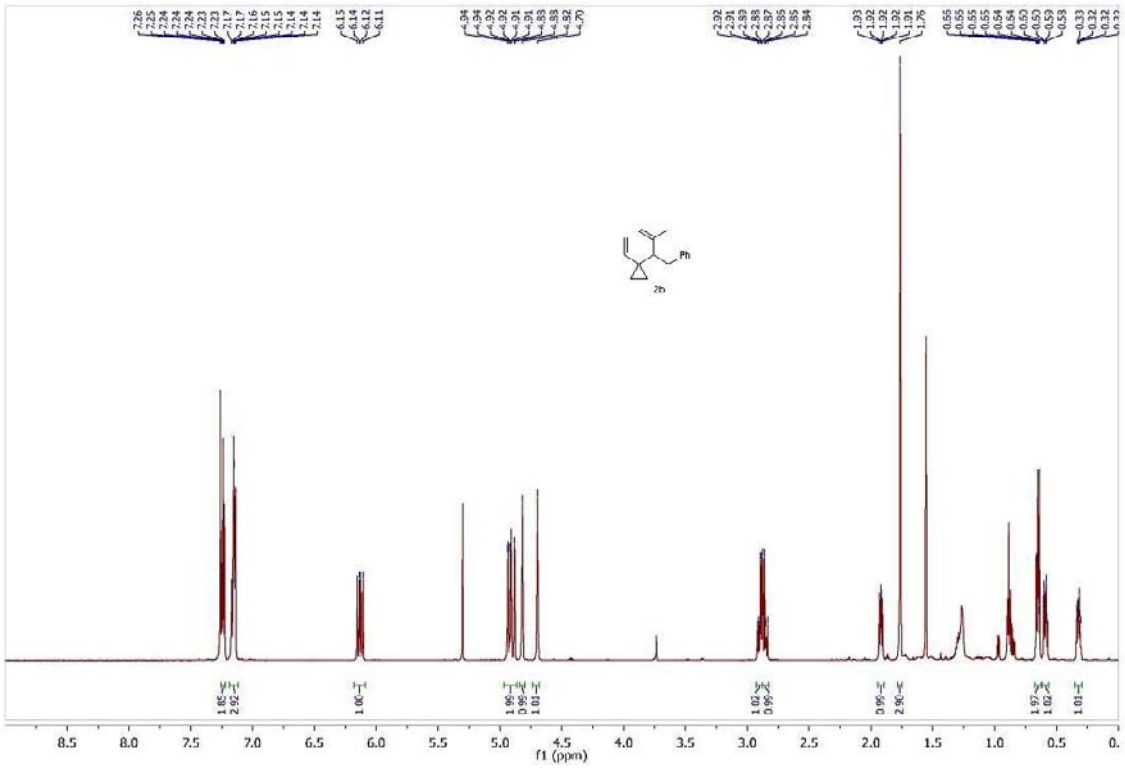


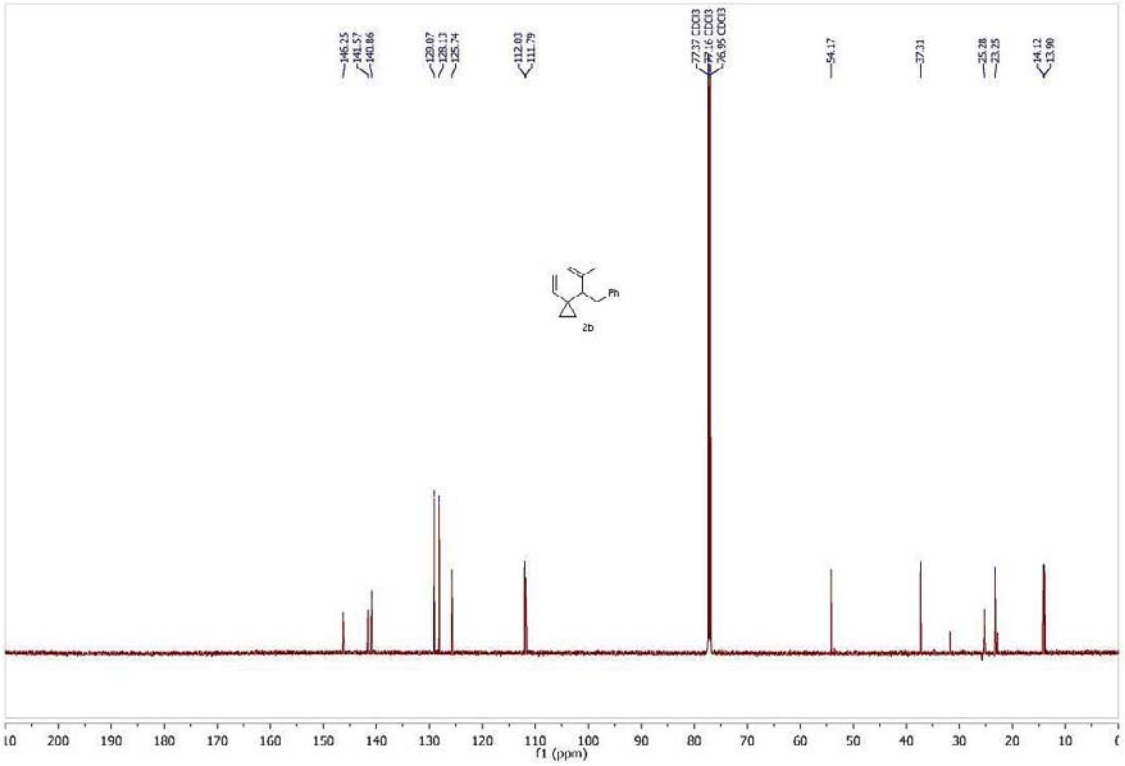


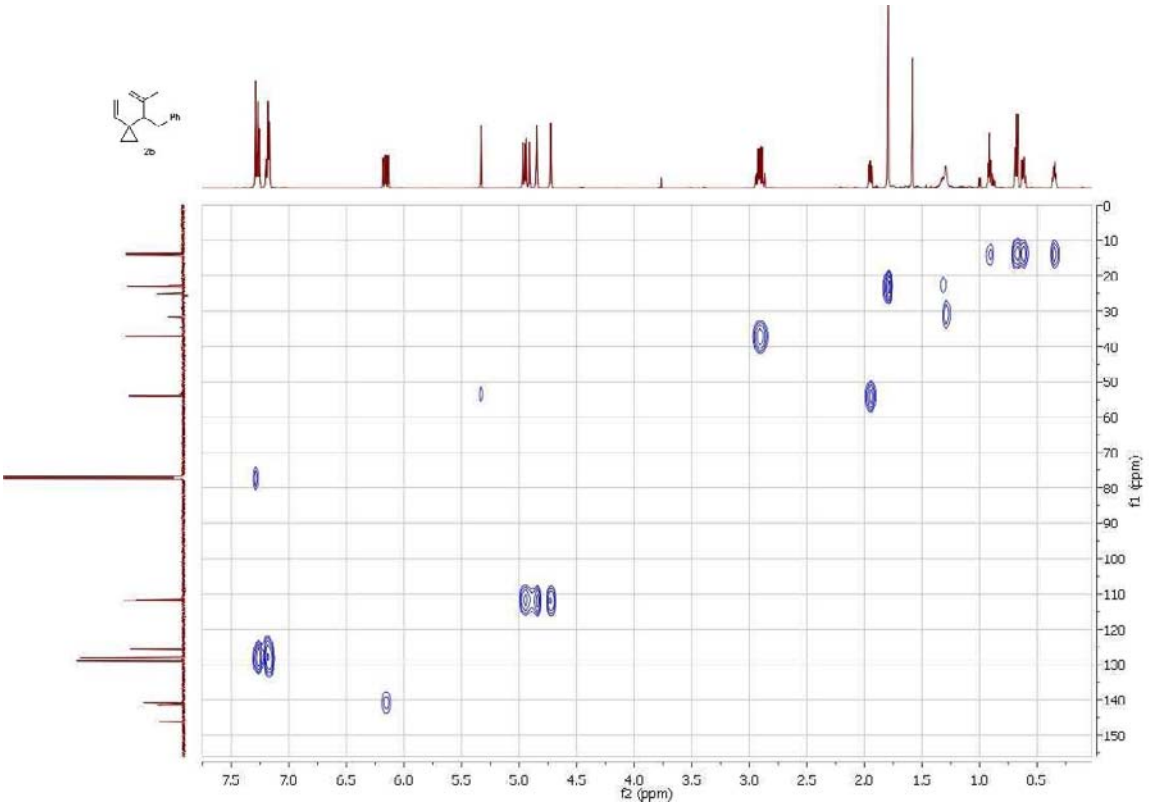


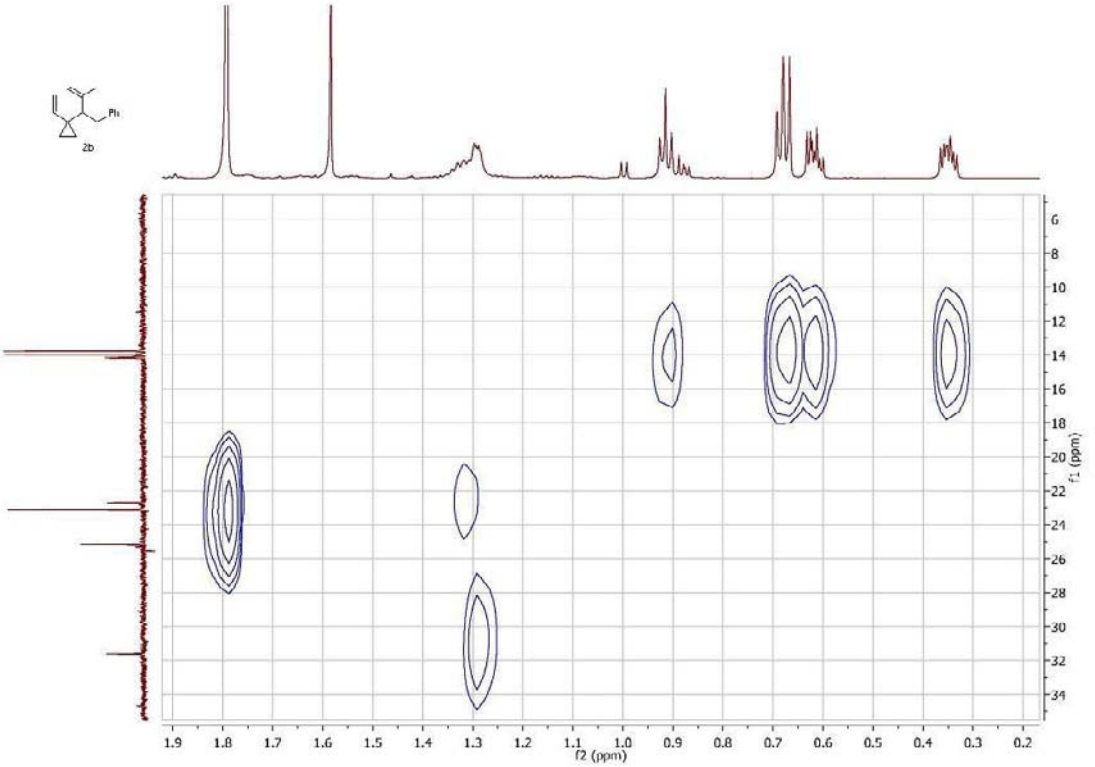


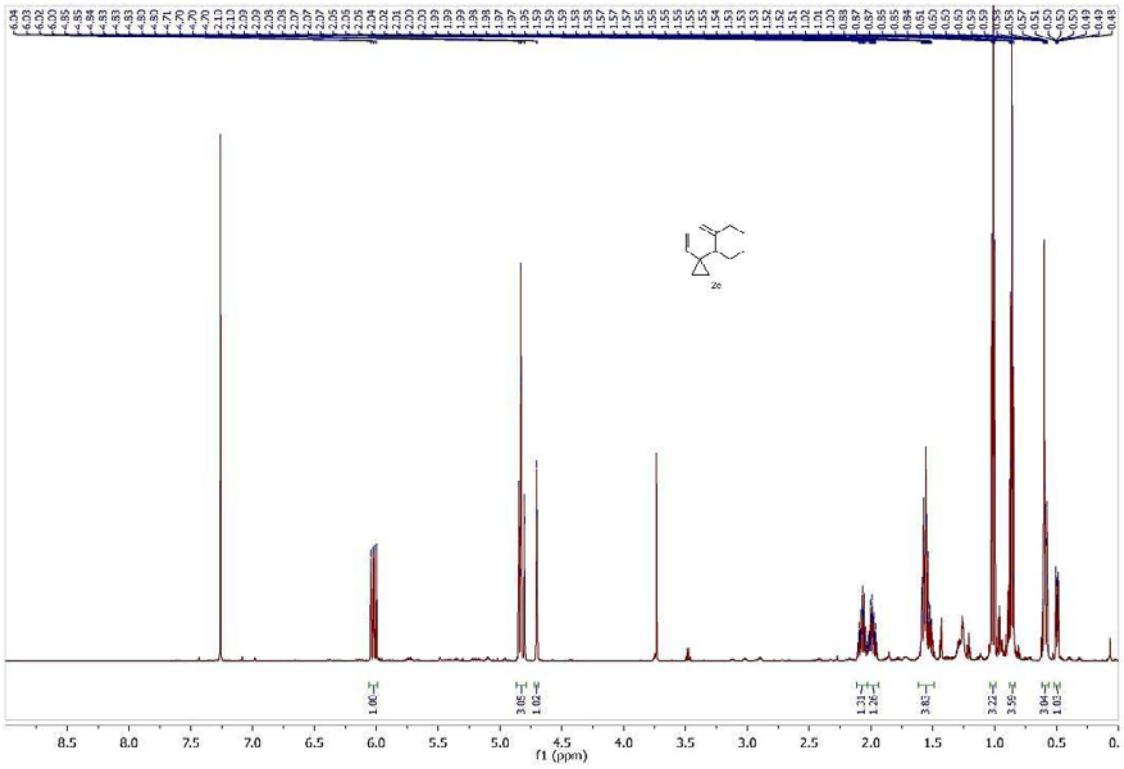


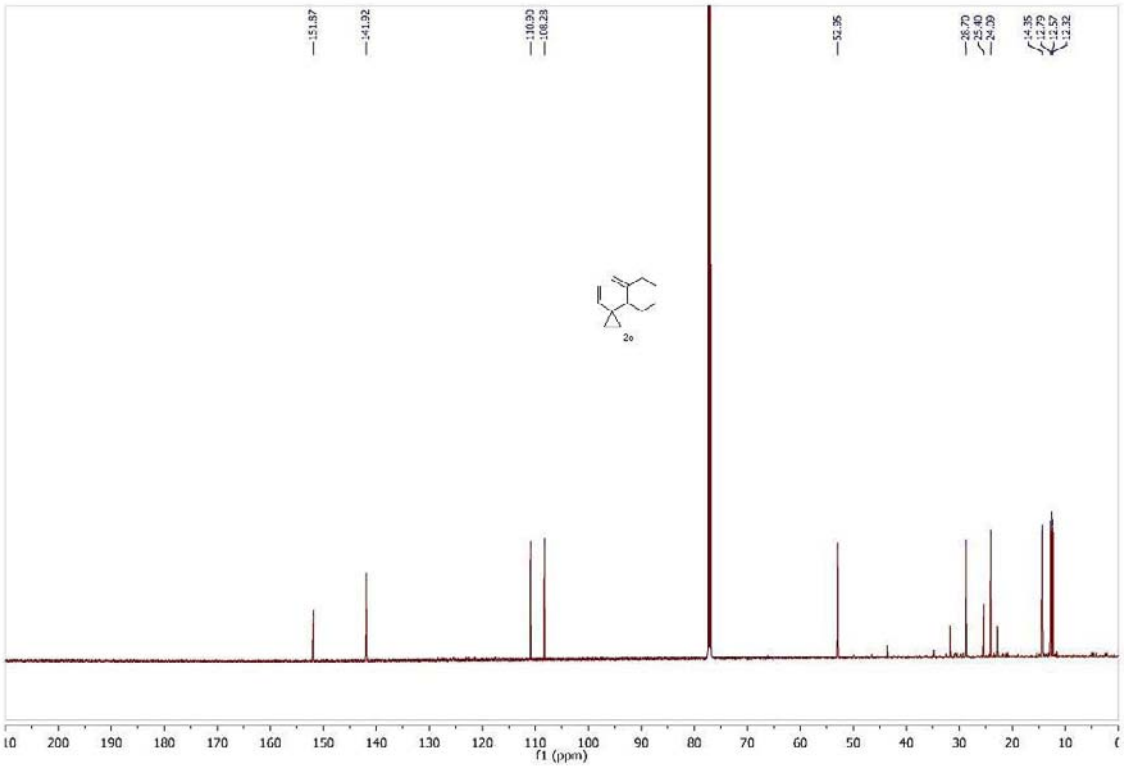


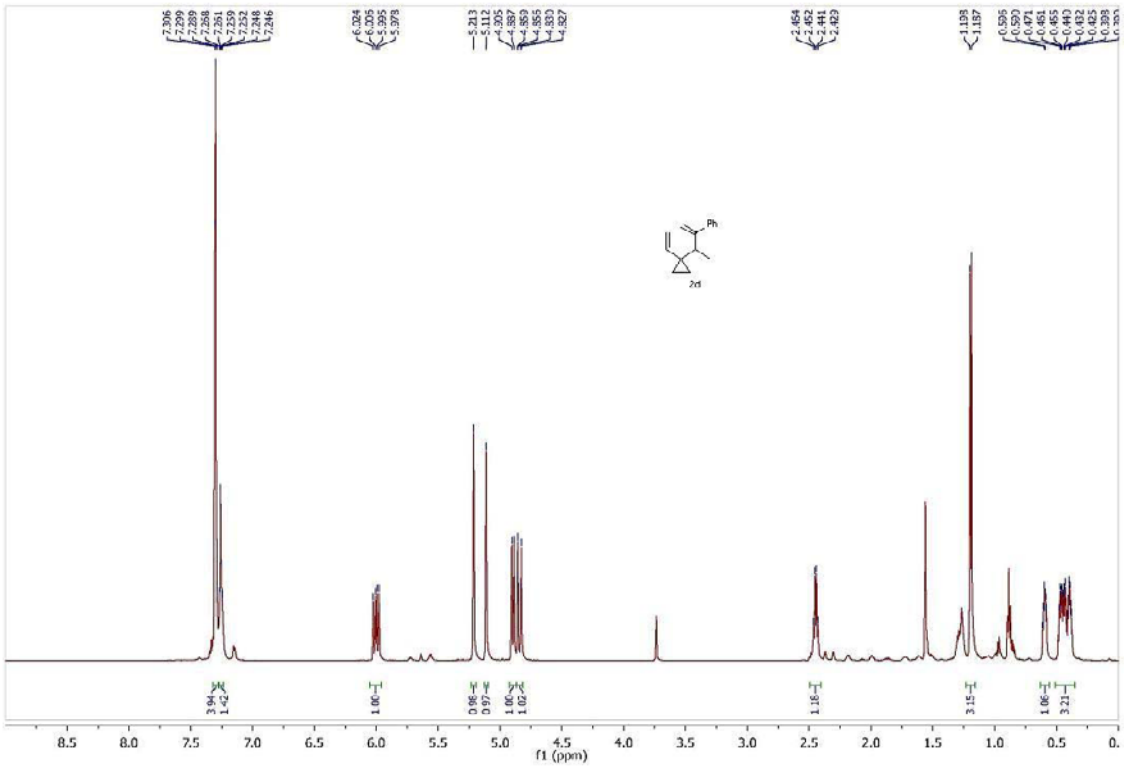


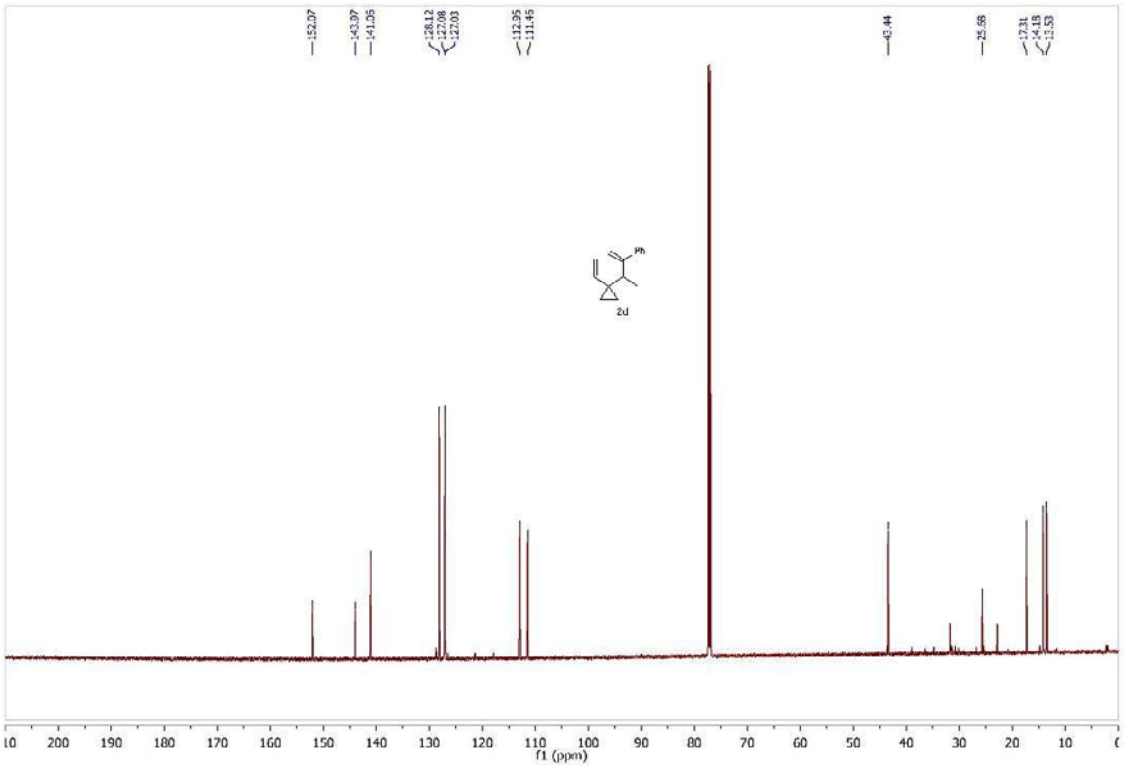


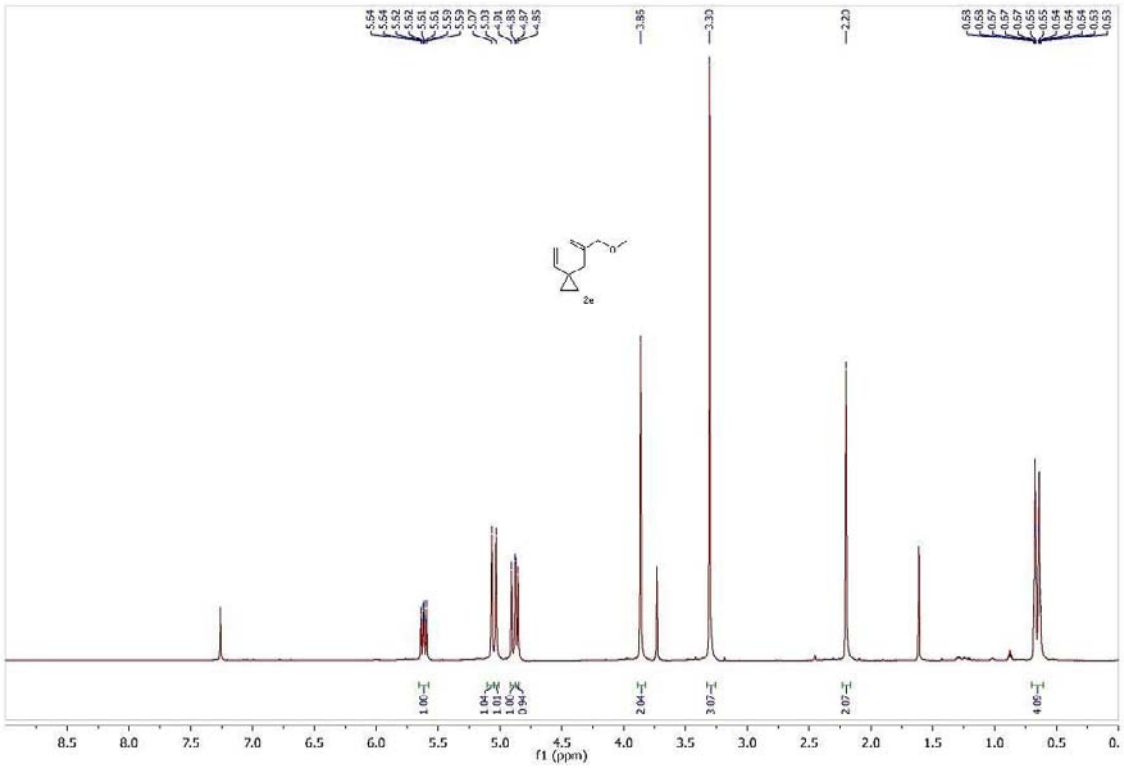


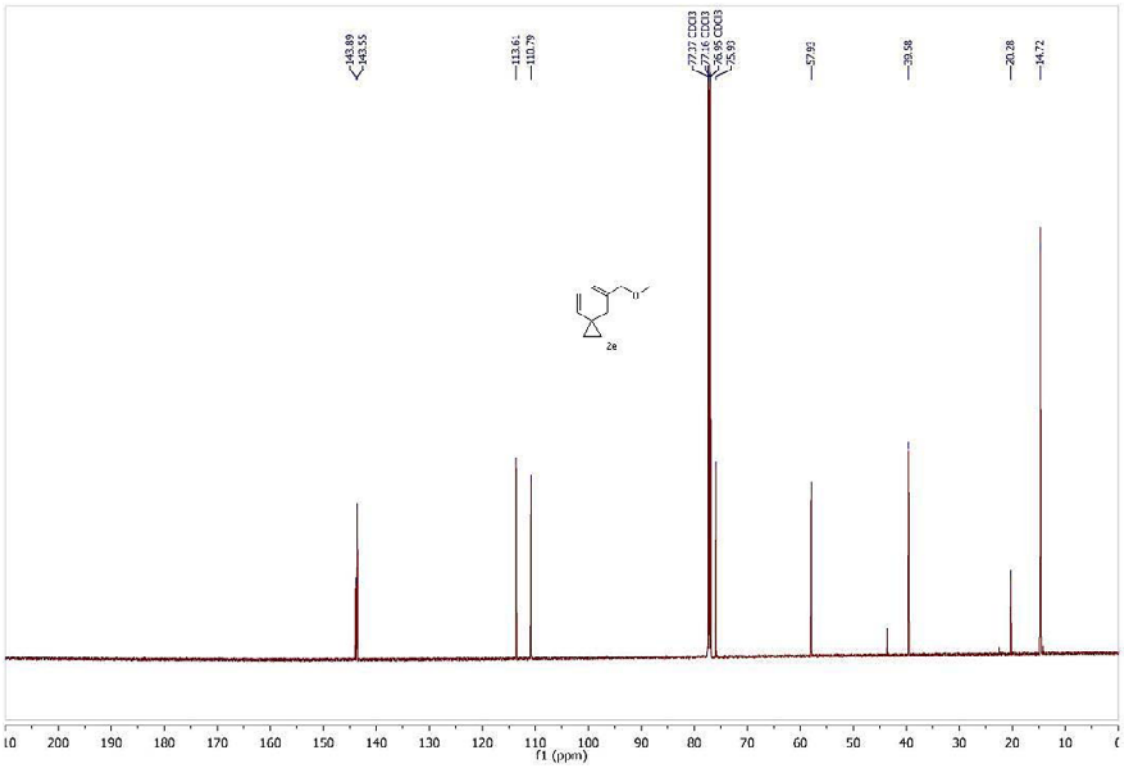


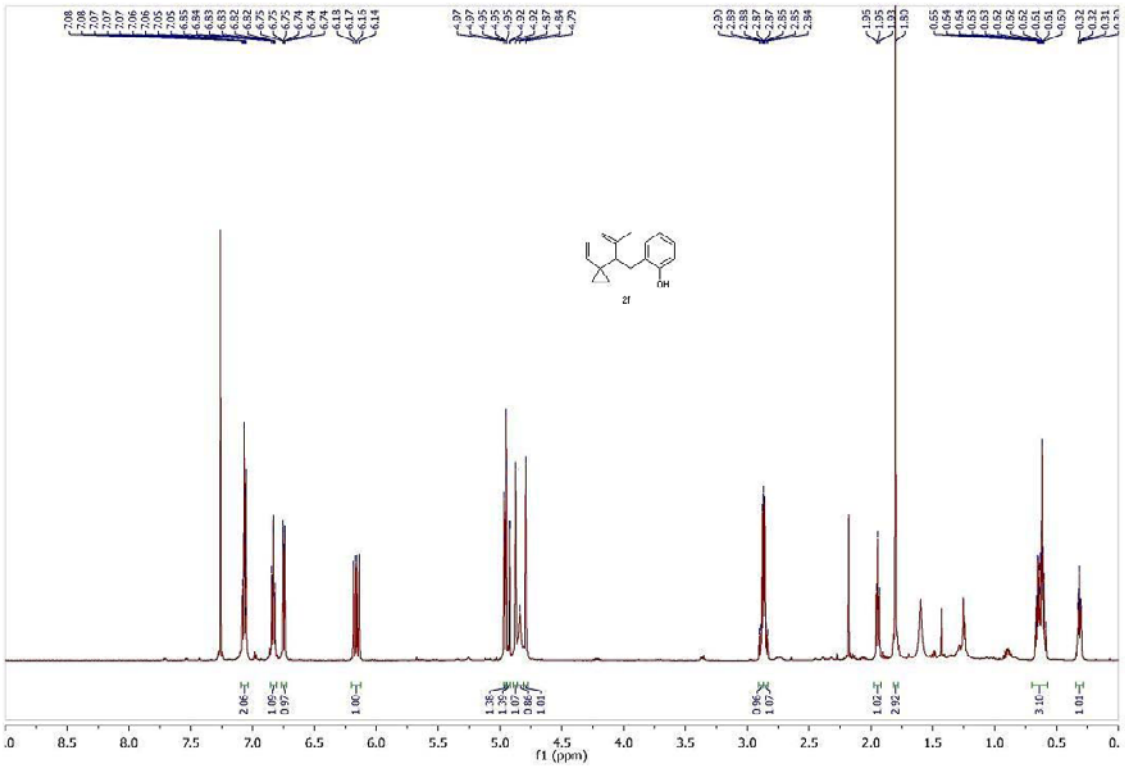


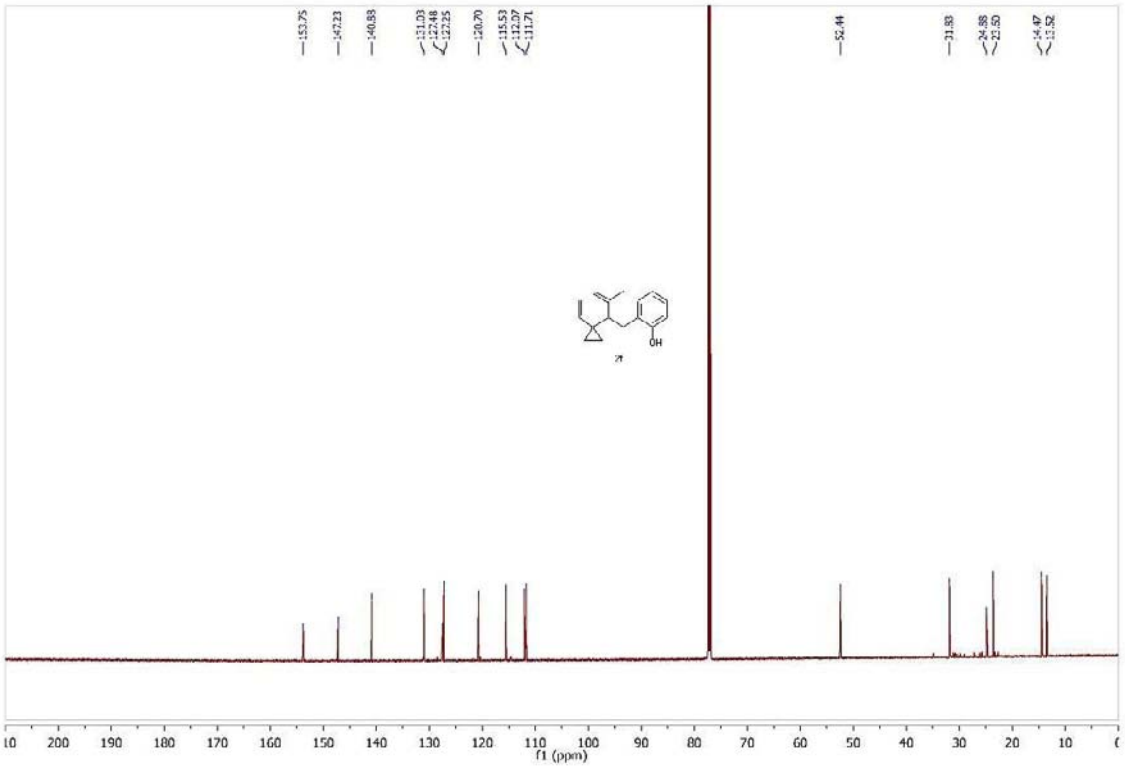


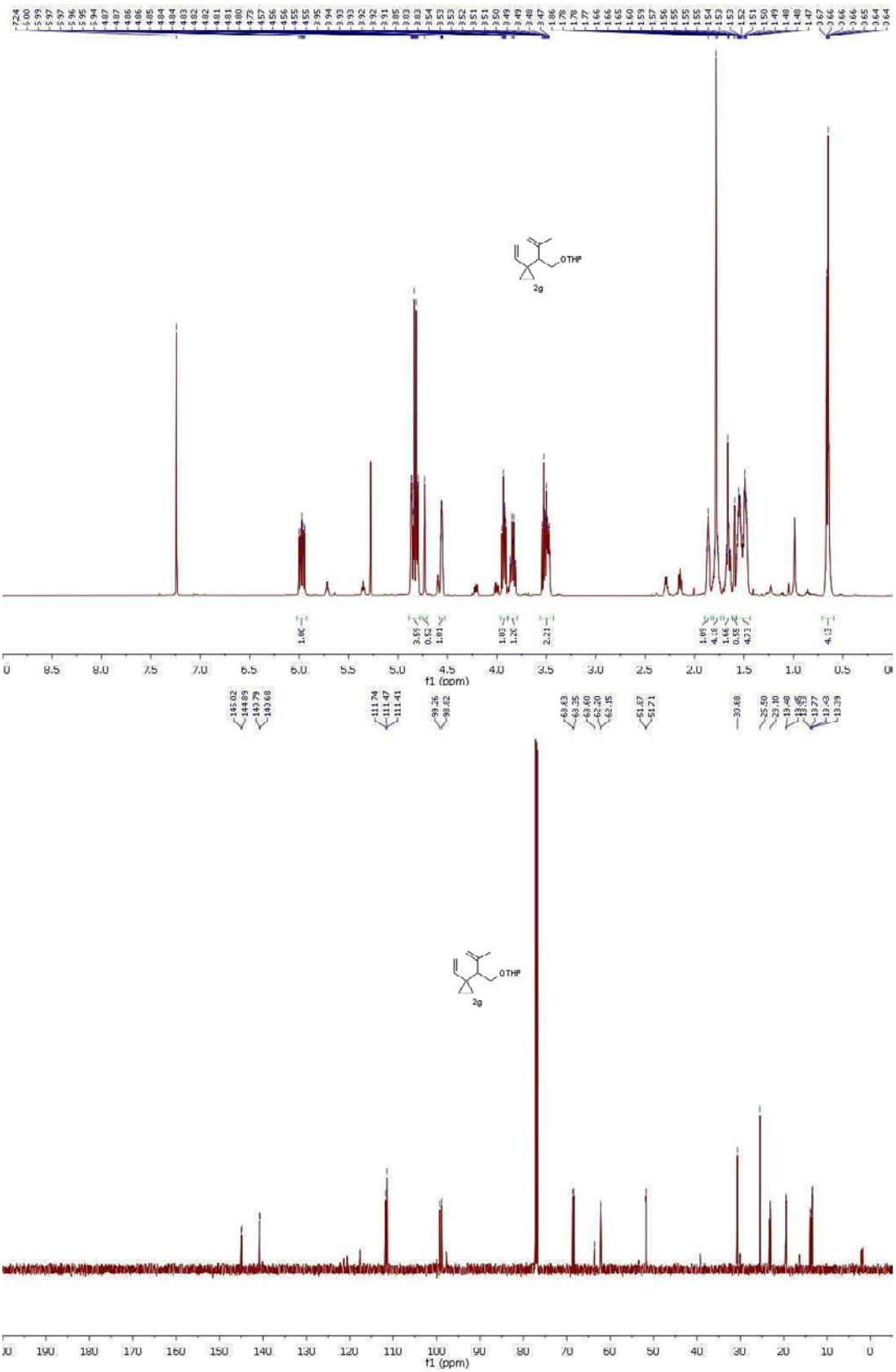


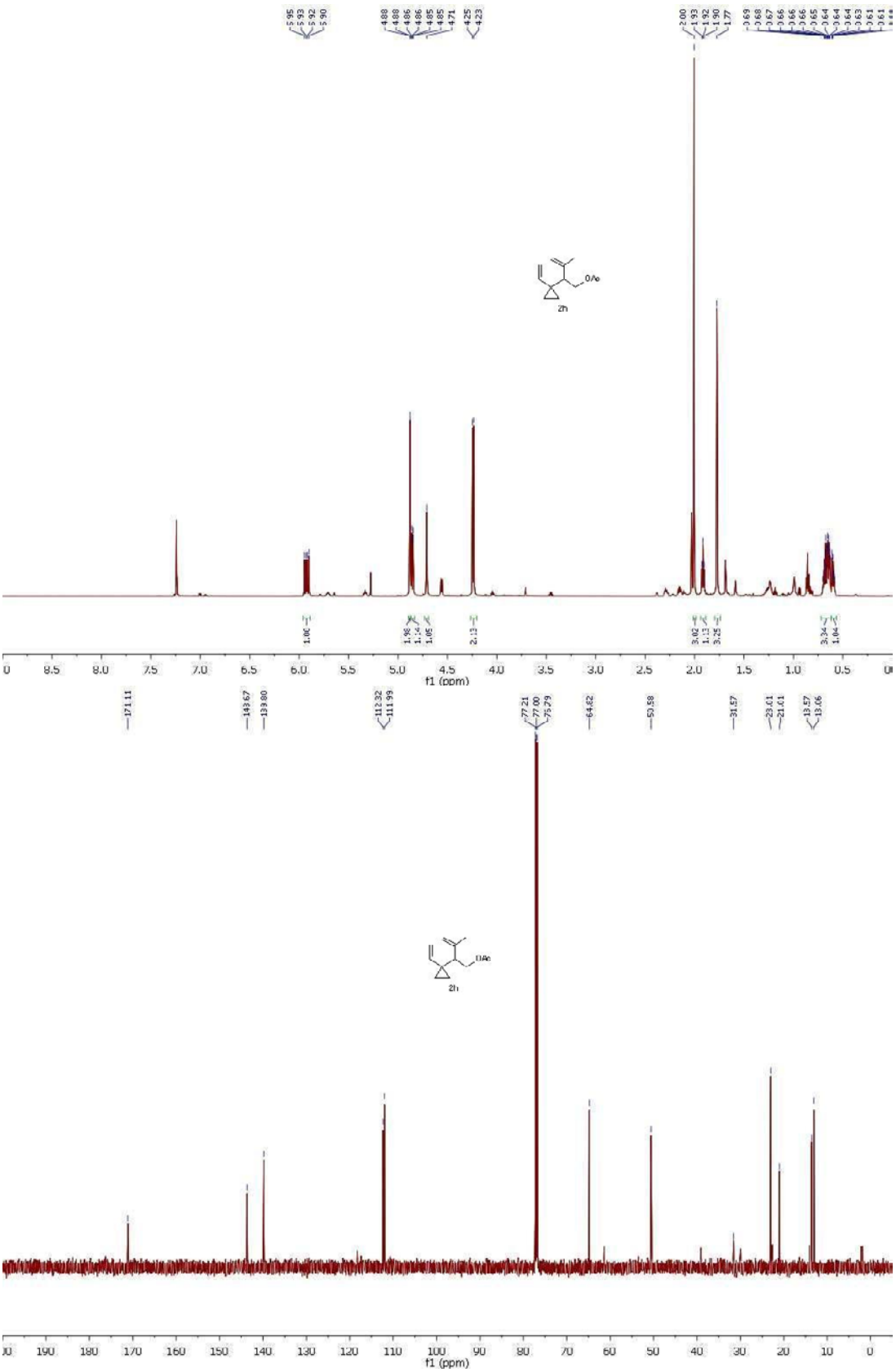


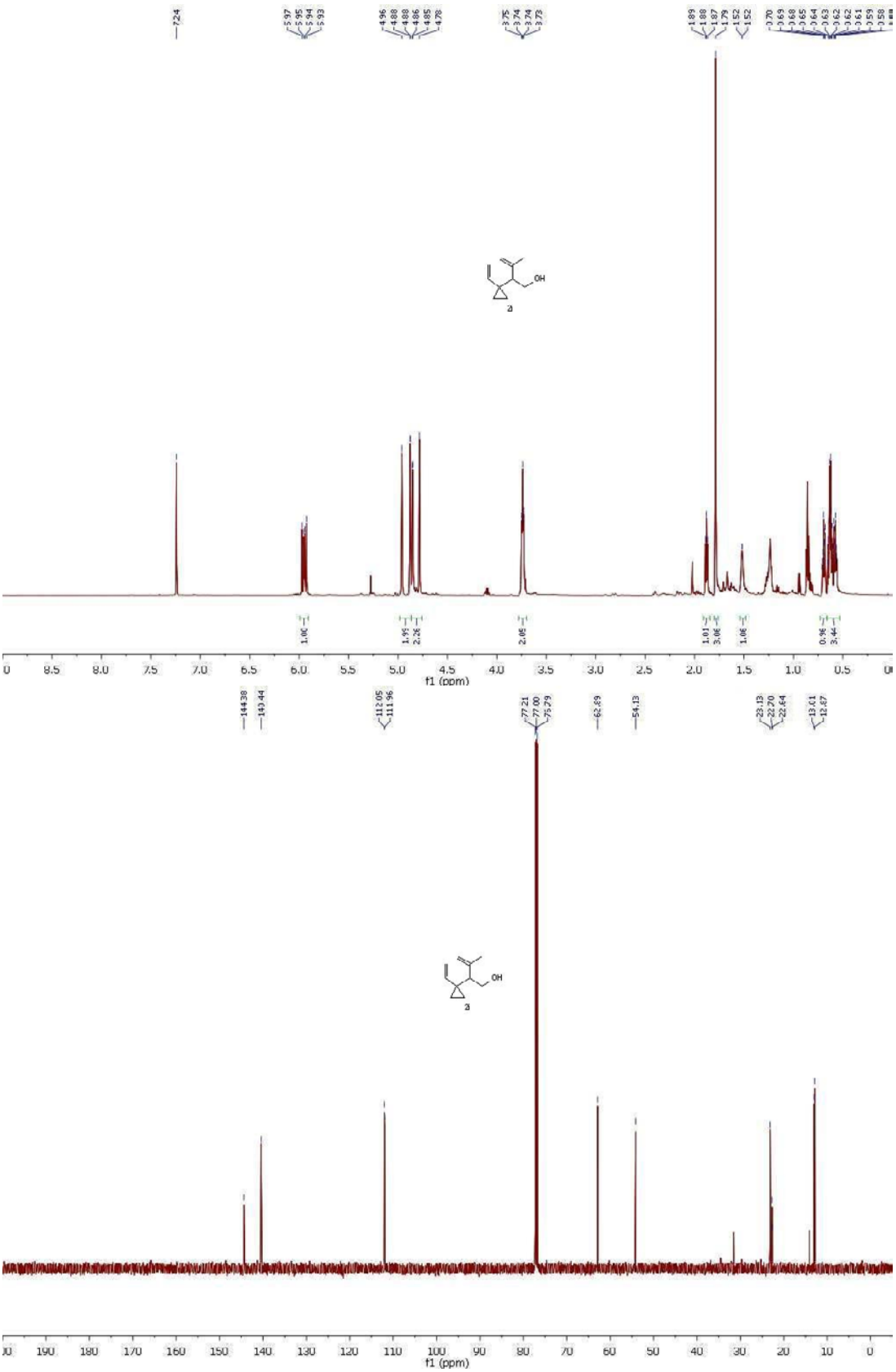


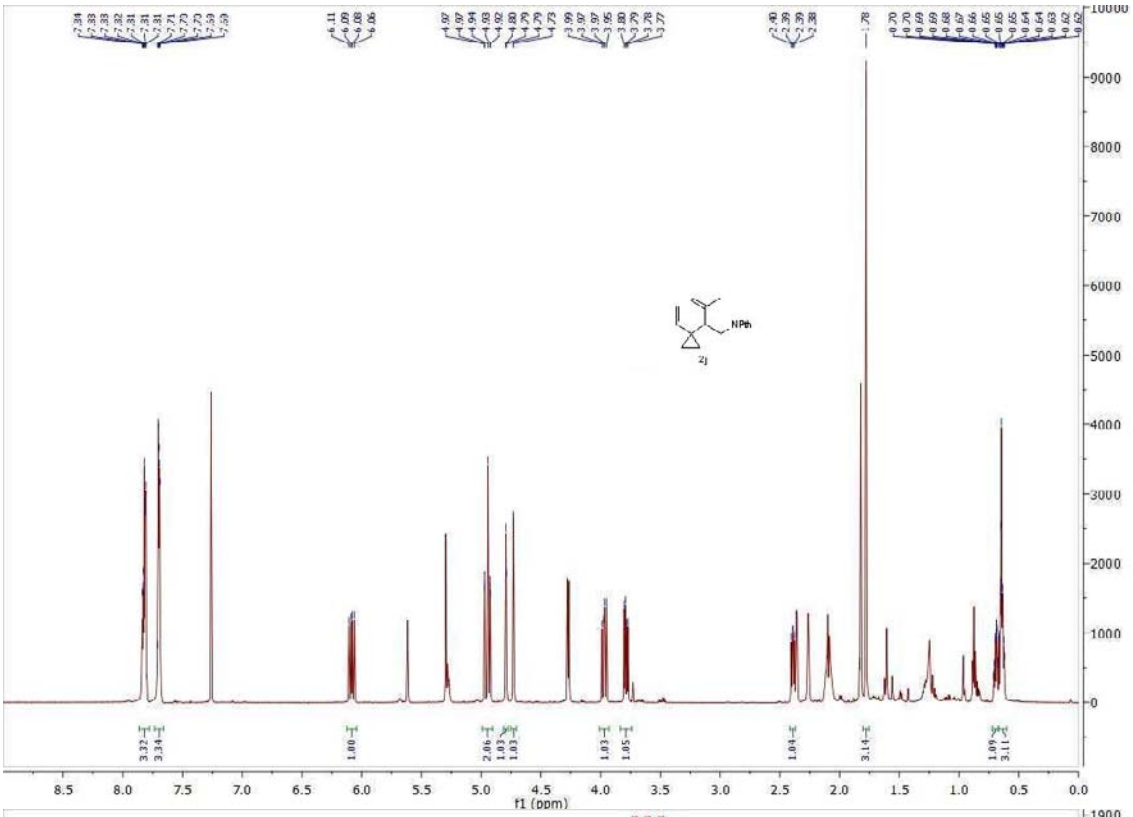


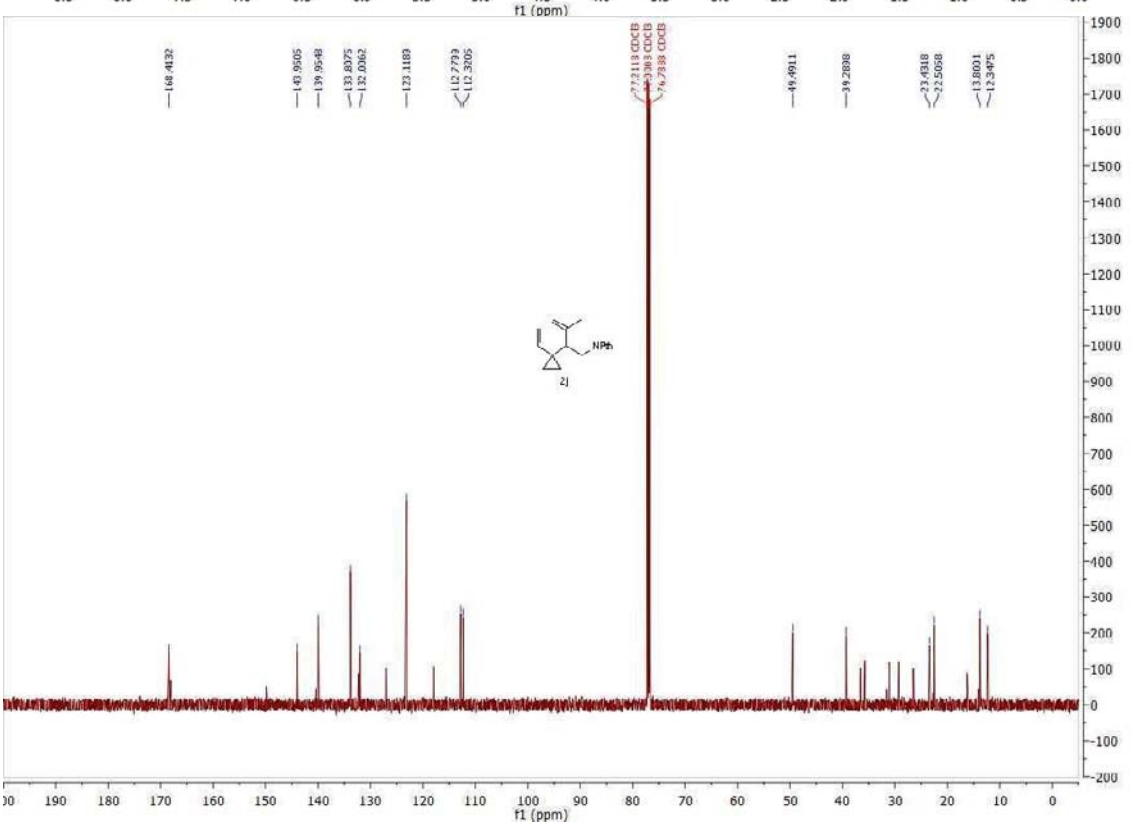


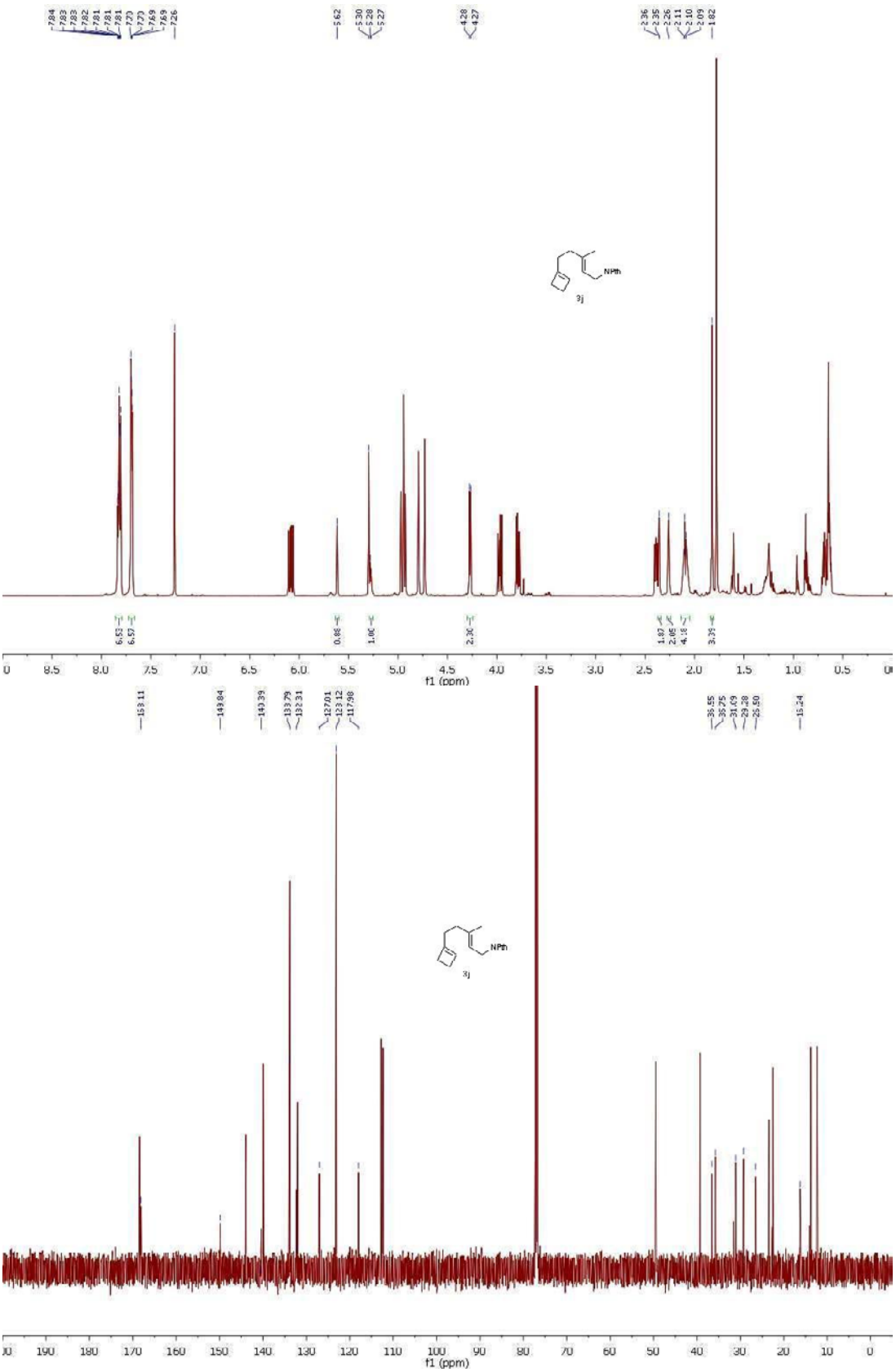


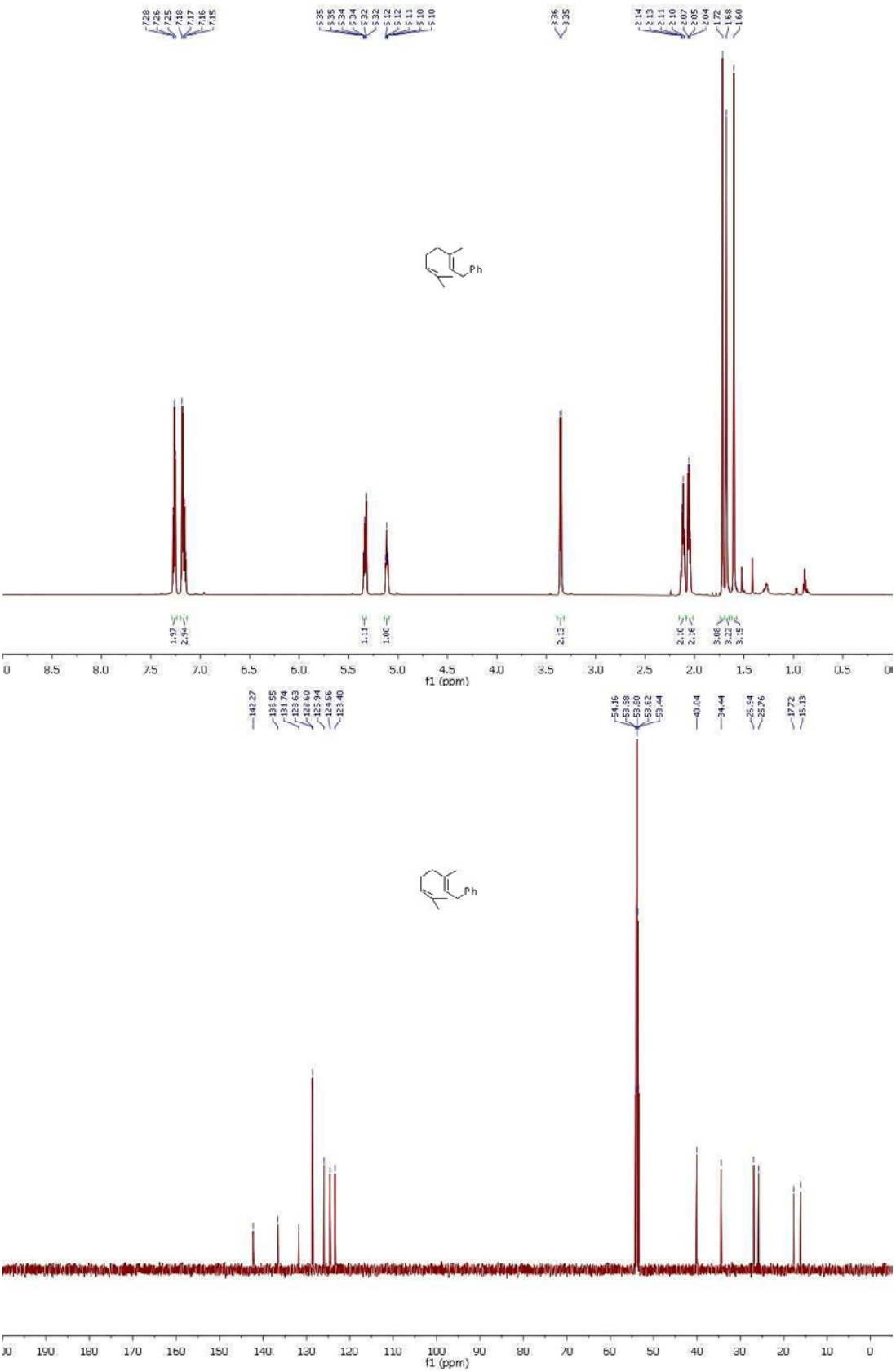


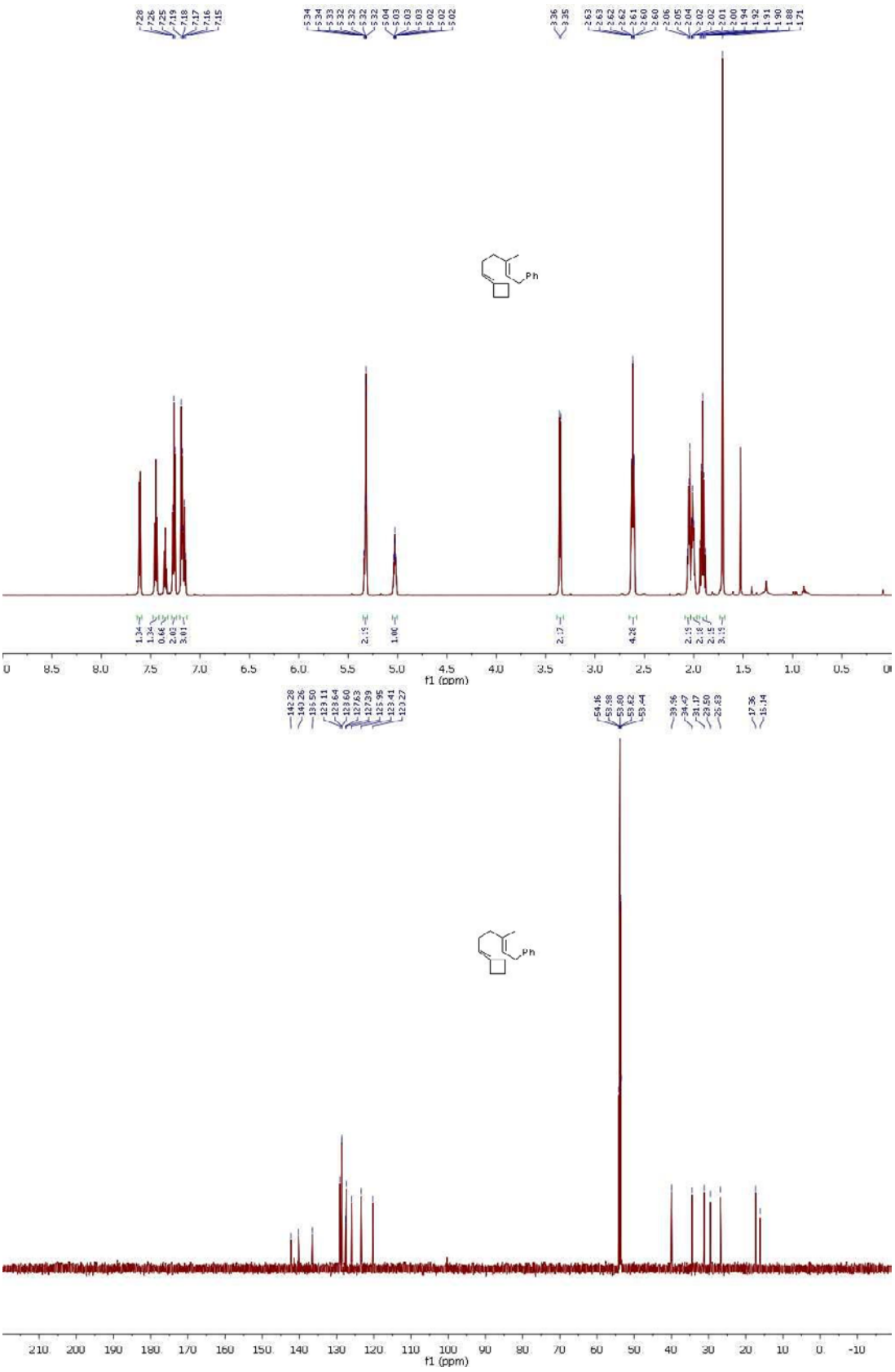


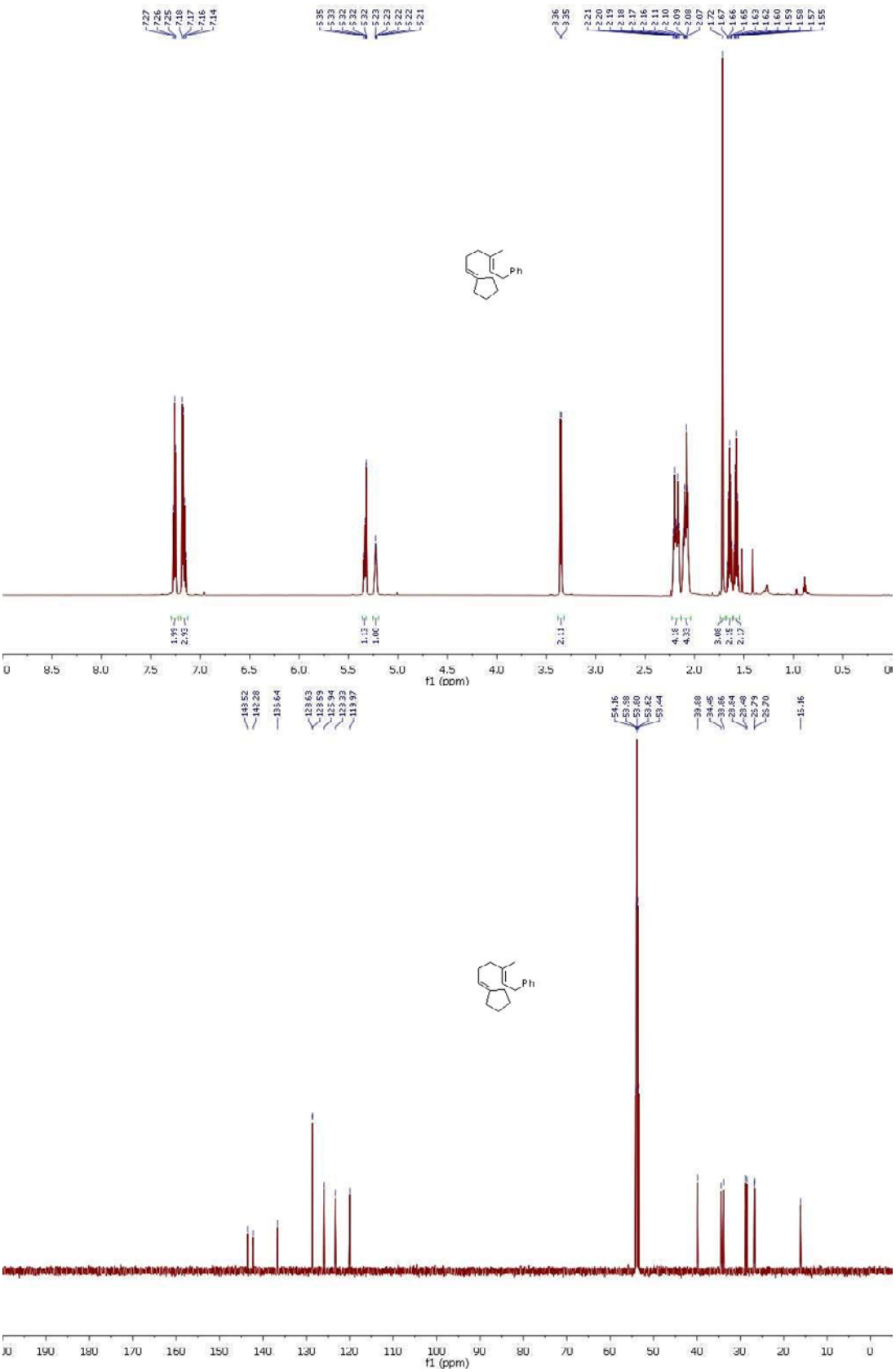






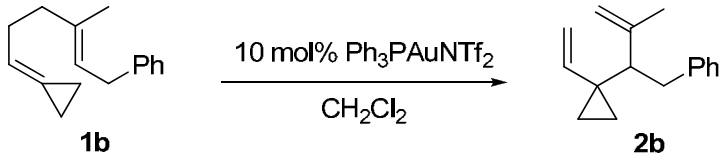






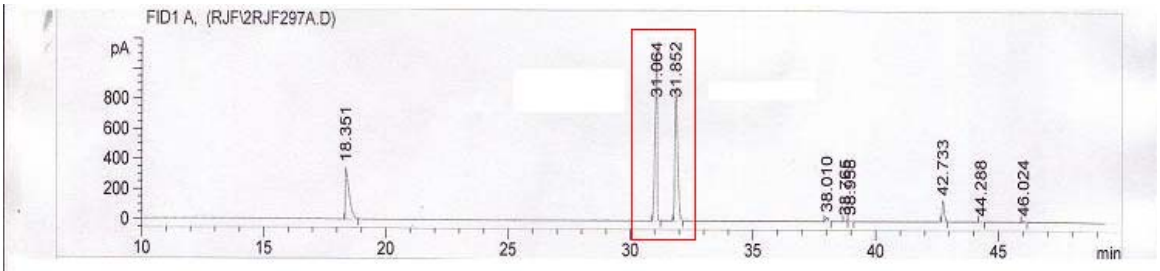
5. Gas Chromatography Results

Enantiomeric excess (ee's) were determined on a HP-6890 GC using an Agilent β-Cyclosil column. Inlet temperature was maintained at 250°C, 19.99 psi H_2.



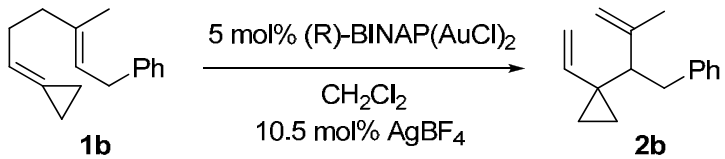
1b **2b**

Initial: 80°C (5 min) *Ramp 1*: 2.0°C/min to 170°C (30 min)



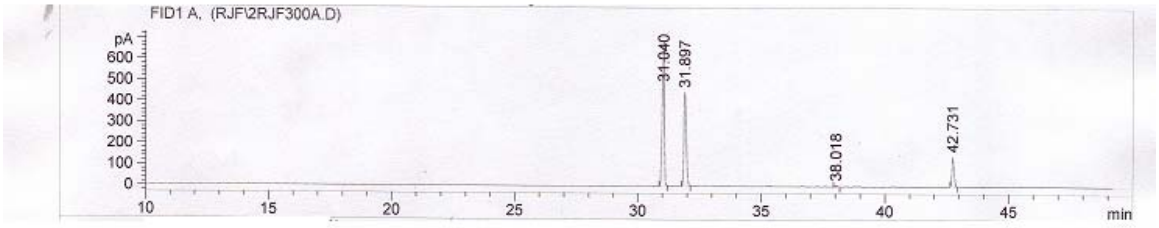
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	18.351	BB	0.1283	3587.17651	343.44250	19.33022
2	31.064	BB	0.0818	6880.26758	1137.30103	37.07570
3	31.852	BB	0.0961	6878.80225	886.57819	37.06780
4	38.010	PB	0.0777	151.59846	25.96917	0.81692
5	38.765	BV	0.0722	34.87588	6.17979	0.18794
6	38.958	VB	0.0740	36.81094	6.43266	0.19836
7	42.733	BB	0.0791	874.75201	138.75943	4.71378
8	44.288	BP	0.0731	28.37593	4.90221	0.15291
9	46.024	BP	0.0664	47.55323	8.67448	0.25625
10	53.411	BB	0.0841	37.13955	5.35386	0.20013
Totals :				1.85574e4	2563.59331	



1b **2b**

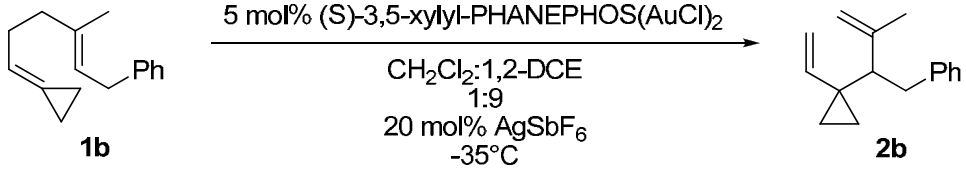
Initial: 80°C (5 min) *Ramp 1*: 2.0°C/min to 170°C (30 min)



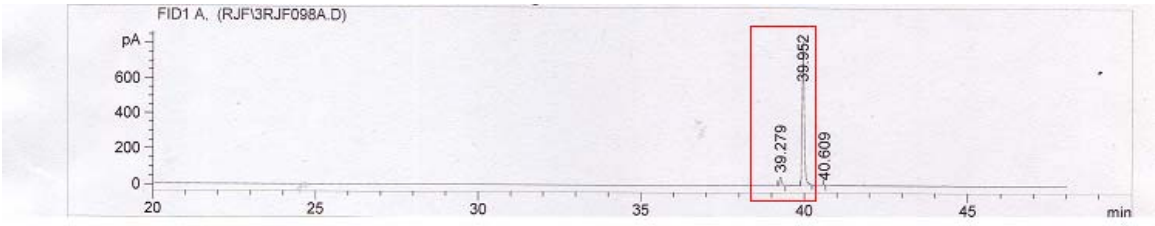
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	31.040	BB	0.0760	4052.35669	687.12292	50.85804
2	31.897	BB	0.0864	2997.06396	446.25327	37.61387
3	38.018	BB	0.0715	37.64063	6.66853	0.47240
4	42.731	BB	0.0801	880.91492	142.46346	11.05569

Totals : 7967.97620 1282.50818



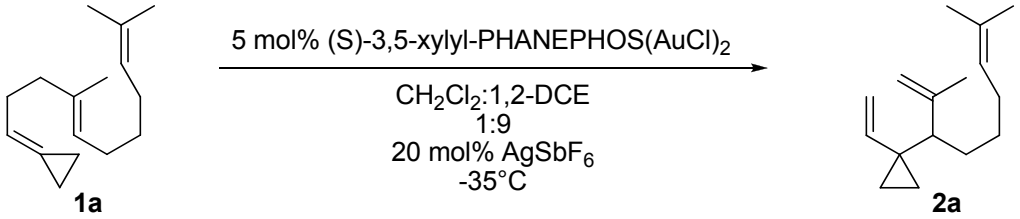
Initial: 80°C (14 min) *Ramp 1*: 2.0°C/min to 130°C (0 min) *Ramp 2*: 20°C/min to 170°C (7 min)



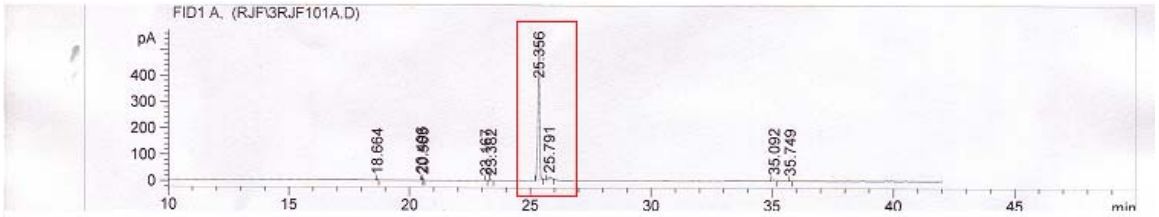
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	39.279	BB	0.0643	239.81931	47.64743	6.49692
2	39.952	PB	0.0583	3447.78027	812.22766	93.40341
3	40.609	BB	0.0293	3.67938	1.75539	0.09968

Totals : 3691.27896 861.63048

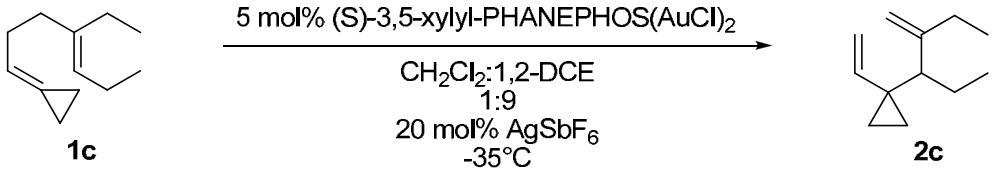


Initial: 60°C (14 min) *Ramp 1*: 5.0°C/min to 100°C (10 min) *Ramp 2*: 10°C/min to 130°C (10 min) *Ramp 3*: 10°C/min to 170°C (0 min)

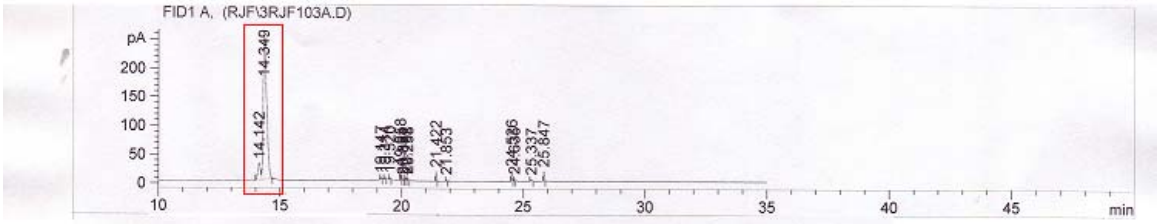


Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	3.689	BB	0.0413	20.53978	7.75835	0.74254
2	18.664	BB	0.0371	9.26258	3.81891	0.33485
3	20.496	BV	0.0330	19.74739	9.52839	0.71389
4	20.563	VB	0.0310	10.96064	5.55833	0.39624
5	23.167	BB	0.0411	4.65947	1.72743	0.16845
6	23.382	PB	0.0474	9.05670	3.12747	0.32741
7	25.356	PB	0.0696	2555.77490	539.78345	92.39462
8	25.791	PB	0.1222	97.33476	9.48041	3.51878
9	35.092	BB	0.0582	26.40583	6.44400	0.95461
10	35.749	PB	0.0525	12.40914	3.37542	0.44861
Totals :				2766.15120	590.60217	

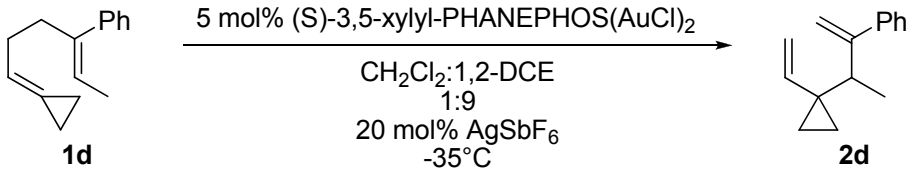


Initial: 60°C (14 min) *Ramp 1*: 10°C/min to 170°C (10 min)

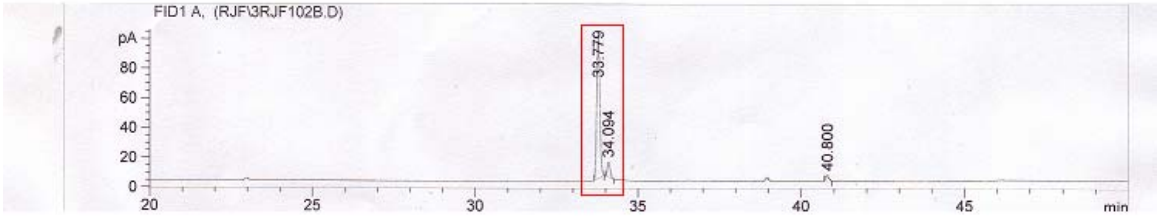


Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	3.693	BB	0.0387	9.44923	3.79004	0.32730
2	14.142	BV	0.1130	218.44730	28.90483	7.56651
3	14.349	VB	0.1450	2463.99634	247.37848	85.34711
4	19.147	BB	0.0370	8.85403	3.65790	0.30668
5	19.314	PB	0.0359	7.43450	3.20224	0.25751
6	19.520	BP	0.0356	7.12740	3.19425	0.24688
7	19.958	BB	0.0313	34.99399	17.49883	1.21211
8	20.054	BB	0.0328	3.94372	1.85828	0.13660
9	20.162	BB	0.0309	7.57995	3.85682	0.26255
10	20.258	BP	0.0310	7.78298	3.94491	0.26958
11	21.422	BB	0.0267	27.71542	16.59258	0.96000
12	21.853	PP	0.0261	5.39276	3.32735	0.18679
13	24.526	BP	0.0320	35.67371	17.95411	1.23565
14	24.635	PB	0.0268	7.60393	4.34342	0.26338
15	25.337	PB	0.0383	8.25134	3.01471	0.28581
16	25.847	BP	0.0322	32.78294	16.36681	1.13553
Totals :				2887.02954	378.88555	

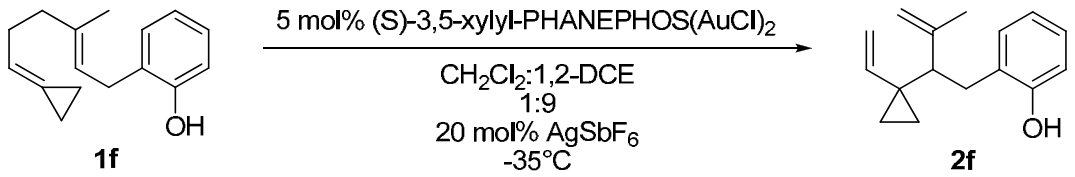


Initial: 80°C (14 min) *Ramp 1*: 2.0°C/min to 130°C (0 min) *Ramp 2*: 20°C/min to 170°C (7 min)



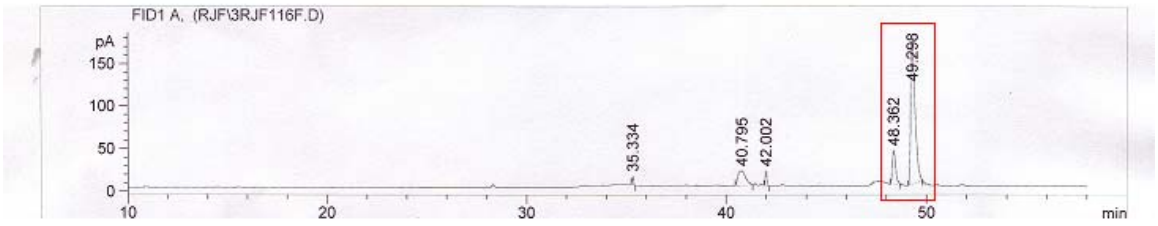
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	33.779	PB	0.0833	638.82385	94.93727	87.86691
2	34.094	PP	0.0782	61.79708	10.03902	8.49987
3	40.800	BB	0.0850	26.41479	3.95970	3.63322
Totals :				727.03573	108.93599	



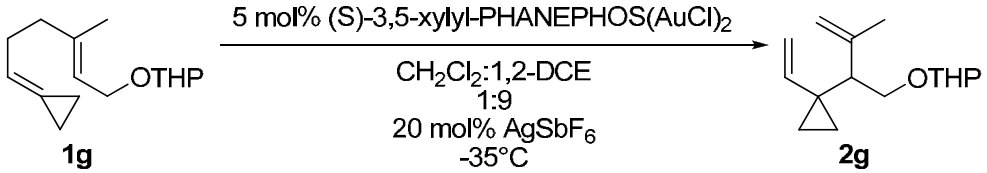
1f 2f

Initial: 100°C (10 min) *Ramp 1*: 2.0°C/min to 130°C (5 min) *Ramp 2*: 5.0°C/min to 170°C (20 min)



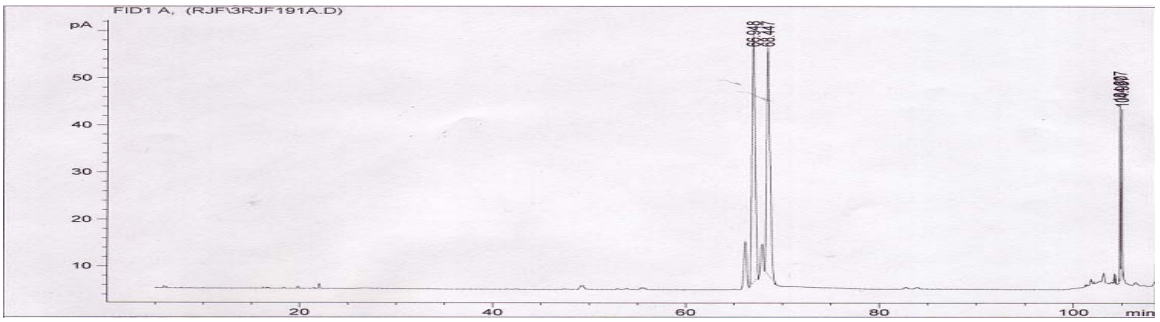
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	2.091	BB	0.0239	4.95926	3.03597	0.13714
2	35.334	BP	0.0631	48.37317	10.23862	1.33770
3	40.795	BB	0.3064	449.57294	17.25171	12.43242
4	42.002	PB	0.0805	96.58465	17.47247	2.67094
5	48.362	PB	0.1344	446.71997	39.49307	12.35352
6	49.298	PB	0.1806	2569.92480	169.01466	71.06828
Totals :				3616.13479	256.50651	



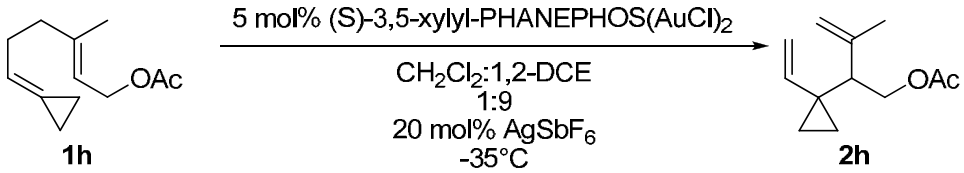
1g 2g

Initial: 80°C (10 min) *Ramp 1*: 1.0°C/min to 100°C (10 min) *Ramp 2*: 1.0°C/min to 110 (15 min) *Ramp 3*: 1.0°C/min to 115°C (12 min) *Ramp 4*: 1°C/min 120 (10 min) *Ramp 5*: 20°C/min to 170°C (7 min)

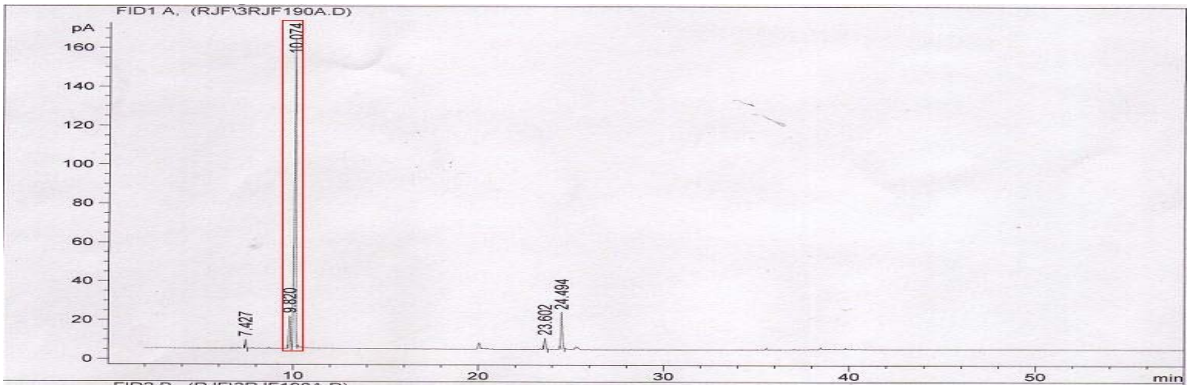


Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	66.147	PV	0.3196	203.32793	10.03438	6.26077
2	66.946	VV	0.3472	1302.15051	53.64042	40.09513
3	67.901	VV	0.3445	204.95366	9.04174	6.31082
4	68.443	VB	0.3930	1312.88062	50.48575	40.42552
5	105.002	VB	0.0959	224.33992	35.60491	6.90776
Totals :				3247.65263	158.80720	

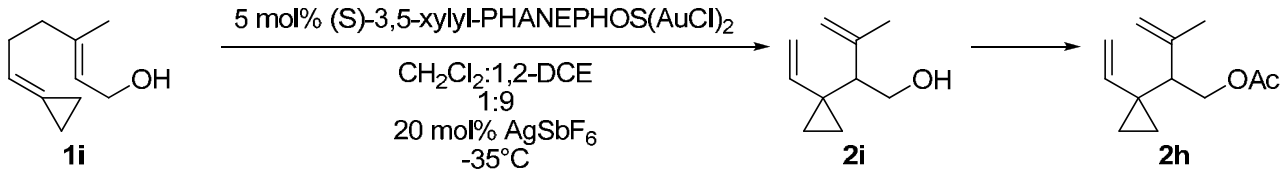


Initial: 100°C (10 min) *Ramp 1*: 2°C/min to 130°C (5 min) *Ramp 2*: 5°C/min to 170°C (20 min)

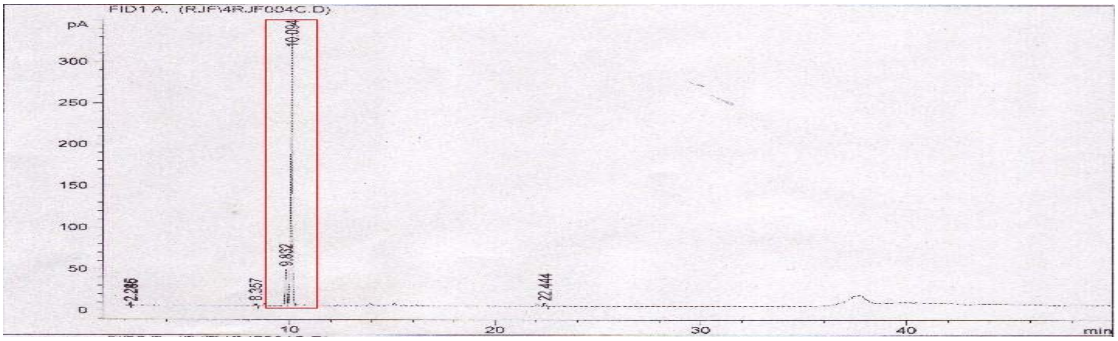


Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	7.427	PB	0.0673	19.44063	4.56688	1.63949
2	9.820	BV	0.0882	93.14408	16.30516	7.85512
3	10.074	VB	0.0909	929.99030	158.30988	78.42885
4	23.602	BB	0.0912	32.36367	5.68944	2.72932
5	24.494	BB	0.0937	110.83716	18.77416	9.34723
Totals :				1185.77584	203.64552	

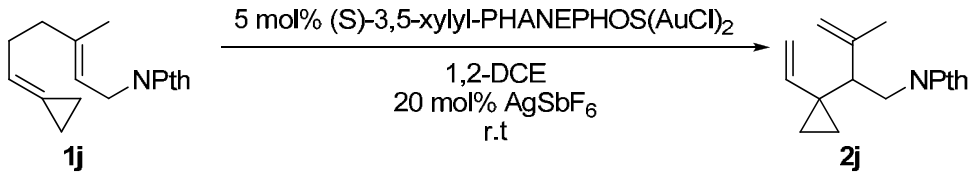


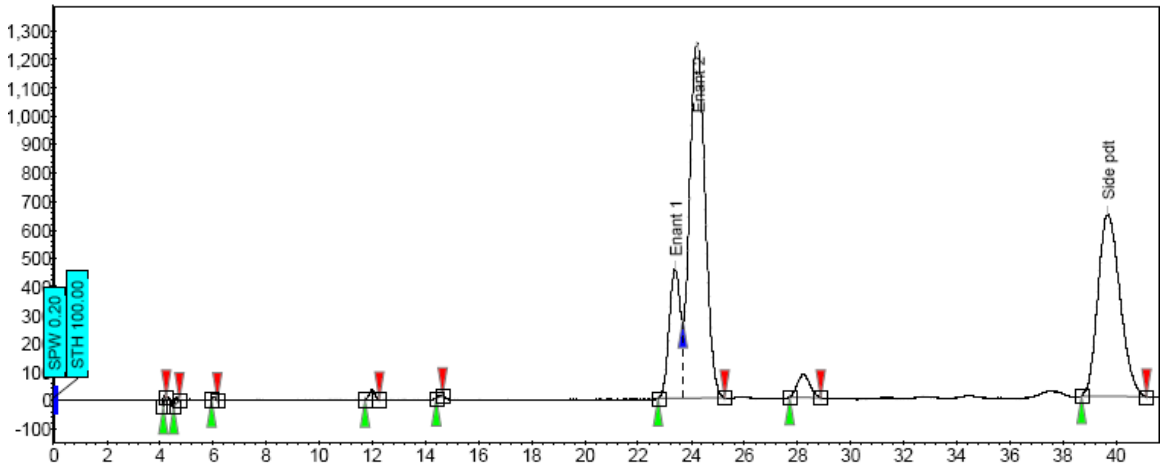
Initial: 100°C (10 min) *Ramp 1*: 2°C/min to 130°C (5 min) *Ramp 2*: 5°C/min to 170°C (20 min)



Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	2.246	PV	0.0280	3.91561	2.11341	0.17742
2	2.285	VB	0.0213	2.41829	1.70988	0.10957
3	8.357	BB	0.0712	13.81585	2.91884	0.62600
4	9.832	BV	0.0930	261.71375	43.74424	11.85830
5	10.094	VB	0.0872	1906.02380	327.19940	86.36231
6	22.444	BB	0.0893	19.12160	3.37252	0.86640
Totals :				2207.00889	381.05829	

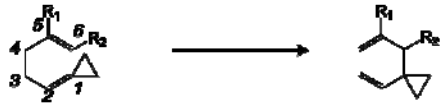




Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.13	4.15	4.24	0.00	0.10	30.0	1.7	0.098
2	UNKNOWN	4.52	4.59	4.73	0.00	0.17	22.3	2.9	0.165
3	UNKNOWN	5.95	6.04	6.16	0.00	0.05	8.0	0.9	0.050
4	UNKNOWN	11.72	11.96	12.25	0.00	0.46	34.2	8.0	0.458
5	UNKNOWN	14.39	14.53	14.63	0.00	0.04	5.4	0.8	0.044
6	Enant 1	22.76	23.39	23.69	0.00	12.77	457.0	224.0	12.774
7	Enant 2	23.69	24.22	25.25	0.00	48.72	1253.8	854.1	48.716
8	UNKNOWN	27.71	28.22	28.87	0.00	2.49	80.4	43.7	2.492
9	Side pdt	38.68	39.68	41.13	0.00	35.20	644.0	617.2	35.203
Total						100.00	2535.0	1753.2	100.000

6. Quantum Calculations and Discussion

Supplementary Table 6. Gas phase free energies (enthalpies in parentheses) for thermal [3,3]-sigmatropic rearrangements of hexadienes at various levels of theory.[a]



Entry	R_1	R_2	ΔG‡ (ΔH‡)	ΔG (ΔH)
1	H	H	35.6 (32.4) 33.4 (30.1) 25.9 (22.4)	-4.1 (-4.9) -7.3 (-8.4) -9.1 (-10.1)
2	Me	H	35.1 (31.9) 32.0 (29.5) 24.2 (20.3)	-2.9 (-2.9) -7.0 (-7.5) -8.2 (-8.8)
3	H	Me	39.5 (36.2) 36.1 (32.4) 28.0 (24.1)	0.9 (-0.3) -4.4 (-6.0) -7.0 (-8.5)
4	Me	Me	38.6 (35.3) 35.1 (30.1) 25.5 (21.1)	3.2 (-0.5) -3.8 (-6.2) -5.4 (-8.3)

[a] B3LYP/6-31G(d) (BLACK), M06-2X/6-31G(d) (BLUE), and MP2/6-31G(d) (RED).

Cope reactions of several model compounds were studied using density functional theory (M06-2X[15a,b] and B3LYP[12c-e]) and Møller-Plesset pertubation theory (MP2)[12f] as implemented in *GAUSSIAN09*[16] with the 6-31G(d) basis set as shown in Supplementary Table 6. First, rearrangement in the absence of catalyst was examined. As shown in Supplementary Table 6, the M06-2X and B3LYP methods predict similar rearrangement

[15] Also, UB3LYP calculations were performed with the guess= (mix,always) keyword and show S^2 value of 0, eliminating the possibility of lower lying diradical-like pathway. (a) Zhao, Y.; Thrular, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215. (b) Zhao, Y.; Thrular, D. G. *Acc. Chem. Res.* **2008**, *41*, 157. (c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5468. (d) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (e) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B*. **1988**, *98*, 785. (f) Binkley, J. S.; Pople, J. A. *Int. J. Quantum Chem.* **1975**, *9*, 229.

[16] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010..

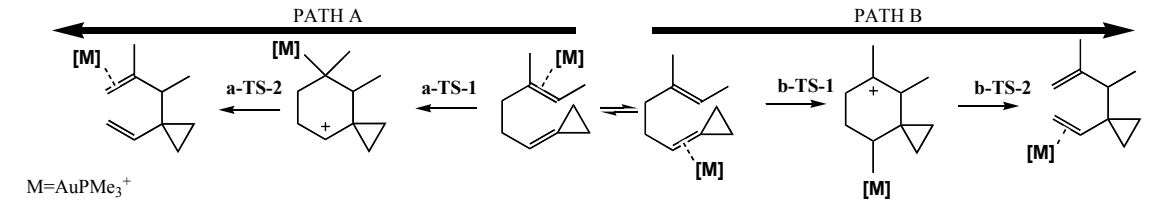
barriers while MP2 appears to underestimate the barriers.[17] In contrast, M06-2X and MP2 predict comparable exergonicities and exothermicities while B3LYP underestimates these. Thus, it appears that M06-2X provides the best estimates of both kinetic *and* thermodynamic parameters for these systems.

The rearrangement of the unsubstituted system (entry 1) is predicted to have a barrier ($\Delta H^{\ddagger}$) of approximately 30 kcal/mol, comparable to that for the Cope reaction of 1,5-hexadiene, and is predicted to be exothermic/exergonic by 7-8 kcal/mol, reflecting the release of strain upon rearrangement.[18] As expected, methyl substitution at the C5 position (R_1) only slightly changes this thermodynamic preference, but greater effects are predicted for alkyl substitution at the C6 position (entries 3 and 4). In sum, this strain relief allows the Cope-like rearrangement of methylenecyclopropane containing dienes, here catalyzed by Au(I) species, to proceed (vide infra).

Supplementary Table 7. Comparison of different functionals for calculated reaction pathways for the Au(I)-catalyzed rearrangement of the substrate corresponding to entry 4 in Table 3 in the main text. Free energies (kcal/mol, at 298 K) are shown. All structures were optimized without constraints using the 6-31G(d) basis set for P, C and H and LANL2DZ for Au, in DCE (using the CPCM solvation model). The ligand (L) was modeled as trimethylphosphine.

[17] A known tendency; see, for example: Wiest, O.; Montiel, D. C.; Houk, K. N. *J. Phys. Chem. A* **1997**, *101*, 8378.

[18] Previous calculations have predicted an 11-12 kcal/mol strain energy for the methylene cyclopropane substructure; see: (a) Johnson, W. T. G.; Borden, W. T. *J. Am. Chem. Soc.* **1997**, *119*, 5930. (b) Bach, R. D.; Dmitrenko, O. *J. Am. Chem. Soc.* **2004**, *126*, 4444.

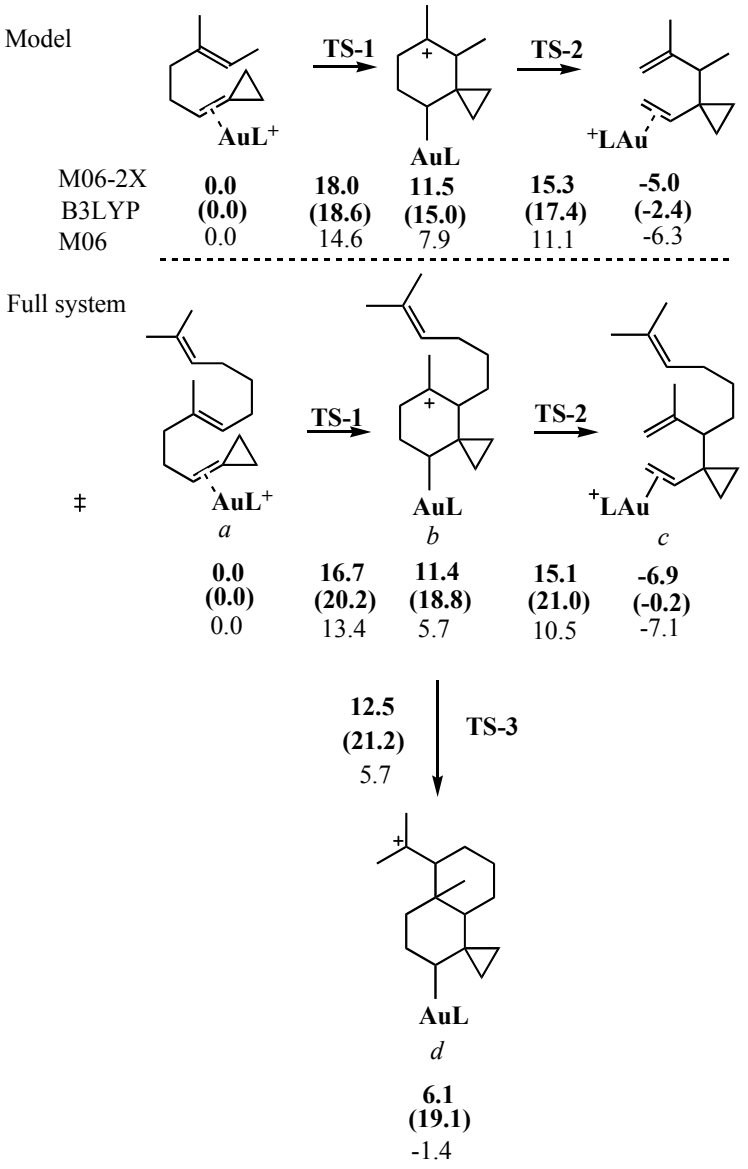


M06-2X	-5.9	28.1	19.5	28.0	0.0	0.8	18.8	12.3	16.1	-5.8
B3LYP	(-1.3)	(28.5)	(21.0)	(29.3)	(0.0)	(-0.4)	(18.2)	(14.6)	(17.0)	(-2.0)
M06	(-5.9)	(19.3)	(15.1)	(25.0)	(0.0)	(0.9)	(15.5)	(8.8)	(12.0)	(-5.4)

Next, the effect of gold on the rearrangement was examined with M06-2X, B3LYP, and M06 functionals using a split basis set (6-31G(d) for P, C and H and LANL2DZ for Au) in for 1,2-dichloroehtane (DCE) solvent (CPCM[19] model) with PMe_3 as a simple model ligand). Recent literature indicates that M06 is appropriate for treatment of organometallic systems.[20] As shown in Supplementary Table 7, the M06 and M06-2X functionals have similar energetics although M06 energies are ca. 3 kcal/mol lower. B3LYP predicts higher barriers and lower thermodynamic drive than the aforementioned functionals. However, all three methods predict the Path B to be favored over Path A by ca. 10 kcal/mol and predict the reaction to be downhill by 2-5 kcal/mol.

[19] (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995. (b) Barone, V.; Cossi, M.; Tomasi, J. *J. Comput. Chem.* **1998,** *19*, 404.

[20] (a) Sieffert, N.; B€uhl, M. *Inorg. Chem*. **2009,** *48*, 4622. (b) Minenkov, Y.; Occhipinti, G.; Jensen, V. R. *J. Phys. Chem. A* **2009**,*113*, 11833. (c) Stewart, I. C.; Benitez, D.; O'leary, D. J.; Tkatchouk, E.; Day, M. W.; Goddard, W. A., III; Grubbs, R. H. *J. Am. Chem. Soc*. **2009,***131*, 1931. (d) Benitez, D.; Tkatchouk, E.; Goddard, W. A., III. *Organometallics* **2009**, *28*, 2643. (e) Fedorov, A.; Couzijn, E. P. A.;Nagornova, N. S.; Boyarkin, O. V.; Rizzo, T. R.; Chen, P. *J. Am. Chem. Soc*. **2010**, *132*, 13789. (f) Takatani, T.; Sears, J. S.; Sherrill, C. D. *J. Phys.Chem. A* **2010***, 114*, 11714. (g) Pratt, L. M.; Voit, S.; Okeke, F. N. *J. Phys.Chem. A* **2011**, *115,* 2281. (h) Kulkarni, A. D.; Truhlar, D. G. *J.Chem.Theory Comput*. **2011***, 7*, 2325.



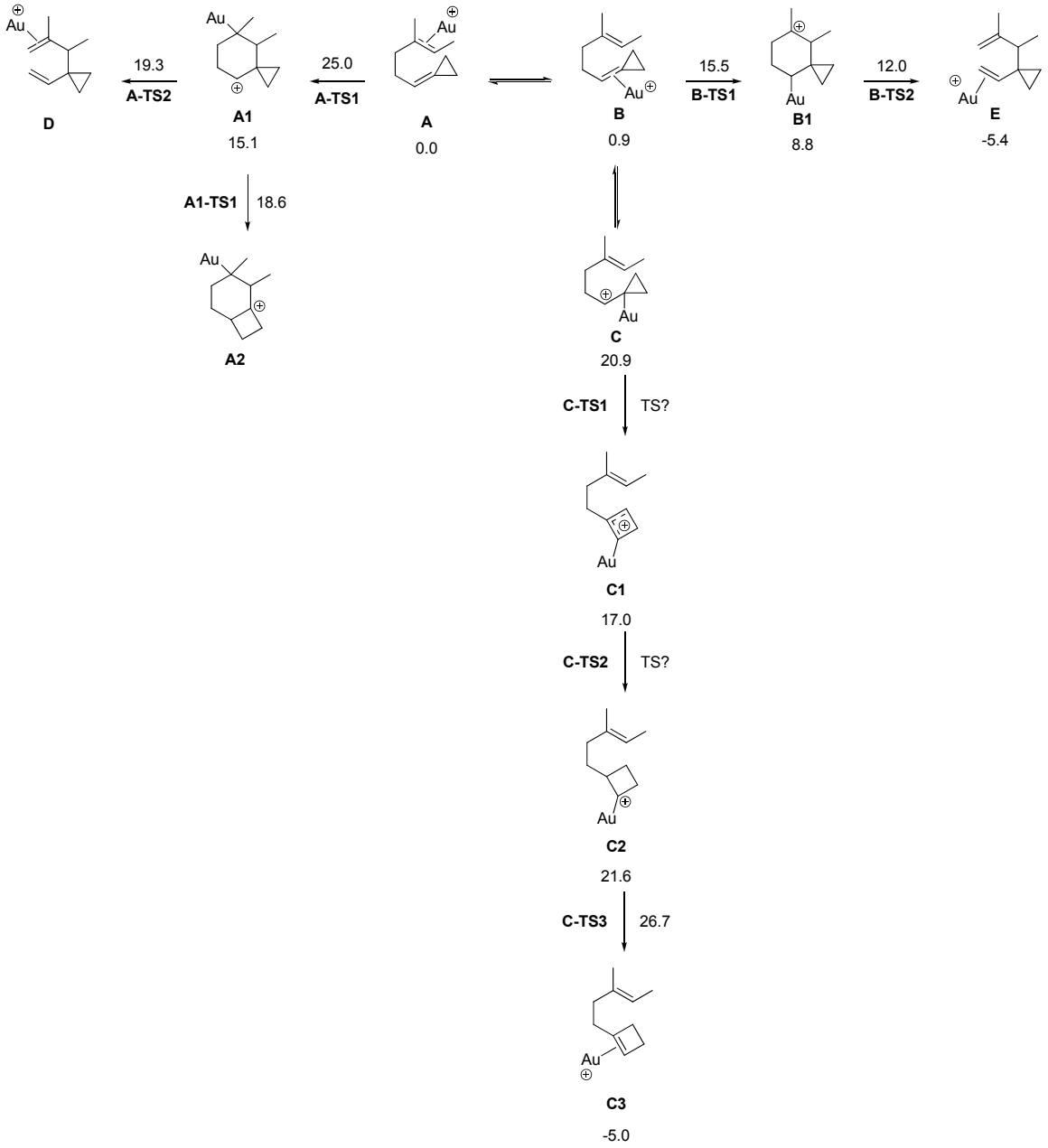
Supplementary Figure 1. Competing pathways for the Au(I)-catalyzed reaction of **1a**. Free energies (kcal/mol; 298K) were calculated with the indicated functionals (M06-2X, B3LYP, M06; from top to bottom). Trimethyl phospine (L) was used as a model ligand. The 6-31G(d) basis set was used for P, C, H and LANL2DZ (ECP) for Au.

Next, we examined the effect of modeling the full susbstrate **1a** and the competing cyclization pathway as shown in Supplementary Figure 1. Only the lowest energy pathway (Path B) was calculated with full substrate given that Path A was much higher in energy. As shown in Supplementary Figure 1, the energetics are very similar for both the

model substrate and the model system with all three functionals. However, as discussed before B3LYP understimates the exergonicities showing rearrangement to be only slightly exergonic in the full system (by 0.2 kcal/mol) while the M06 suite functionals both show the Cope-like rearrangement to be exergonic by ca. 7 kcal/mol. Given that susbtrate **1a** failed to undergo cyclization, we wondered if perhaps this was due to a kinetic preference for Cope-like rearrangement rather than cyclization. The barrier leading to cyclization (**TS-3**) is nearly the same or lower (within the M06 suite functionals) than energy to undergo the Cope-like rearrangement (**TS-2**). Although, the magnitude of exergonicities/endergonicities varies with the level of theory, there seems to be a thermodynamic preference leading to Cope-like product (*c*) than to cyclized product (*d*). This suggests the failure to cyclize and the preference to undergo the rearrangement is due to a thermodynamic preference.

As shown in Supplementary Figure 2 (below), formation of intermediate **A1**, which can proceed to the Cope-like product **D** or ring-open to form intermediate **A2,** is kinetically disfavored by over 10 kcal/mol with respect to formation of intermediate **B1**. Furthermore, although Au(I) can complex to the carbon bearing the cyclopropyl group (**C**), this is 20 kcal/mol higher in energy and the subsequent pathway way leading to the cyclobutene product **C3** proceeds through a high-energy transition state (**C-TS3**) that corresponds to a proton shift. Although we could not find transition state structures **C-TS1** and **C-TS2** due to convergence problems, the intermediates leading to the cyclobutene product are much higher in energy than those leading to the Cope product **E** and therefore we conclude that this pathway is kinetically unfeasible (but it cannot be ruled out, given that for one substrate [the naphthlimide substituted compound **1j**] some

amount of this product was observed). Calculations on this substrate are underway.



Supplementary Figure 2. Relative free energies (298.15K) calculated using M06/6-31G(d)-LANL2DZ(Au) in DCE (CPCM;UA0).

Coordinates and energies:

B3LYP/6-31G(d)

XYZ Coordinates

C	3.67298700	0.89444800	-0.19680900
H	4.63193000	1.08953500	0.27617100
H	3.36160300	1.59492200	-0.96957800
C	2.91822300	-0.15005100	0.14619500
H	3.27200300	-0.82345600	0.92981900
C	1.57876700	-0.48814400	-0.44854000
H	1.33520300	0.21726400	-1.25251100
H	1.62407000	-1.48702700	-0.90952800
C	0.44141000	-0.48436600	0.60105000
H	0.72169100	-1.16459700	1.42035300
H	0.35155400	0.51641800	1.03864700
C	-1.96859600	-0.15345100	-0.01830600
C	-0.88267800	-0.91136900	0.02391200
H	-0.92784900	-1.91733200	-0.39870400
C	-2.60886400	1.13157400	0.30241800
H	-2.86094700	1.35544200	1.33851000
H	-2.35733500	2.01262700	-0.28714800
C	-3.38004000	-0.00398100	-0.39621400
H	-4.14174200	-0.53002200	0.17849000
H	-3.63731400	0.12825900	-1.44675400

Zero-point correction=	0.176237 (Hartree/Particle)
Thermal correction to Energy=	0.185385
Thermal correction to Enthalpy=	0.186330
Thermal correction to Gibbs Free Energy=	0.141307
Sum of electronic and zero-point Energies=	-311.809980
Sum of electronic and thermal Energies=	-311.800831
Sum of electronic and thermal Enthalpies=	-311.799887
Sum of electronic and thermal Free Energies=	-311.844910

M06-2X/6-31G(d)

XYZ Coordinates

C	3.61158800	0.92153000	-0.18411000
H	4.56717100	1.12980200	0.28680400
H	3.26890400	1.62903800	-0.93562300
C	2.89065400	-0.14875100	0.13541000
H	3.26381300	-0.83483800	0.89732500
C	1.55614000	-0.49200400	-0.45946300
H	1.29673500	0.23111400	-1.24123700
H	1.60883600	-1.47840100	-0.94161900
C	0.44082300	-0.52049500	0.60013300
H	0.73303200	-1.21558600	1.39995000
H	0.34382300	0.47101600	1.05531500
C	-1.94817200	-0.16378600	-0.01893100
C	-0.87959600	-0.93963600	0.01843400
H	-0.93475600	-1.93933400	-0.41447300
C	-2.54998900	1.13147300	0.31571300
H	-2.79604500	1.34307500	1.35323200
H	-2.26914300	2.00613300	-0.26553300
C	-3.34924800	0.03530100	-0.39482700
H	-4.12242300	-0.47429900	0.17445600
H	-3.59314400	0.19048600	-1.44275000

Zero-point correction=	0.178081 (Hartree/Particle)
Thermal correction to Energy=	0.187164
Thermal correction to Enthalpy=	0.188108
Thermal correction to Gibbs Free Energy=	0.143239
Sum of electronic and zero-point Energies=	-311.648692
Sum of electronic and thermal Energies=	-311.639608
Sum of electronic and thermal Enthalpies=	-311.638664
Sum of electronic and thermal Free Energies=	-311.683533

MP2/6-31G(d)

B3LYP/6-31G(d)

XYZ Coordinates

C	3.58427000	0.94912300	-0.17293400
H	4.54121700	1.16238700	0.29232100
H	3.21842700	1.67465400	-0.89454700
C	2.88706400	-0.15549000	0.12100100
H	3.28832100	-0.85758700	0.85313600
C	1.55157800	-0.49930500	-0.46716000
H	1.28079400	0.23754400	-1.23262000
H	1.60370200	-1.47568000	-0.96838200
C	0.44621100	-0.54559900	0.60176600
H	0.74275900	-1.25031000	1.39125400
H	0.35297200	0.44085900	1.06955900
C	-1.94230100	-0.16127700	-0.01467900
C	-0.87614300	-0.95436500	0.02280200
H	-0.94336400	-1.95497100	-0.40839200
C	-2.53238000	1.14051900	0.31781900
H	-2.78377800	1.35801200	1.35345100
H	-2.24830000	2.01456500	-0.26390900
C	-3.34207400	0.04375600	-0.39562200
H	-4.12311900	-0.45494300	0.17373500
H	-3.58698200	0.20128800	-1.44356200

Zero-point correction= 0.179534 (Hartree/Particle)
Thermal correction to Energy= 0.188593
Thermal correction to Enthalpy= 0.189537
Thermal correction to Gibbs Free Energy= 0.144676
Sum of electronic and zero-point Energies= -310.681338
Sum of electronic and thermal Energies= -310.672279
Sum of electronic and thermal Enthalpies= -310.671335
Sum of electronic and thermal Free Energies= -310.716196

XYZ Coordinates

C	-0.86064900	-0.20209100	-0.16961700
C	0.02269200	-1.24366800	-0.49266100
C	1.22023700	-1.37949500	0.26231000
C	2.19764400	0.16580600	-0.03642800
C	1.31541700	1.23106300	0.28952000
C	0.15357600	1.40917700	-0.48242500
H	1.90409500	-2.17322000	-0.04338900
H	0.02964300	-1.59705300	-1.52553800
H	2.44526900	0.04151200	-1.09095600
H	3.07770300	0.03876500	0.59593500
H	1.29832200	1.57698700	1.32289400
H	-0.54261600	2.19420400	-0.18579600
H	1.11889000	-1.33558800	1.34664200
H	0.24221000	1.32433200	-1.56461300
C	-2.31555100	-0.01533300	-0.43369900
H	-2.65638400	0.93289100	-0.84473700
H	-2.90017300	-0.87148700	-0.76270300
C	-1.77608800	-0.00181200	0.99592300
H	-1.98388800	-0.86158600	1.62876900
H	-1.77673900	0.94835700	1.52596000

Zero-point correction= 0.175878 (Hartree/Particle)
Thermal correction to Energy= 0.183491
Thermal correction to Enthalpy= 0.184435
Thermal correction to Gibbs Free Energy= 0.144564
Sum of electronic and zero-point Energies= -311.756864
Sum of electronic and thermal Energies= -311.749251
Sum of electronic and thermal Enthalpies= -311.748307
Sum of electronic and thermal Free Energies= -311.788178

M06-2X/6-31G(d)

XYZ Coordinates

C	-0.84934700	-0.21630700	-0.18382500
C	0.04109500	-1.23840800	-0.51588900
C	1.21721100	-1.36292800	0.26267300
C	2.17218900	0.18645600	-0.02595000
C	1.27037600	1.22763500	0.29806500
C	0.13466600	1.39698100	-0.50070700
H	1.92358400	-2.14133200	-0.02593200
H	0.06314700	-1.58366700	-1.54940300
H	2.42269200	0.06924300	-1.07974900
H	3.04467000	0.06073600	0.61467400
H	1.22579900	1.56391800	1.33259600
H	-0.58952800	2.16089400	-0.21810300
H	1.08813800	-1.30872100	1.34302300
H	0.24684000	1.29983600	-1.57900700
C	-2.30133000	-0.01854400	-0.41067900
H	-2.64162400	0.93337500	-0.80910100
H	-2.89528600	-0.87193900	-0.72254200
C	-1.72799700	-0.01463000	0.99919600
H	-1.92647800	-0.87772600	1.62742400
H	-1.70313200	0.93385300	1.52880900

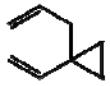
Zero-point correction=	0.177441 (Hartree/Particle)
Thermal correction to Energy=	0.184922
Thermal correction to Enthalpy=	0.185867
Thermal correction to Gibbs Free Energy=	0.146256
Sum of electronic and zero-point Energies=	-311.599170
Sum of electronic and thermal Energies=	-311.591689
Sum of electronic and thermal Enthalpies=	-311.590745
Sum of electronic and thermal Free Energies=	-311.630356

MP2/6-31G(d)

XYZ Coordinates

C	-0.85924600	-0.22222600	-0.18632000
C	0.03958000	-1.23731400	-0.51211300
C	1.25674000	-1.30296400	0.26460200
C	2.14190600	0.12095300	-0.02849000
C	1.28309100	1.23589400	0.29677000
C	0.14719700	1.42392300	-0.49801600
H	1.92531300	-2.12502800	-0.00511500
H	0.07534600	-1.57639700	-1.55006100
H	2.40735700	0.05932700	-1.08644700
H	3.04327800	0.03738100	0.58387400
H	1.23748800	1.55421200	1.33877700
H	-0.56604600	2.19940400	-0.21674100
H	1.09042400	-1.29518300	1.34388400
H	0.25312500	1.31329200	-1.57573600
C	-2.31490200	-0.03972900	-0.41261300
H	-2.66571700	0.90722100	-0.81558200
H	-2.90491600	-0.89897300	-0.71962300
C	-1.73568700	-0.01771100	0.99972300
H	-1.92392600	-0.87596900	1.63943800
H	-1.72379600	0.93575600	1.52207300

Zero-point correction=	0.179443 (Hartree/Particle)
Thermal correction to Energy=	0.186705
Thermal correction to Enthalpy=	0.187650
Thermal correction to Gibbs Free Energy=	0.148420
Sum of electronic and zero-point Energies=	-310.643847
Sum of electronic and thermal Energies=	-310.636585
Sum of electronic and thermal Enthalpies=	-310.635641
Sum of electronic and thermal Free Energies=	-310.674870



B3LYP/6-31G(d)

XYZ Coordinates

C	-3.00666100	-0.40361300	0.55781100
H	-2.83443700	-1.05952500	1.40911900
C	-2.07595100	-0.21276900	-0.37892000
C	-0.71759600	-0.86051500	-0.38639500
H	-0.68021400	-1.63477800	0.39108500
H	-0.58105700	-1.38013000	-1.34789700
C	0.48976700	0.07601300	-0.18436100
C	2.79063300	-0.73879900	0.48650000
C	1.79008200	-0.63350400	-0.38942800
H	1.89459600	-1.11584500	-1.36429700
H	-3.97873900	0.07995600	0.50681800
H	-2.30290900	0.44646500	-1.21741200
H	2.73914400	-0.29777100	1.47876300
H	3.70391400	-1.27396900	0.24068400
C	0.41364100	1.52269000	-0.64796200
H	-0.50372900	1.88285900	-1.10503100
H	1.31904800	1.96076100	-1.05896600
C	0.39801900	1.19154800	0.82572700
H	1.27634400	1.44086600	1.41343000
H	-0.54357400	1.30480100	1.35587000

Zero-point correction= 0.176719 (Hartree/Particle)
Thermal correction to Energy= 0.185549
Thermal correction to Enthalpy= 0.186493
Thermal correction to Gibbs Free Energy= 0.142884
Sum of electronic and zero-point Energies= -311.817537
Sum of electronic and thermal Energies= -311.808707
Sum of electronic and thermal Enthalpies= -311.807762
Sum of electronic and thermal Free Energies= -311.851371

M06-2X/6-31G(d)

XYZ Coordinates

C	-2.93513000	-0.35045200	0.59572900
H	-2.71277700	-0.90920100	1.50207800
C	-2.05320200	-0.26914800	-0.39697500
C	-0.69407700	-0.90819700	-0.37359800
H	-0.65066900	-1.64422500	0.43862200
H	-0.54088500	-1.46086400	-1.31125900
C	0.47903800	0.06133100	-0.19696700
C	2.77832800	-0.66632600	0.51666500
C	1.80205900	-0.60300500	-0.38399600
H	1.94276900	-1.08044400	-1.35557900
H	-3.90801000	0.12782600	0.53861600
H	-2.31394400	0.29353900	-1.29285700
H	2.67313300	-0.22229000	1.50276100
H	3.71668600	-1.16701900	0.30053200
C	0.35346500	1.48527000	-0.68158200
H	-0.57870300	1.80375500	-1.13678900
H	1.24417900	1.94439700	-1.09772100
C	0.35227900	1.18023800	0.79189900
H	1.22538600	1.46739000	1.36742000
H	-0.59371600	1.26886400	1.31711800

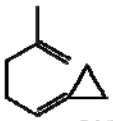
Zero-point correction= 0.178081 (Hartree/Particle)
Thermal correction to Energy= 0.187164
Thermal correction to Enthalpy= 0.188108
Thermal correction to Gibbs Free Energy= 0.143339
Sum of electronic and zero-point Energies= -311.648692
Sum of electronic and thermal Energies= -311.639608
Sum of electronic and thermal Enthalpies= -311.638664
Sum of electronic and thermal Free Energies= -311.683533

MP2/6-31G(d)

XYZ Coordinates

C	-2.91596400	-0.40179500	0.59981100
H	-2.67617500	-0.99761000	1.47657100
C	-2.04452700	-0.26225200	-0.40864600
C	-0.67959800	-0.88389000	-0.42958200
H	-0.62083500	-1.66217500	0.34251600
H	-0.52620800	-1.38610800	-1.39571900
C	0.48237100	0.08735700	-0.20797100
C	2.74564000	-0.73116300	0.52195900
C	1.80715500	-0.55799600	-0.41826000
H	1.99399800	-0.93007500	-1.42797000
H	-3.89608800	0.06401300	0.57742600
H	-2.33147100	0.33338800	-1.27463700
H	2.59979700	-0.39512700	1.54384000
H	3.68956800	-1.21717500	0.29626500
C	0.34393600	1.53167800	-0.62850400
H	-0.59023800	1.86231600	-1.07070400
H	1.22944800	2.01916700	-1.02522100
C	0.34577300	1.16151100	0.83299000
H	1.21776700	1.42659000	1.42119300
H	-0.59828900	1.22210000	1.36565900

Zero-point correction=	0.179783 (Hartree/Particle)
Thermal correction to Energy=	0.188454
Thermal correction to Enthalpy=	0.189398
Thermal correction to Gibbs Free Energy=	0.146221
Sum of electronic and zero-point Energies=	-310.697113
Sum of electronic and thermal Energies=	-310.688442
Sum of electronic and thermal Enthalpies=	-310.687498
Sum of electronic and thermal Free Energies=	-310.730675



B3LYP/6-31G(d)

XYZ Coordinates

C	2.97332700	1.48508700	-0.16077100
H	3.94608100	1.73850500	0.25421200
H	2.40739700	2.30170900	-0.60296200
C	2.49786200	0.23553200	-0.13179200
C	1.13964100	-0.10485400	-0.70933300
H	0.75820800	0.74784100	-1.28284200
H	1.24234900	-0.94058400	-1.41875700
C	0.08382100	-0.49335900	0.35594800
H	0.45525800	-1.35123000	0.93521200
H	-0.04245800	0.33649700	1.06079600
C	-2.37647100	-0.19278900	-0.04220300
C	-1.24507400	-0.84764000	-0.25829200
H	-1.25406500	-1.69974700	-0.94125200
C	-3.07372500	0.90261700	0.64913200
H	-3.27485800	0.81435400	1.71632600
H	-2.91397300	1.92799400	0.31712700
C	-3.81506100	-0.05369500	-0.30380300
H	-4.50626800	-0.77311800	0.13429500
H	-4.14410800	0.34075500	-1.26475400
C	3.28963200	-0.90065500	0.47027900
H	4.26393900	-0.56251300	0.83628400
H	2.75879200	-1.36664000	1.31083800
H	3.45999200	-1.69539000	-0.26951500

Zero-point correction=	[illegible] (Hartree/Particle)
Thermal correction to Energy=	0.215117
Thermal correction to Enthalpy=	0.216061
Thermal correction to Gibbs Free Energy=	0.167398
Sum of electronic and zero-point Energies=	-351.100071
Sum of electronic and thermal Energies=	-351.089534
Sum of electronic and thermal Enthalpies=	-351.088590
Sum of electronic and thermal Free Energies=	-351.137254

M06-2X/6-31G(d)

XYZ Coordinates

C	2.99486300	1.46746000	-0.15962500
H	3.96242700	1.68616300	0.28400800
H	2.47637100	2.29234200	-0.64045400
C	2.46930500	0.24351300	-0.11938500
C	1.12864800	-0.06185200	-0.74102300
H	0.73450600	0.83459800	-1.23186500
H	1.25649700	-0.82485400	-1.52318900
C	0.08848700	-0.57249900	0.27273500
H	0.45633100	-1.49976800	0.73170900
H	-0.03198000	0.16365300	1.07556800
C	-2.35089400	-0.18245900	-0.06843300
C	-1.24159800	-0.82985500	-0.37717900
H	-1.26896100	-1.58364600	-1.16533300
C	-2.99959600	0.83263600	0.76847500
H	-3.19332700	0.60512000	1.81369300
H	-2.80194000	1.88249600	0.56735600
C	-3.78115300	0.04292200	-0.28560500
H	-4.48889100	-0.70292600	0.06720100
H	-4.09772700	0.57398400	-1.17971400
C	3.17892800	-0.90532300	0.54878100
H	4.19014000	-0.62527400	0.85385700
H	2.63802500	-1.24176600	1.44085800
H	3.24659000	-1.76737600	-0.12612600

Zero-point correction=	0.206277 (Hartree/Particle)
Thermal correction to Energy=	0.216020
Thermal correction to Enthalpy=	0.216964
Thermal correction to Gibbs Free Energy=	0.170489
Sum of electronic and zero-point Energies=	-350.918737
Sum of electronic and thermal Energies=	-350.908995
Sum of electronic and thermal Enthalpies=	-350.908051
Sum of electronic and thermal Free Energies=	-350.954526

MP2/6-31G(d)

XYZ Coordinates

C	2.90592200	1.50665800	-0.16371500
H	3.86923900	1.78108800	0.25686400
H	2.32135800	2.30703000	-0.60834600
C	2.45975300	0.24115100	-0.14042400
C	1.11532000	-0.12548600	-0.71464700
H	0.70824100	0.72444300	-1.27445500
H	1.23317300	-0.95201700	-1.43011900
C	0.09275800	-0.53794500	0.35977900
H	0.47978900	-1.39413200	0.92709900
H	-0.03883100	0.28851700	1.06758100
C	-2.34934600	-0.20457500	-0.03743200
C	-1.23226900	-0.89401900	-0.24719400
H	-1.25867500	-1.75747300	-0.91460000
C	-3.00327300	0.92180300	0.63858800
H	-3.20521200	0.85333100	1.70517800
H	-2.81379100	1.93131100	0.28587800
C	-3.78023500	-0.02320000	-0.29463900
H	-4.49040400	-0.70860700	0.16232100
H	-4.09845900	0.37073300	-1.25721600
C	3.26839800	-0.87362000	0.46776700
H	4.24617800	-0.51571200	0.80110200
H	2.75905800	-1.31673500	1.33011600
H	3.42616800	-1.67820700	-0.25989900

Zero-point correction=	0.208414 (Hartree/Particle)
Thermal correction to Energy=	0.218889
Thermal correction to Enthalpy=	0.219833
Thermal correction to Gibbs Free Energy=	0.171186
Sum of electronic and zero-point Energies=	-349.823704
Sum of electronic and thermal Energies=	-349.813229
Sum of electronic and thermal Enthalpies=	-349.812285
Sum of electronic and thermal Free Energies=	-349.860932

B3LYP/6-31G(d)

XYZ Coordinates

C	-1.12734800	0.20314700	0.10455900
C	-0.61628600	1.50645500	-0.03660400
C	0.66615300	1.66075800	-0.64297700
C	1.85870000	0.76544100	0.38553400
C	1.35621600	-0.57197700	0.46289200
C	0.13507800	-0.73474000	1.15684400
H	1.05797000	2.67913900	-0.68444000
H	-0.92904600	2.25535400	0.69309700
H	1.83451000	1.34264300	1.30985400
H	2.80984600	0.89948700	-0.13442900
H	-0.28268500	-1.74102400	1.21491900
H	0.80863500	1.14947100	-1.59906900
H	0.01420400	-0.18959600	2.09153100
C	-2.52624500	-0.26904500	0.31493700
H	-2.71714300	-1.01233800	1.08661100
H	-3.34116300	0.43714400	0.17390500
C	-1.73268600	-0.72483000	-0.90755800
H	-2.00206900	-0.30810300	-1.87521800
H	-1.42346600	-1.76694800	-0.94435300
C	1.75293300	-1.55409800	-0.60806900
H	1.37022600	-1.24187000	-1.59637900
H	2.84238800	-1.63379900	-0.70317600
H	1.35871200	-2.55622100	-0.41019800

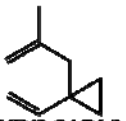
Zero-point correction= 0.203763 (Hartree/Particle)
Thermal correction to Energy= 0.212947
Thermal correction to Enthalpy= 0.213891
Thermal correction to Gibbs Free Energy= 0.170293
Sum of electronic and zero-point Energies= -351.047889
Sum of electronic and thermal Energies= -351.038705
Sum of electronic and thermal Enthalpies= -351.037761
Sum of electronic and thermal Free Energies= -351.081359

M06-2X/6-31G(d)

XYZ Coordinates

C	-1.09984000	0.24952900	0.11428800
C	-0.55209700	1.52706000	-0.03717900
C	0.71920400	1.61249700	-0.66365200
C	1.87978400	0.69794800	0.37880100
C	1.31190800	-0.60314600	0.47860800
C	0.11391200	-0.70070900	1.20467100
H	1.16228900	2.60585100	-0.73918400
H	-0.84191800	2.30256400	0.67082900
H	1.88606100	1.29531200	1.28938000
H	2.82343500	0.78072400	-0.16277300
H	-0.36206700	-1.67926100	1.28066800
H	0.82543800	1.05485600	-1.59839300
H	0.02555100	-0.11804200	2.11933600
C	-2.49742000	-0.21525100	0.29092500
H	-2.70707600	-0.94538700	1.06792600
H	-3.30157900	0.49077100	0.10939400
C	-1.67011400	-0.69127200	-0.89389200
H	-1.90848000	-0.28685800	-1.87315500
H	-1.36097800	-1.73309900	-0.89795800
C	1.59202800	-1.58584000	-0.62163600
H	1.13923100	-1.23679300	-1.56634300
H	2.66496500	-1.70393800	-0.80106600
H	1.17093200	-2.57159700	-0.40426200

Zero-point correction= 0.205981 (Hartree/Particle)
Thermal correction to Energy= 0.214805
Thermal correction to Enthalpy= 0.215749
Thermal correction to Gibbs Free Energy= 0.173263
Sum of electronic and zero-point Energies= -350.870773
Sum of electronic and thermal Energies= -350.861949
Sum of electronic and thermal Enthalpies= -350.861005
Sum of electronic and thermal Free Energies= -350.903491



MP2/6-31G(d)

XYZ Coordinates

C	-1.13403100	0.24995700	0.10360600
C	-0.57381700	1.51715400	-0.03009900
C	0.73996200	1.59155200	-0.63509100
C	1.82661100	0.76295200	0.34620600
C	1.33666300	-0.59826400	0.47940300
C	0.15547000	-0.73912900	1.21694300
H	1.13052400	2.60836200	-0.73397900
H	-0.85351500	2.28530700	0.69403600
H	1.84527400	1.31961400	1.28613800
H	2.79881200	0.84826100	-0.14846400
H	-0.30240600	-1.72703100	1.28855700
H	0.80434300	1.07655100	-1.59929400
H	0.04007900	-0.14601800	2.12185100
C	-2.52815700	-0.22366200	0.28396100
H	-2.73519400	-0.95091600	1.06555000
H	-3.34273400	0.47059400	0.09568600
C	-1.68943500	-0.70536400	-0.89795600
H	-1.93061200	-0.31577100	-1.88387900
H	-1.37529200	-1.74568900	-0.89252500
C	1.65295300	-1.56673300	-0.62242300
H	1.22355000	-1.22685600	-1.57927900
H	2.73344500	-1.66679000	-0.76980700
H	1.24641500	-2.56040200	-0.41188300

Zero-point correction=	0.208175 (Hartree/Particle)
Thermal correction to Energy=	0.216889
Thermal correction to Enthalpy=	0.217833
Thermal correction to Gibbs Free Energy=	0.175402
Sum of electronic and zero-point Energies=	-349.789615
Sum of electronic and thermal Energies=	-349.780901
Sum of electronic and thermal Enthalpies=	-349.779957
Sum of electronic and thermal Free Energies=	-349.822388

B3LYP/6-31G(d)

XYZ Coordinates

C	2.39951400	0.81211200	-0.99530400
H	1.91733600	1.32955600	-1.82135300
C	1.79680300	-0.18794500	-0.34203500
C	0.39621700	-0.64637000	-0.70037600
H	0.20960200	-0.46894500	-1.76690000
H	0.33763100	-1.73510400	-0.55644300
C	-0.76999600	-0.00419400	0.08421400
C	-3.19919700	-0.40109000	-0.51491400
C	-2.02661400	-0.80905700	-0.02688800
H	-1.93647700	-1.83977100	0.32441500
H	3.40280900	1.14245500	-0.73675300
H	-3.34783600	0.60542100	-0.89772900
H	-4.05905700	-1.06474000	-0.54920400
C	-0.52585400	0.70599500	1.40831000
H	0.48927400	0.77719400	1.78688100
H	-1.28853000	0.60594700	2.17586800
C	-0.86479300	1.49831900	0.17031400
H	-1.84290000	1.96566300	0.10895200
H	-0.06233700	2.07563000	-0.28058600
C	2.49050900	-0.95077700	0.76156400
H	2.67416600	-1.98909100	0.45115200
H	3.45329200	-0.50193600	1.02552700
H	1.87349900	-1.00423400	1.66686300

Zero-point correction=	0.205086 (Hartree/Particle)
Thermal correction to Energy=	0.215233
Thermal correction to Enthalpy=	0.216178
Thermal correction to Gibbs Free Energy=	0.169685
Sum of electronic and zero-point Energies=	-351.106420
Sum of electronic and thermal Energies=	-351.096273
Sum of electronic and thermal Enthalpies=	-351.095328
Sum of electronic and thermal Free Energies=	-351.141821

M06-2X/6-31G(d)

XYZ Coordinates

C	2.36510000	0.88451400	-0.91110200
H	1.88289500	1.45354500	-1.70194400
C	1.77275100	-0.17389000	-0.35707600
C	0.38560800	-0.61334200	-0.76131700
H	0.19678000	-0.35977600	-1.81085200
H	0.32619600	-1.70808200	-0.68666600
C	-0.75434900	-0.01604600	0.07642100
C	-3.18095600	-0.34873100	-0.50217200
C	-2.01936700	-0.80054800	-0.03893300
H	-1.94462900	-1.84082100	0.28350900
H	3.35526000	1.20986000	-0.60402400
H	-3.29682800	0.67257300	-0.85410700
H	-4.05771800	-0.98679200	-0.54865800
C	-0.47205800	0.62732500	1.41426700
H	0.55466800	0.68115200	1.76146500
H	-1.21707300	0.49681400	2.19240000
C	-0.83865900	1.47301900	0.22797700
H	-1.81593200	1.94298800	0.21697500
H	-0.04159000	2.06085000	-0.21697300
C	2.44515100	-1.01309100	0.69719300
H	2.69249300	-2.00068100	0.28834500
H	3.36764400	-0.55202100	1.05928000
H	1.77850400	-1.18486900	1.54970100

Zero-point correction= 0.207282 (Hartree/Particle)
Thermal correction to Energy= 0.217204
Thermal correction to Enthalpy= 0.218148
Thermal correction to Gibbs Free Energy= 0.172470
Sum of electronic and zero-point Energies= -350.930908
Sum of electronic and thermal Energies= -350.920986
Sum of electronic and thermal Enthalpies= -350.920041
Sum of electronic and thermal Free Energies= -350.965719

MP2/6-31G(d)

XYZ Coordinates

C	2.39951400	0.81211200	-0.99530400
H	1.91733600	1.32955600	-1.82135300
C	1.79680300	-0.18794500	-0.34203500
C	0.39621700	-0.64637000	-0.70037600
H	0.20960200	-0.46894500	-1.76690000
H	0.33763100	-1.73510400	-0.55644300
C	-0.76999600	-0.00419400	0.08421400
C	-3.19919700	-0.40109000	-0.51491400
C	-2.02661400	-0.80905700	-0.02688800
H	-1.93647700	-1.83977100	0.32441500
H	3.40280900	1.14245500	-0.73675300
H	-3.34783600	0.60542100	-0.89772900
H	-4.05905700	-1.06474000	-0.54920400
C	-0.52585400	0.70599500	1.40831000
H	0.48927400	0.77719400	1.78688100
H	-1.28853000	0.60594700	2.17586800
C	-0.86479300	1.49831900	0.17031400
H	-1.84290000	1.96566300	0.10895200
H	-0.06233700	2.07563000	-0.28058600
C	2.49050900	-0.95077700	0.76156400
H	2.67416600	-1.98909100	0.45115200
H	3.45329200	-0.50193600	1.02552700
H	1.87349900	-1.00423400	1.66686300

Zero-point correction= 0.205086 (Hartree/Particle)
Thermal correction to Energy= 0.215233
Thermal correction to Enthalpy= 0.216178
Thermal correction to Gibbs Free Energy= 0.169685
Sum of electronic and zero-point Energies= -351.106420
Sum of electronic and thermal Energies= -351.096273
Sum of electronic and thermal Enthalpies= -351.095328
Sum of electronic and thermal Free Energies= -351.141821

B3LYP/6-31G(d)

XYZ Coordinates

C	3.10601400	0.43440600	-0.38965800
H	2.77760100	1.06721900	-1.21695200
C	2.27553900	-0.50851700	0.06361300
C	0.89202700	-0.77613900	-0.46264900
H	0.68511700	-0.12971800	-1.32464500
C	-0.20744900	-0.56807000	0.60693500
H	0.03507000	-1.19290000	1.48062100
H	-0.19089500	0.47291900	0.94949500
C	-2.59595500	-0.07094700	0.01373200
C	-1.58261900	-0.91990800	0.10343200
H	-1.73267100	-1.95163400	-0.22174500
C	-3.10620300	1.29238100	0.22569900
H	-3.30546400	1.63327600	1.24120800
H	-2.79363500	2.08808000	-0.44982900
C	-3.99869800	0.17473500	-0.34595000
H	-4.78770600	-0.22260200	0.29195600
H	-4.27470800	0.23352000	-1.39843800
C	4.48407400	0.70789100	0.14250400
H	5.24602800	0.58623100	-0.63963900
H	4.57346400	1.74026400	0.50767100
H	4.73759800	0.03435300	0.96833600
H	2.60081100	-1.14085500	0.89370100

Zero-point correction= 0.204542 (Hartree/Particle)
Thermal correction to Energy= 0.215199
Thermal correction to Enthalpy= 0.216143
Thermal correction to Gibbs Free Energy= 0.167359
Sum of electronic and zero-point Energies= -351.101082
Sum of electronic and thermal Energies= -351.090426
Sum of electronic and thermal Enthalpies= -351.089482
Sum of electronic and thermal Free Energies= -351.138265

M06-2X/6-31G(d)

XYZ Coordinates

C	3.07551300	0.43180300	-0.39758500
H	2.74562400	1.04629000	-1.23671800
C	2.25600400	-0.50992700	0.06502600
C	0.87979600	-0.79118900	-0.46352100
H	0.66903700	-0.14898000	-1.32653700
C	-0.20626200	-0.57888200	0.60589400
H	0.03961200	-1.19588400	1.48178900
H	-0.19530000	0.46545200	0.93623500
C	-2.57631700	-0.07675900	0.01207100
C	-1.57598700	-0.93494400	0.10164000
H	-1.72980200	-1.96415100	-0.22574300
C	-3.05676800	1.29211600	0.22941800
H	-3.24836800	1.62531700	1.24632900
H	-2.72505400	2.07769500	-0.44483300
C	-3.96848000	0.20363500	-0.34444900
H	-4.75972200	-0.17900800	0.29525700
H	-4.23677300	0.27409300	-1.39555400
C	4.44321800	0.72171000	0.14583400
H	5.21160000	0.59021900	-0.62438500
H	4.51825400	1.75719400	0.49689400
H	4.68365100	0.06021600	0.98296900
H	2.58103600	-1.12421700	0.90796700
H	0.82190100	-1.82961900	-0.81963300

Zero-point correction= 0.206529 (Hartree/Particle)
Thermal correction to Energy= 0.217150
Thermal correction to Enthalpy= 0.218094
Thermal correction to Gibbs Free Energy= 0.169269
Sum of electronic and zero-point Energies= -350.917663
Sum of electronic and thermal Energies= -350.907042
Sum of electronic and thermal Enthalpies= -350.906098
Sum of electronic and thermal Free Energies= -350.954924

MP2/6-31G(d)

XYZ Coordinates

C	3.03885900	0.46534100	-0.37755500
H	2.67146100	1.13675700	-1.15524100
C	2.24939700	-0.53846500	0.03119800
C	0.86677200	-0.80015300	-0.48516200
H	0.64115900	-0.11521200	-1.31137000
C	-0.20041600	-0.63345300	0.61052500
H	0.05388300	-1.28601200	1.45752100
H	-0.17985800	0.39741700	0.98151600
C	-2.56048000	-0.07131700	0.02010200
C	-1.57598300	-0.96022400	0.10882600
H	-1.75578400	-1.98543600	-0.22033500
C	-3.00880700	1.30895400	0.23751900
H	-3.20205600	1.64850800	1.25262300
H	-2.66109500	2.09058200	-0.43423800
C	-3.94588600	0.23609600	-0.34429000
H	-4.75191300	-0.12476900	0.29056700
H	-4.21037200	0.31689900	-1.39621100
C	4.41246200	0.74245500	0.15497800
H	5.16403900	0.69324600	-0.64062700
H	4.47347800	1.74531300	0.59190900
H	4.68611500	0.01766900	0.92690000
H	2.61238600	-1.21107700	0.81159500
H	0.80304900	-1.81929200	-0.89144600

Zero-point correction= 0.208524 (Hartree/Particle)
Thermal correction to Energy= 0.219098
Thermal correction to Enthalpy= 0.220042
Thermal correction to Gibbs Free Energy= 0.171385
Sum of electronic and zero-point Energies= -349.822999
Sum of electronic and thermal Energies= -349.812425
Sum of electronic and thermal Enthalpies= -349.811481
Sum of electronic and thermal Free Energies= -349.860138

B3LYP/6-31G(d)

XYZ Coordinates

C	-0.57249700	-0.74099100	-0.16830500
C	0.59599700	-1.42718500	-0.54204700
C	1.77012000	-1.27229700	0.21477400
C	2.23759100	0.61497800	-0.02574600
C	1.06850400	1.30617700	0.33512000
C	-0.11167000	1.19247500	-0.43077400
H	2.67290800	-1.77701300	-0.12898300
H	0.69735900	-1.71405600	-1.59064500
H	2.49740300	0.56445900	-1.08135100
H	3.11246200	0.72029300	0.61537600
H	1.67851000	-1.26066900	1.29902100
H	0.03101700	1.10478100	-1.50822600
C	-1.99707200	-1.09383300	-0.42474300
H	-2.68754100	-0.33422100	-0.78405600
H	-2.21887000	-2.09213600	-0.79614500
C	-1.47613300	-0.93930800	1.00337600
H	-1.33996300	-1.83498600	1.60563000
H	-1.83063900	-0.07937000	1.56741300
C	-1.30479300	2.05749500	-0.06801900
H	-2.24437000	1.67517400	-0.47887000
H	-1.41850500	2.15242400	1.01784800
H	-1.17104800	3.06859100	-0.47290400
H	0.96099800	1.62166900	1.37407500

Zero-point correction= 0.203803 (Hartree/Particle)
Thermal correction to Energy= 0.213033
Thermal correction to Enthalpy= 0.213977
Thermal correction to Gibbs Free Energy= 0.170470
Sum of electronic and zero-point Energies= -351.042047
Sum of electronic and thermal Energies= -351.032817
Sum of electronic and thermal Enthalpies= -351.031873
Sum of electronic and thermal Free Energies= -351.075380

M06-2X/6-31G(d)

XYZ Coordinates

C	-0.53874200	-0.73860900	-0.17513700
C	0.64170700	-1.39834500	-0.53636800
C	1.79551100	-1.18922700	0.23593000
C	2.20036900	0.64810500	-0.03750700
C	1.01873000	1.31560100	0.32251700
C	-0.15079900	1.16177500	-0.44266200
H	2.71759000	-1.67655500	-0.07820500
H	0.76032000	-1.69610200	-1.57833800
H	2.45229600	0.60462800	-1.09521300
H	3.07604500	0.78858100	0.59448200
H	1.67359200	-1.16986700	1.31724200
H	-0.00877700	1.08304600	-1.52081300
C	-1.94839600	-1.13146500	-0.41948000
H	-2.65943000	-0.40005400	-0.79165600
H	-2.13418800	-2.14282900	-0.76818300
C	-1.43007400	-0.93841400	0.99716000
H	-1.26691000	-1.82034200	1.60950200
H	-1.80310200	-0.07485800	1.54141400
C	-1.36745800	1.97933900	-0.06081100
H	-2.30555700	1.53165400	-0.39884800
H	-1.42284000	2.11644000	1.02375400
H	-1.30382700	2.97286100	-0.51644300
H	0.89969300	1.63083400	1.35944600

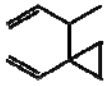
Zero-point correction=	0.205767 (Hartree/Particle)
Thermal correction to Energy=	0.214753
Thermal correction to Enthalpy=	0.215698
Thermal correction to Gibbs Free Energy=	0.172717
Sum of electronic and zero-point Energies=	-350.864320
Sum of electronic and thermal Energies=	-350.855334
Sum of electronic and thermal Enthalpies=	-350.854390
Sum of electronic and thermal Free Energies=	-350.897370

MP2/6-31G(d)

XYZ Coordinates

C	-0.52636400	-0.72412100	-0.18538800
C	0.66188100	-1.37726900	-0.55749700
C	1.83770400	-1.06980700	0.21130300
C	2.16878900	0.60146700	-0.02066200
C	0.98469500	1.33392300	0.33784100
C	-0.18389000	1.14644200	-0.43412100
H	2.74611200	-1.59288200	-0.09920500
H	0.79083300	-1.64141200	-1.61008400
H	2.43449900	0.66193900	-1.07794600
H	3.04550800	0.81274900	0.59682700
H	1.70106300	-1.15389300	1.29114200
H	-0.01948900	1.09078000	-1.51239000
C	-1.92963500	-1.17474000	-0.39848700
H	-2.67956400	-0.46660200	-0.73804500
H	-2.08478000	-2.18728900	-0.76078500
C	-1.38156500	-0.97840300	1.00946800
H	-1.16437300	-1.86051000	1.60595600
H	-1.77676200	-0.14097500	1.57827900
C	-1.41169300	1.96063400	-0.07780700
H	-2.32988700	1.54100400	-0.49534400
H	-1.52747300	2.04258300	1.00681200
H	-1.30816200	2.97400800	-0.47891400
H	0.85293600	1.61174600	1.38580600

Zero-point correction=	0.208388 (Hartree/Particle)
Thermal correction to Energy=	0.217053
Thermal correction to Enthalpy=	0.217997
Thermal correction to Gibbs Free Energy=	0.175641
Sum of electronic and zero-point Energies=	-349.782712
Sum of electronic and thermal Energies=	-349.774047
Sum of electronic and thermal Enthalpies=	-349.773103
Sum of electronic and thermal Free Energies=	-349.815459



B3LYP/6-31G(d)

XYZ Coordinates

C	-2.79775900	-0.54791600	-0.96057000
H	-2.58465700	-0.33426500	-2.00627100
C	-1.97134800	-0.16710400	0.01480400
C	-0.69657300	0.61695700	-0.18573200
H	-0.61832900	0.85110300	-1.25675200
C	0.59123100	-0.16659500	0.18205600
C	2.74764000	0.26625000	-1.05281900
C	1.85509300	0.58410700	-0.11325500
H	2.03710000	1.46766300	0.49982200
H	-3.72089300	-1.08320000	-0.75344300
H	2.61935100	-0.59956900	-1.69806600
H	3.64341100	0.86147700	-1.20982700
C	0.60330900	-1.04884100	1.41817000
H	-0.30033100	-1.13103200	2.01652900
H	1.52205000	-1.08879600	1.99760500
C	0.61024800	-1.67040000	0.04097200
H	1.52740200	-2.14473500	-0.29485800
H	-0.29843800	-2.15752000	-0.29940100
C	-0.79441800	1.94897300	0.58915100
H	0.06039600	2.60041400	0.38164800
H	-1.70389100	2.48997100	0.30706400
H	-0.82889400	1.77064600	1.67097400
H	-2.23881500	-0.39474400	1.04831200

Zero-point correction=	0.204928 (Hartree/Particle)
Thermal correction to Energy=	0.215150
Thermal correction to Enthalpy=	0.216094
Thermal correction to Gibbs Free Energy=	0.169295
Sum of electronic and zero-point Energies=	-351.101154
Sum of electronic and thermal Energies=	-351.090932
Sum of electronic and thermal Enthalpies=	-351.089988
Sum of electronic and thermal Free Energies=	-351.136786

M06-2X/6-31G(d)

XYZ Coordinates

C	-2.76664400	-0.55460700	-0.88981500
H	-2.49422500	-0.51336600	-1.94208000
C	-1.97323100	-0.04493500	0.04811100
C	-0.66380800	0.64846600	-0.22098400
H	-0.58671200	0.81367200	-1.30462700
C	0.56488500	-0.18824800	0.18121200
C	2.74940800	0.20962700	-0.97856400
C	1.86917900	0.51384600	-0.02901900
H	2.08661600	1.33632300	0.65297700
H	-3.71342800	-1.02656400	-0.64593200
H	2.56674800	-0.60031900	-1.68025300
H	3.68097800	0.75621000	-1.08778600
C	0.48014900	-1.10261900	1.37645700
H	-0.45648800	-1.16734000	1.92108400
H	1.36897200	-1.20066500	1.99180700
C	0.52916200	-1.67534400	-0.01557600
H	1.44365700	-2.17168800	-0.32179300
H	-0.38491900	-2.10611300	-0.41057600
C	-0.66124300	2.01175200	0.48422600
H	0.20881900	2.60865300	0.19816500
H	-1.56080000	2.57860900	0.22780700
H	-0.64063100	1.87686600	1.57223400
H	-2.28572500	-0.09190600	1.09268800

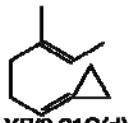
Zero-point correction=	0.206957 (Hartree/Particle)
Thermal correction to Energy=	0.216985
Thermal correction to Enthalpy=	0.217930
Thermal correction to Gibbs Free Energy=	0.171682
Sum of electronic and zero-point Energies=	-350.926605
Sum of electronic and thermal Energies=	-350.916577
Sum of electronic and thermal Enthalpies=	-350.915632
Sum of electronic and thermal Free Energies=	-350.961880

MP2/6-31G(d)

XYZ Coordinates

C	-2.75282600	-0.54132700	-0.94492000
H	-2.48285100	-0.42959400	-1.99169600
C	-1.95976400	-0.08320900	0.03327700
C	-0.66354300	0.64039000	-0.19602200
H	-0.57450900	0.83616900	-1.27487500
C	0.57343400	-0.18229800	0.19649600
C	2.70234600	0.23736000	-1.05379400
C	1.86561400	0.52312300	-0.04663500
H	2.12493100	1.32729600	0.64283700
H	-3.69537100	-1.03639500	-0.73268800
H	2.48487600	-0.55369900	-1.76552000
H	3.62816000	0.78596400	-1.19710700
C	0.51538600	-1.08412100	1.40568700
H	-0.41033600	-1.15131900	1.96849800
H	1.41389300	-1.16442100	2.01085200
C	0.54939500	-1.67659800	0.01934800
H	1.46448700	-2.16597200	-0.29752900
H	-0.36333800	-2.12532600	-0.35872500
C	-0.69487800	1.98499400	0.54217500
H	0.17624000	2.59766500	0.29593300
H	-1.59289700	2.54813500	0.27076800
H	-0.70601300	1.82235700	1.62538300
H	-2.27825800	-0.20074900	1.07019600

Zero-point correction=	0.208605 (Hartree/Particle)
Thermal correction to Energy=	0.218623
Thermal correction to Enthalpy=	0.219567
Thermal correction to Gibbs Free Energy=	0.173305
Sum of electronic and zero-point Energies=	-349.835989
Sum of electronic and thermal Energies=	-349.825972
Sum of electronic and thermal Enthalpies=	-349.825027
Sum of electronic and thermal Free Energies=	-349.871290



B3LYP/6-31G(d)

XYZ Coordinates

C	2.63254200	0.92705100	-0.34173800
H	2.07317400	1.70832600	-0.85974100
C	2.02505300	-0.26113200	-0.19455500
C	0.61983100	-0.46578500	-0.72799500
H	0.33548900	0.38394400	-1.35974500
C	-0.45610400	-0.63682000	0.37399500
H	-0.18499300	-1.49012900	1.01248900
H	-0.46197500	0.25196400	1.01566200
C	-2.86785700	-0.05711100	-0.01766800
C	-1.83137900	-0.86294700	-0.19696900
H	-1.96130900	-1.75386000	-0.81505400
C	-3.40941200	1.16441900	0.59761200
H	-3.59970900	1.17974100	1.67035700
H	-3.12934300	2.13482000	0.18885000
C	-4.28267700	0.24257300	-0.27426100
H	-5.04979900	-0.35049900	0.22287700
H	-4.57879600	0.60505200	-1.25829600
C	2.64600100	-1.46116300	0.48121800
H	3.68520600	-1.29650000	0.77481700
H	2.09071900	-1.74542900	1.38495900
H	2.62125100	-2.33421800	-0.18568000
C	4.00123300	1.34846200	0.11494000
H	4.60940300	1.68849500	-0.73465900
H	3.93554500	2.19817000	0.80874900
H	4.55322100	0.55214300	0.62126800
H	0.59852600	-1.35729700	-1.37434000

Zero-point correction=	0.232956 (Hartree/Particle)
Thermal correction to Energy=	0.245117
Thermal correction to Enthalpy=	0.246061
Thermal correction to Gibbs Free Energy=	0.193514
Sum of electronic and zero-point Energies=	-390.387980
Sum of electronic and thermal Energies=	-390.375819
Sum of electronic and thermal Enthalpies=	-390.374875
Sum of electronic and thermal Free Energies=	-390.427422

M06-2X/6-31G(d)

XYZ Coordinates

C	2.64869500	0.91088700	-0.37613200
H	2.13840500	1.68599500	-0.94897900
C	1.99963400	-0.24480600	-0.20015700
C	0.61361500	-0.43679100	-0.76886800
H	0.32596300	0.44072100	-1.35829900
C	-0.45631300	-0.68101200	0.31117800
H	-0.19238600	-1.58089500	0.88301400
H	-0.46421700	0.15991800	1.01394900
C	-2.84539700	-0.05088500	-0.03668600
C	-1.82414900	-0.85062800	-0.28706900
H	-1.95761700	-1.67652200	-0.98713600
C	-3.35582600	1.11494500	0.69285100
H	-3.54544400	1.02409800	1.75942400
H	-3.04909700	2.10822300	0.37495500
C	-4.24712400	0.31009400	-0.25761400
H	-5.02392200	-0.30940500	0.18349100
H	-4.52629500	0.77518900	-1.19970000
C	2.54659600	-1.42109100	0.56885800
H	3.62782000	-1.37041600	0.70782600
H	2.08748700	-1.49345200	1.56224600
H	2.31837700	-2.35725700	0.04558200
C	4.00977800	1.29257000	0.12798600
H	4.66586200	1.57874000	-0.70208200
H	3.94422000	2.16215400	0.79229900
H	4.49880400	0.48978200	0.68296300
H	0.61498400	-1.29657600	-1.45564200

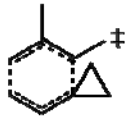
Zero-point correction=	0.234925 (Hartree/Particle)
Thermal correction to Energy=	0.247071
Thermal correction to Enthalpy=	0.248016
Thermal correction to Gibbs Free Energy=	0.195288
Sum of electronic and zero-point Energies=	-390.185043
Sum of electronic and thermal Energies=	-390.172896
Sum of electronic and thermal Enthalpies=	-390.171952
Sum of electronic and thermal Free Energies=	-390.224680

MP2/6-31G(d)

XYZ Coordinates

C	2.58841500	0.93496600	-0.36066900
H	2.03100100	1.70350200	-0.89833400
C	1.99178700	-0.26346300	-0.21009900
C	0.59895500	-0.48336600	-0.74565200
H	0.29176700	0.37901500	-1.34901100
C	-0.44648900	-0.69979500	0.36352300
H	-0.16472700	-1.57098800	0.96900000
H	-0.45024600	0.17156300	1.02875300
C	-2.83045900	-0.06069000	-0.01496900
C	-1.82026000	-0.90409600	-0.20349300
H	-1.97658500	-1.78858600	-0.82399600
C	-3.31312400	1.17650200	0.60929200
H	-3.50037900	1.19025800	1.68068500
H	-2.99717700	2.13382600	0.20082700
C	-4.22918000	0.29894700	-0.26165400
H	-5.01534500	-0.25995500	0.24090400
H	-4.51185900	0.68301900	-1.23922200
C	2.60687100	-1.44155900	0.50042900
H	3.68372000	-1.33256800	0.64036400
H	2.15702200	-1.59359200	1.48799500
H	2.43566100	-2.35891100	-0.07429600
C	3.94178900	1.36327000	0.12379700
H	4.57092100	1.68576500	-0.71352500
H	3.85346700	2.21918300	0.80254200
H	4.47028000	0.57178400	0.65753100
H	0.59265200	-1.35761700	-1.41324100

Zero-point correction=	0.237291 (Hartree/Particle)
Thermal correction to Energy=	0.249471
Thermal correction to Enthalpy=	0.250415
Thermal correction to Gibbs Free Energy=	0.197529
Sum of electronic and zero-point Energies=	-388.962728
Sum of electronic and thermal Energies=	-388.950548
Sum of electronic and thermal Enthalpies=	-388.949604
Sum of electronic and thermal Free Energies=	-389.002490



B3LYP/6-31G(d)

XYZ Coordinates

C	-1.06584400	-0.52178600	-0.07521200
C	-0.45394400	-1.75531100	-0.36942300
C	0.81129300	-2.04263500	0.18565400
C	1.97732000	-0.72058000	-0.54027000
C	1.37973900	0.51441000	-0.19206300
C	0.15034600	0.83884600	-0.82819100
H	1.28876200	-2.97836400	-0.10741600
H	-0.72131100	-2.23775500	-1.31149100
H	1.94167500	-1.01871900	-1.58642000
H	2.93466400	-0.96352600	-0.07768700
H	0.95578800	-1.82067800	1.24339400
H	0.07498000	0.49152600	-1.85834700
C	-2.51775800	-0.18194800	-0.09383100
H	-2.85191500	0.74624300	-0.55080900
H	-3.23205000	-0.99679300	-0.18930100
C	-1.70986100	-0.06278500	1.19661500
H	-1.86892600	-0.80223600	1.97835200
H	-1.53343900	0.94236200	1.57112200
C	1.76912000	1.18094400	1.10507500
H	1.04029600	0.97164200	1.90470300
H	2.74656000	0.83161800	1.45301600
H	1.82535300	2.27232600	1.00804400
C	-0.46483600	2.21757600	-0.65613300
H	-1.45931800	2.27563200	-1.10813100
H	-0.55195000	2.51501100	0.39355200
H	0.15738200	2.97132900	-1.15589400

Zero-point correction=	0.231954 (Hartree/Particle)
Thermal correction to Energy=	0.242775
Thermal correction to Enthalpy=	0.243720
Thermal correction to Gibbs Free Energy=	0.196536
Sum of electronic and zero-point Energies=	-390.330414
Sum of electronic and thermal Energies=	-390.319593
Sum of electronic and thermal Enthalpies=	-390.318649
Sum of electronic and thermal Free Energies=	-390.365832

M06-2X/6-31G(d)

XYZ Coordinates

C	-0.97669400	-0.62037000	-0.09329600
C	-0.24590600	-1.77854800	-0.38776500
C	1.03832700	-1.90190000	0.18212500
C	2.02564300	-0.50719400	-0.54198900
C	1.29368200	0.65195000	-0.19893100
C	0.05240900	0.84039900	-0.84801800
H	1.62457200	-2.78210500	-0.08036500
H	-0.45828200	-2.30002300	-1.32064300
H	2.03217300	-0.79730300	-1.59084100
H	3.00151300	-0.63618800	-0.07351300
H	1.12909800	-1.64484900	1.23946800
H	0.02353000	0.49174700	-1.88014200
C	-2.44684600	-0.41815600	-0.06986300
H	-2.87327900	0.47833600	-0.50884000
H	-3.07981800	-1.29680500	-0.14715600
C	-1.62101200	-0.22835700	1.19277800
H	-1.68488600	-0.98770600	1.96668000
H	-1.53355100	0.78684600	1.56790600
C	1.55107100	1.30390700	1.13134800
H	0.87130800	0.89887200	1.89896300
H	2.57496000	1.12423900	1.46995100
H	1.39381500	2.38714400	1.10118200
C	-0.71879700	2.13203100	-0.66149000
H	-1.68941800	2.09655300	-1.16150000
H	-0.88454800	2.37482100	0.39198600
H	-0.15845000	2.96385100	-1.10252700

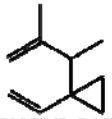
Zero-point correction=	0.233902 (Hartree/Particle)
Thermal correction to Energy=	0.243742
Thermal correction to Enthalpy=	0.244686
Thermal correction to Gibbs Free Energy=	0.199881
Sum of electronic and zero-point Energies=	-390.134704
Sum of electronic and thermal Energies=	-390.124865
Sum of electronic and thermal Enthalpies=	-390.123921
Sum of electronic and thermal Free Energies=	-390.168725

MP2/6-31G(d)

XYZ Coordinates

C	-0.97886500	-0.62805700	-0.09423900
C	-0.22999300	-1.77385900	-0.39300400
C	1.10789200	-1.82998800	0.14337700
C	1.98331800	-0.54490700	-0.52874900
C	1.28985100	0.68328100	-0.20138000
C	0.04248100	0.86159600	-0.84427700
H	1.66116300	-2.74012100	-0.10494200
H	-0.43574300	-2.29604100	-1.33017400
H	2.01794800	-0.76620400	-1.59781600
H	2.98915000	-0.62091200	-0.10518800
H	1.15908300	-1.64354600	1.22083600
H	0.02064000	0.50559600	-1.87592500
C	-2.45672200	-0.46806200	-0.04581000
H	-2.91685700	0.41428900	-0.48087000
H	-3.06842900	-1.36390200	-0.11216400
C	-1.61159200	-0.24941400	1.20449300
H	-1.64278200	-1.00529600	1.98534600
H	-1.54543200	0.76958800	1.57443700
C	1.55719500	1.29843600	1.14169700
H	1.01552600	0.75976100	1.93726400
H	2.62325800	1.25530800	1.38473000
H	1.24833000	2.34662500	1.18899400
C	-0.75018200	2.14110200	-0.67437700
H	-1.73313700	2.06479100	-1.14501600
H	-0.89210100	2.41101700	0.37422400
H	-0.22091500	2.96826900	-1.16012500

Zero-point correction= 0.208175 (Hartree/Particle)
Thermal correction to Energy= 0.216889
Thermal correction to Enthalpy= 0.217833
Thermal correction to Gibbs Free Energy= 0.175402
Sum of electronic and zero-point Energies= -349.789615
Sum of electronic and thermal Energies= -349.780901
Sum of electronic and thermal Enthalpies= -349.779957
Sum of electronic and thermal Free Energies= -349.822388



B3LYP/6-31G(d) XYZ Coordinates

C	-2.23147900	-0.83394600	-1.28441600
H	-1.68494300	-1.03183400	-2.20357700
C	-1.73044700	-0.04962400	-0.32227800
C	-0.35421000	0.59291400	-0.48131800
H	-0.13330000	0.60525100	-1.55735700
C	0.81459900	-0.21907300	0.15624900
C	3.17979500	0.30314900	-0.55775600
C	2.11251500	0.53328600	0.20925700
H	2.16255200	1.33888100	0.94296900
H	-3.21060500	-1.29885200	-1.19427500
H	3.18889400	-0.48245100	-1.30961100
H	4.08771000	0.89264900	-0.45935400
C	0.57841000	-1.19761600	1.29499400
H	-0.42936300	-1.34638100	1.66778200
H	1.35174000	-1.27622900	2.05511800
C	0.89124300	-1.70749900	-0.09055200
H	1.86682400	-2.15033800	-0.26643100
H	0.07825900	-2.17179000	-0.64040900
C	-2.54155500	0.26725200	0.91567300
H	-2.88932200	1.30834400	0.90122000
H	-3.42470600	-0.37579200	0.98193900
H	-1.96159000	0.14932800	1.83788700
C	-0.36691300	2.06352000	-0.01464800
H	0.55514300	2.57339200	-0.30821600
H	-1.20353200	2.60276100	-0.47264900
H	-0.46550700	2.14888500	1.07373800

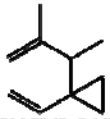
Zero-point correction= 0.233813 (Hartree/Particle)
Thermal correction to Energy= 0.245141
Thermal correction to Enthalpy= 0.246085
Thermal correction to Gibbs Free Energy= 0.197128
Sum of electronic and zero-point Energies= -390.386308
Sum of electronic and thermal Energies= -390.374980
Sum of electronic and thermal Enthalpies= -390.374036
Sum of electronic and thermal Free Energies= -390.422992

MP2/6-31G(d)

XYZ Coordinates

C	-0.97886500	-0.62805700	-0.09423900
C	-0.22999300	-1.77385900	-0.39300400
C	1.10789200	-1.82998800	0.14337700
C	1.98331800	-0.54490700	-0.52874900
C	1.28985100	0.68328100	-0.20138000
C	0.04248100	0.86159600	-0.84427700
H	1.66116300	-2.74012100	-0.10494200
H	-0.43574300	-2.29604100	-1.33017400
H	2.01794800	-0.76620400	-1.59781600
H	2.98915000	-0.62091200	-0.10518800
H	1.15908300	-1.64354600	1.22083600
H	0.02064000	0.50559600	-1.87592500
C	-2.45672200	-0.46806200	-0.04581000
H	-2.91685700	0.41428900	-0.48087000
H	-3.06842900	-1.36390200	-0.11216400
C	-1.61159200	-0.24941400	1.20449300
H	-1.64278200	-1.00529600	1.98534600
H	-1.54543200	0.76958800	1.57443700
C	1.55719500	1.29843600	1.14169700
H	1.01552600	0.75976100	1.93726400
H	2.62325800	1.25530800	1.38473000
H	1.24833000	2.34662500	1.18899400
C	-0.75018200	2.14110200	-0.67437700
H	-1.73313700	2.06479100	-1.14501600
H	-0.89210100	2.41101700	0.37422400
H	-0.22091500	2.96826900	-1.16012500

Zero-point correction= 0.208175 (Hartree/Particle)
Thermal correction to Energy= 0.216889
Thermal correction to Enthalpy= 0.217833
Thermal correction to Gibbs Free Energy= 0.175402
Sum of electronic and zero-point Energies= -349.789615
Sum of electronic and thermal Energies= -349.780901
Sum of electronic and thermal Enthalpies= -349.779957
Sum of electronic and thermal Free Energies= -349.822388



B3LYP/6-31G(d) XYZ Coordinates

C	-2.23147900	-0.83394600	-1.28441600
H	-1.68494300	-1.03183400	-2.20357700
C	-1.73044700	-0.04962400	-0.32227800
C	-0.35421000	0.59291400	-0.48131800
H	-0.13330000	0.60525100	-1.55735700
C	0.81459900	-0.21907300	0.15624900
C	3.17979500	0.30314900	-0.55775600
C	2.11251500	0.53328600	0.20925700
H	2.16255200	1.33888100	0.94296900
H	-3.21060500	-1.29885200	-1.19427500
H	3.18889400	-0.48245100	-1.30961100
H	4.08771000	0.89264900	-0.45935400
C	0.57841000	-1.19761600	1.29499400
H	-0.42936300	-1.34638100	1.66778200
H	1.35174000	-1.27622900	2.05511800
C	0.89124300	-1.70749900	-0.09055200
H	1.86682400	-2.15033800	-0.26643100
H	0.07825900	-2.17179000	-0.64040900
C	-2.54155500	0.26725200	0.91567300
H	-2.88932200	1.30834400	0.90122000
H	-3.42470600	-0.37579200	0.98193900
H	-1.96159000	0.14932800	1.83788700
C	-0.36691300	2.06352000	-0.01464800
H	0.55514300	2.57339200	-0.30821600
H	-1.20353200	2.60276100	-0.47264900
H	-0.46550700	2.14888500	1.07373800

Zero-point correction= 0.233813 (Hartree/Particle)
Thermal correction to Energy= 0.245141
Thermal correction to Enthalpy= 0.246085
Thermal correction to Gibbs Free Energy= 0.197128
Sum of electronic and zero-point Energies= -390.386308
Sum of electronic and thermal Energies= -390.374980
Sum of electronic and thermal Enthalpies= -390.374036
Sum of electronic and thermal Free Energies= -390.422992

M06-2X/6-31G(d)

XYZ Coordinates

C	-2.24407800	-0.88541500	-1.19377300
H	-1.72280900	-1.13536800	-2.11433400
C	-1.71677300	-0.04335900	-0.30385100
C	-0.34891300	0.57708500	-0.52841300
H	-0.14326300	0.53921000	-1.60656800
C	0.79524800	-0.22189700	0.13952700
C	3.17149000	0.28954600	-0.48053200
C	2.08413200	0.53213200	0.24607300
H	2.10404300	1.34341100	0.97449200
H	-3.21728600	-1.34393300	-1.04005400
H	3.19107400	-0.50403300	-1.22318300
H	4.07896000	0.87292500	-0.35909800
C	0.51620100	-1.20970700	1.24727800
H	-0.50820900	-1.36967200	1.56486000
H	1.25899200	-1.29766000	2.03410500
C	0.88753200	-1.69663300	-0.12519500
H	1.87120000	-2.13172800	-0.26333900
H	0.09569000	-2.15082500	-0.71221200
C	-2.47229300	0.35178400	0.94154200
H	-2.84453600	1.37952100	0.85795100
H	-3.33103800	-0.30466400	1.10387700
H	-1.83630900	0.32065100	1.83233200
C	-0.33753300	2.05449700	-0.11218000
H	0.58490300	2.54154100	-0.43821700
H	-1.17832900	2.58597900	-0.56865600
H	-0.41315600	2.16644300	0.97517900

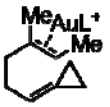
Zero-point correction=	0.235830 (Hartree/Particle)
Thermal correction to Energy=	0.247017
Thermal correction to Enthalpy=	0.247961
Thermal correction to Gibbs Free Energy=	0.199298
Sum of electronic and zero-point Energies=	-390.193908
Sum of electronic and thermal Energies=	-390.182722
Sum of electronic and thermal Enthalpies=	-390.181777
Sum of electronic and thermal Free Energies=	-390.230441

MP2/6-31G(d)

XYZ Coordinates

C	-2.20357000	-0.86245600	-1.25977000
H	-1.65473500	-1.08638600	-2.17028500
C	-1.70263500	-0.04071800	-0.32136100
C	-0.33444600	0.58694100	-0.49691100
H	-0.10540600	0.57892800	-1.57274900
C	0.79988400	-0.22076500	0.16823400
C	3.14184800	0.29588800	-0.56344300
C	2.09771200	0.51361900	0.24815300
H	2.17846400	1.28370400	1.01630200
H	-3.18122200	-1.32505300	-1.15287400
H	3.10645300	-0.45672000	-1.34563500
H	4.06228700	0.86408900	-0.47031900
C	0.52177200	-1.19370100	1.29159500
H	-0.49851400	-1.33755400	1.62735400
H	1.27194200	-1.27693100	2.07328300
C	0.87361000	-1.70386800	-0.08033100
H	1.85244300	-2.14819300	-0.22648200
H	0.07274400	-2.15842300	-0.65439200
C	-2.51148500	0.32335800	0.89922300
H	-2.88626500	1.34984100	0.82515500
H	-3.37429200	-0.34097600	1.00191700
H	-1.92103900	0.26643600	1.81771300
C	-0.33520200	2.05301700	-0.04530000
H	0.59322300	2.54774700	-0.34025000
H	-1.16530400	2.59404500	-0.51033000
H	-0.43571200	2.13754900	1.04105300

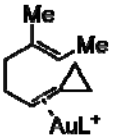
Zero-point correction=	0.237990 (Hartree/Particle)
Thermal correction to Energy=	0.249098
Thermal correction to Enthalpy=	0.250042
Thermal correction to Gibbs Free Energy=	0.201689
Sum of electronic and zero-point Energies=	-388.974827
Sum of electronic and thermal Energies=	-388.963719
Sum of electronic and thermal Enthalpies=	-388.962775
Sum of electronic and thermal Free Energies=	-389.011129



Gtot(B3LYP)=-986.796812
Gtot(M06-2X)=-986.341187
Gtot(M06)=-986.312685

XYZ Coordinates

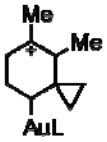
C	1.45618500	0.24980300	0.35363200
C	1.71452000	1.61680500	-0.22303000
C	3.21091800	1.97439200	-0.13247300
C	4.06330700	1.03684900	-0.92887700
C	4.90309800	0.16433200	-0.39419800
H	1.12981200	2.37326000	0.32110900
H	3.53616600	1.97713900	0.91804400
H	3.32694200	3.00370200	-0.50224200
H	1.39705700	1.65002400	-1.27611900
Au	-0.88371900	-0.11365700	-0.07725700
P	-3.21451900	0.15260900	0.00833900
H	3.94514700	1.06986900	-2.01649500
C	1.29800200	-0.83649300	-0.48125800
H	1.35313000	-0.63461000	-1.55628500
C	5.89891800	-0.88748100	-0.56583000
H	6.88669500	-0.61907000	-0.94292300
H	5.57166600	-1.88746400	-0.85399400
C	5.50838200	-0.38196600	0.82125700
H	6.23510500	0.21953300	1.36896200
H	4.92074600	-1.05083600	1.45314000
C	1.39473700	-2.27650000	-0.08212400
H	0.77882000	-2.91041800	-0.72962200
H	2.43678600	-2.61396500	-0.19119100
H	1.09669900	-2.45542200	0.95681800
C	1.66624900	0.11008500	1.83150900
H	1.17110000	-0.76988300	2.25529500
H	2.74333700	0.00921000	2.03528200
H	1.31369500	1.00161600	2.36483600
C	-4.05693900	-1.12210100	0.99725900
H	-3.67403100	-1.10767300	2.02339800
H	-5.13731800	-0.92952600	1.00974200
H	-3.86988200	-2.11086800	0.56450200
C	-4.01318200	0.09742100	-1.62577300
H	-3.82210700	-0.87252300	-2.09766900
H	-5.09581700	0.24066800	-1.51634500
H	-3.60536000	0.88745100	-2.26549500
C	-3.72341000	1.73917900	0.74093000
H	-4.81876000	1.80202300	0.77041600
H	-3.32744100	1.81894400	1.75909600
H	-3.32753200	2.56707500	0.14291200



Gtot(B3LYP)=-986.797451
Gtot(M06-2X)=-986.339889
Gtot(M06)=-986.311227

XYZ Coordinates

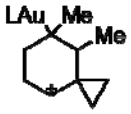
C	1.32515200	0.82607000	-0.17057000
C	1.34501300	-0.35821500	-0.84056300
C	1.78829200	-1.65075400	-0.22302500
C	3.26994100	-1.90548200	-0.56847500
C	4.19628000	-0.91546400	0.08553300
C	4.68661300	0.11802600	-0.61573100
H	1.17873200	-2.48275500	-0.60070100
H	1.24708400	-0.33338900	-1.93131100
H	3.38602600	-1.87556700	-1.66233200
H	3.51999600	-2.92929100	-0.25038600
H	1.64959700	-1.61198000	0.86743400
H	4.40426900	0.17661700	-1.67262300
C	1.47801000	2.27878800	-0.25549200
H	2.31708100	2.65369500	-0.84252900
H	0.59206700	2.91274900	-0.27151200
C	1.76154100	1.52387900	1.04069300
H	1.05453300	1.67054000	1.85693100
H	2.79085300	1.37724200	1.34649700
Au	-0.87888400	0.03601600	-0.20226200
P	-3.19520800	-0.16577500	0.13053300
C	4.47617200	-1.18014600	1.53481100
H	4.96708600	-2.15663900	1.66091300
H	5.11388900	-0.42312300	2.00278300
H	3.54351000	-1.22905400	2.11748500
C	5.57951700	1.21714300	-0.14352300
H	6.51957700	1.23556200	-0.71329000
H	5.10938300	2.20000700	-0.29748200
H	5.83717200	1.13761200	0.91864900
C	-4.06905800	-0.77702400	-1.34375800
H	-5.14362400	-0.85534200	-1.13525700
H	-3.91006500	-0.08580100	-2.17841200
H	-3.67973500	-1.76222900	-1.62262300
C	-4.00404700	1.40863700	0.55444000
H	-3.83698300	2.14030600	-0.24337200
H	-5.08234100	1.24867500	0.68232700
H	-3.58221900	1.80014100	1.48643100
C	-3.64543000	-1.31000400	1.47168000
H	-4.73760500	-1.36124200	1.56599900
H	-3.25165000	-2.30880700	1.25512300
H	-3.21566700	-0.95858800	2.41593700



Gtot(B3LYP)=-986.773535
Gtot(M06-2X)=-986.321557
Gtot(M06)=-986.298606

XYZ Coordinates

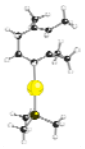
C	2.12112800	0.66334000	-0.26899700
C	1.23235900	-0.50309700	-0.57378800
C	1.69745600	-1.69517000	0.21182600
C	3.25301200	-1.99919000	-0.10527400
C	3.90845500	-0.74573100	0.18002300
C	3.65140300	0.36026300	-0.72472500
H	1.17098400	-2.62463500	-0.03796200
H	1.29647600	-0.73098400	-1.65164300
H	3.29517100	-2.27276100	-1.16505600
H	3.58955000	-2.82318400	0.53230000
H	1.61063900	-1.53686000	1.29674400
H	3.55502800	0.00030700	-1.75674400
C	1.67828400	2.09633400	-0.37994100
H	2.38910400	2.84597000	-0.71910700
H	0.65855500	2.25706200	-0.72602000
C	1.90394400	1.48889800	0.96900800
H	1.04284700	1.22699500	1.58388000
H	2.76273200	1.85057400	1.53374300
Au	-0.85320400	-0.21461300	-0.19786300
P	-3.18637600	0.06905800	0.18589500
C	4.60324900	-0.56529500	1.46076100
H	4.55080100	0.45585400	1.85152500
H	4.27062100	-1.28914300	2.21365100
H	5.67275100	-0.76975300	1.27338100
C	4.59868200	1.54498000	-0.66580200
H	4.37368600	2.24495500	-1.47631100
H	4.55184700	2.09652200	0.28105200
H	5.63344600	1.20834500	-0.80258000
C	-3.60013400	1.26795900	1.49870100
H	-4.68883800	1.34723000	1.61394400
H	-3.15906400	0.94146200	2.44721100
H	-3.19095800	2.25193800	1.24383700
C	-4.12409200	0.65817700	-1.26498500
H	-5.18672500	0.77101900	-1.01380500
H	-3.72537700	1.62392100	-1.59555000
H	-4.02066700	-0.06093800	-2.08527700
C	-4.06169300	-1.45165400	0.69079500
H	-5.12958400	-1.24531600	0.84005700
H	-3.94616400	-2.21992500	-0.08196400
H	-3.63261500	-1.82955000	1.62564400



Gtot(B3LYP)=-986.76329
Gtot(M06-2X)=-986.310046
Gtot(M06)=-986.288615

XYZ Coordinates

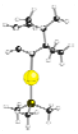
C	-2.09239500	0.68958500	-0.26256700
C	-1.29679400	-0.49939500	0.31905300
C	-1.66004600	-1.75757800	-0.47838200
C	-3.14670200	-2.10916300	-0.39261200
C	-4.02732100	-0.94843100	-0.46067900
C	-3.59078200	0.36139700	-0.35028800
H	-1.07468800	-2.62807900	-0.13148600
H	-3.39826300	-2.58960800	0.57556800
H	-3.47672100	-2.85511100	-1.13263600
H	-5.10085900	-1.12800700	-0.56981200
H	-1.40207800	-1.61507600	-1.53941100
Au	0.80235400	-0.16335300	0.08626200
P	3.16419900	0.20423800	-0.16215400
C	-4.58164600	1.40455200	-1.02013400
H	-4.00962800	2.24177000	-1.41719200
H	-5.32937300	0.98961900	-1.69125400
C	-4.71446700	1.24374500	0.39498000
H	-5.55381000	0.69194100	0.80944000
H	-4.23739400	1.94337000	1.07614300
H	-1.77311300	0.81330000	-1.31317300
C	-1.60650900	-0.70523700	1.80445500
H	-1.19389300	0.09601900	2.43131500
H	-2.68940900	-0.75092500	2.02894400
H	-1.16461000	-1.64760000	2.16009300
C	-1.81229200	2.00814700	0.44626100
H	-0.73494600	2.21492000	0.39901600
H	-2.32589800	2.86204100	-0.01610700
H	-2.08891200	1.97700200	1.50829400
C	3.94460300	-0.65828500	-1.57232600
H	5.01865700	-0.43400100	-1.61185600
H	3.80555200	-1.74017500	-1.46699300
H	3.47430200	-0.33596200	-2.50828600
C	4.18667800	-0.30240000	1.26595100
H	4.05543400	-1.37394400	1.45434900
H	5.24712400	-0.09705500	1.06904900
H	3.87309000	0.24941900	2.15945300
C	3.63324600	1.95175500	-0.42129000
H	4.72191400	2.04619200	-0.52640600
H	3.14942000	2.33344200	-1.32761100
H	3.29987200	2.55418600	0.43140300



Gtot(B3LYP)=-986.767852
Gtot(M06-2X)=-986.311297
Gtot(M06)=-986.287934

XYZ Coordinates

C	1.93100700	0.68590200	-0.14298100
C	1.22971600	-0.42800000	-0.68602500
C	1.66149600	-1.73466400	-0.07754300
C	3.18002300	-1.96236300	-0.38893800
C	3.95250700	-0.78394400	0.06632800
C	4.01194200	0.33117700	-0.73655100
H	1.09403900	-2.58646200	-0.47184800
H	1.25122000	-0.44176500	-1.78604200
H	3.28495600	-2.11219000	-1.47088200
H	3.51273100	-2.87420800	0.12331700
H	1.52107000	-1.72220600	1.01414500
H	3.70739400	0.19677600	-1.77645500
C	1.79023900	2.15135200	-0.13553900
H	2.63585600	2.77848200	-0.41169800
H	0.82359900	2.55467200	-0.43593200
C	1.92278900	1.37356000	1.16149100
H	1.05023100	1.21992300	1.79695600
H	2.85399600	1.50901100	1.71119100
Au	-0.87840900	-0.10763500	-0.25003300
P	-3.19266300	0.09529100	0.16143500
C	4.49776800	-0.82767600	1.44866000
H	4.90411600	0.12691200	1.79567600
H	3.72839800	-1.16748700	2.15903100
H	5.30587400	-1.57193500	1.49701500
C	4.86044400	1.53568100	-0.46889100
H	4.64834800	2.33460800	-1.18726200
H	4.73908700	1.94449100	0.54261300
H	5.92349900	1.28097500	-0.58083700
C	-3.82755600	1.80411100	0.15790400
H	-4.90668000	1.80234700	0.35858800
H	-3.31601400	2.38945200	0.92981600
H	-3.64047100	2.26748500	-0.81702200
C	-3.71525000	-0.58060000	1.77214900
H	-4.79925400	-0.46112100	1.89730200
H	-3.45872200	-1.64436900	1.82577900
H	-3.19664100	-0.05343600	2.58049000
C	-4.22820600	-0.77927200	-1.05780200
H	-3.96731100	-1.84334500	-1.06881900
H	-5.28953600	-0.66808600	-0.80079700
H	-4.05240100	-0.36453900	-2.05659900



Gtot(B3LYP)=-986.769742
Gtot(M06-2X)=-986.315581
Gtot(M06)=-986.293575

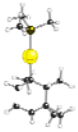
XYZ Coordinates

C	2.15707100	0.79863100	-0.25856100
C	1.27194200	-0.32236500	-0.70026300
C	1.52772200	-1.54968900	-0.02433600
C	3.51285400	-2.03129600	-0.46619000
C	3.92391300	-0.85507900	0.10367100
C	3.64868900	0.42823700	-0.60738900
H	1.15568300	-2.48994100	-0.43573800
H	1.24549200	-0.43057300	-1.79477100
H	3.33931800	-2.09366000	-1.54016200
H	3.67186400	-2.97849100	0.04993700
H	1.61437200	-1.54071700	1.06433800
H	3.65503800	0.23336500	-1.69077400
C	1.69653400	2.22068200	-0.33952800
H	2.41328200	2.99512800	-0.60532300
H	0.68944600	2.39308800	-0.71805100
C	1.85566400	1.56216900	1.00095700
H	0.96283500	1.28329300	1.56173900
H	2.67971700	1.90644400	1.62456600
Au	-0.85173500	-0.17915100	-0.20982000
P	-3.16649000	0.07554500	0.20011000
C	4.40135900	-0.81690700	1.51071800
H	3.78092100	-0.14430300	2.12120800
H	4.40234600	-1.81230100	1.96742200
H	5.42460400	-0.41748800	1.55585800
C	4.66426200	1.52551700	-0.31578300
H	4.47948300	2.40275600	-0.94456700
H	4.65553400	1.84859000	0.73241700
H	5.67745400	1.17206400	-0.54245400
C	-3.88156200	-1.18220500	1.30937300
H	-4.95542200	-0.99859200	1.44331600
H	-3.73540100	-2.17978300	0.88080700
H	-3.38270800	-1.14140400	2.28383500
C	-3.61681200	1.66740700	0.96487700
H	-3.30334400	2.49258100	0.31598900
H	-4.70268200	1.71793800	1.11686500
H	-3.11072300	1.76901400	1.93125800
C	-4.18468500	-0.01368100	-1.30958800
H	-5.24442400	0.12847500	-1.06157200
H	-3.86977500	0.76461100	-2.01343300
H	-4.05179600	-0.99156200	-1.78574500

Gtot(B3LYP)=-986.750043
Gtot(M06-2X)=-986.296636
Gtot(M06)=-986.27279

XYZ Coordinates

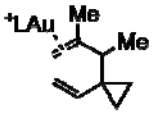
C	1.90003600	-0.65300700	-0.40941900
C	1.36695300	0.42428800	0.39968500
C	1.59826400	1.76593100	-0.21556100
C	3.18280700	2.08058900	-0.25380100
C	3.78323000	0.99950300	-1.00337700
C	3.85730400	-0.27186200	-0.46918100
H	1.13613200	2.58265800	0.35382100
H	3.52179500	2.11296900	0.78957000
H	3.31130500	3.06028900	-0.72369700
H	3.90761300	1.11993800	-2.08326300
H	1.23632900	1.82418200	-1.24991700
Au	-0.80048400	0.10449700	0.09489500
P	-3.13120600	-0.17251400	-0.14737300
C	4.81054600	-1.36945200	-0.71290700
H	4.45002600	-2.37678500	-0.91383700
H	5.73948900	-1.12229500	-1.22548900
C	4.58614200	-0.83282200	0.69228000
H	5.35455800	-0.21066600	1.15087000
H	4.07310700	-1.49476900	1.38827700
H	1.70615200	-0.53343900	-1.48021000
C	1.61281900	0.38125900	1.89606800
H	1.28072900	-0.55921300	2.35321300
H	2.68342200	0.50274800	2.13714700
H	1.07164700	1.19428100	2.39701700
C	1.82568500	-2.09605400	0.01696500
H	2.48679600	-2.73026600	-0.58155300
H	2.05624400	-2.24427200	1.07724100
H	0.80743200	-2.46742800	-0.15533100
C	-4.07343100	1.38334100	-0.02879000
H	-3.73187200	2.08217300	-0.80027000
H	-5.14492400	1.18797800	-0.16454600
H	-3.91021400	1.83879800	0.95429000
C	-3.88551600	-1.26497200	1.10127000
H	-3.71075100	-0.85898200	2.10362700
H	-4.96591500	-1.34680100	0.92605500
H	-3.43287800	-2.26086600	1.04117900
C	-3.62789300	-0.89417500	-1.74580600
H	-4.71967400	-0.99964100	-1.78852000
H	-3.29403000	-0.24754700	-2.56473100
H	-3.16408600	-1.87958900	-1.86503900



Gtot(B3LYP)=-986.75146
Gtot(M06-2X)=-986.296438
Gtot(M06)=-986.28187

XYZ Coordinates

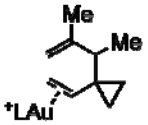
C	1.96094200	-0.95422000	0.48065200
C	1.39212800	0.39637100	0.15531800
C	1.83947600	0.82887200	-1.20862300
C	3.50022200	0.89079300	-1.19578200
C	4.02259900	-0.37154300	-0.79161500
C	3.53917700	-0.99661700	0.39539600
H	3.66031600	1.66064500	-0.42241300
H	3.87635800	1.24143800	-2.16069100
H	4.69610600	-0.92178800	-1.45495800
H	1.59187000	0.05846900	-1.95263300
Au	-0.75985100	0.09153700	0.04024200
P	-3.11351700	-0.24643800	-0.03729200
C	4.26678000	-2.12576200	1.04405500
H	3.65411300	-2.90580900	1.49449400
H	5.18710600	-2.47554800	0.57755300
C	4.29045300	-0.79288900	1.71705800
H	5.20958200	-0.21131500	1.68962200
H	3.66659100	-0.62741600	2.59449300
H	1.69450400	-1.28831400	1.49440700
H	1.60641100	-1.72399600	-0.22038200
C	-3.62761500	-1.97680800	0.22686700
H	-3.27819800	-2.32154000	1.20644900
H	-4.72138600	-2.05776600	0.18273100
H	-3.18596500	-2.61547000	-0.54621500
C	-4.05660200	0.69520000	1.20880300
H	-5.12984800	0.48878900	1.10643600
H	-3.72819800	0.41045800	2.21457600
H	-3.87965400	1.76794600	1.07347400
C	-3.88640400	0.21128000	-1.62548400
H	-3.43487400	-0.37099600	-2.43641200
H	-4.96583000	0.01381300	-1.59471100
H	-3.71868600	1.27568300	-1.82457600
C	1.64059500	1.41292100	1.25299700
H	1.32139600	1.02143700	2.22830100
H	2.71660100	1.66739600	1.35083000
H	1.10334800	2.35527500	1.08663900
C	1.38706300	2.18920600	-1.71182300
H	1.80879200	2.39767300	-2.70241200
H	0.29340000	2.22338400	-1.79788800
H	1.70087000	2.99620900	-1.03719800



Gtot(B3LYP)=-986.798849
Gtot(M06-2X)=-986.350628
Gtot(M06)=-986.322158

XYZ Coordinates

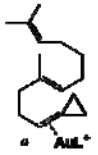
C	-2.18085800	0.61617600	-0.45728400
C	-1.56700000	-0.57496200	0.25209200
C	-1.05215300	-1.63042400	-0.46386800
C	-5.05030800	-1.58472200	-0.05029600
C	-4.26693300	-0.76301400	-0.74581500
C	-3.70635600	0.53465300	-0.27647500
H	-0.82095200	-2.57350000	0.03639900
H	-5.34872700	-1.37115700	0.97644200
H	-5.43118400	-2.50735600	-0.48350500
H	-3.98728600	-1.03561200	-1.76953500
H	-1.14934100	-1.65832500	-1.55103000
Au	0.91509700	-0.52666400	-0.18039800
P	3.07156300	0.38486900	-0.04053500
C	-4.55040600	1.75222200	-0.56357800
H	-4.06514400	2.68430300	-0.84741600
H	-5.50273300	1.57204600	-1.05986500
C	-4.39119200	1.26207300	0.84278300
H	-5.24518500	0.78964700	1.32460100
H	-3.78270300	1.86033900	1.51876000
H	-1.98363800	0.48524800	-1.53563400
C	-1.54916500	1.93841400	-0.03128100
H	-0.47109800	1.93151200	-0.24671400
H	-1.98129100	2.77629500	-0.58939500
H	-1.66894000	2.14494400	1.03890100
C	-1.69212600	-0.64851200	1.73934600
H	-2.75799000	-0.71991800	2.00171000
H	-1.17438700	-1.52344400	2.14682600
H	-1.30233500	0.25236000	2.22948500
C	3.13800100	1.80461700	1.09711800
H	2.83917300	1.48671700	2.10191800
H	4.15617900	2.21287900	1.13050700
H	2.44548200	2.58120300	0.75302300
C	3.70495300	1.01327500	-1.62609700
H	3.02411200	1.77708300	-2.01738400
H	4.70080700	1.45191100	-1.48222200
H	3.77033100	0.19477400	-2.35111500
C	4.33720400	-0.77640100	0.55891100
H	5.31215300	-0.27450700	0.60331400
H	4.06662100	-1.13320300	1.55857300
H	4.40178500	-1.63609700	-0.11668800



Gtot(B3LYP)=-986.79992
Gtot(M06-2X)=-986.350436
Gtot(M06)=-986.321323

XYZ Coordinates

C	2.32583100	-0.84199200	0.49775900
C	1.58618300	-1.18229700	-0.73697400
C	0.77453800	-2.26368000	-0.96095400
C	2.27012000	2.27620600	-1.15664600
C	3.00954500	1.37080300	-0.51090400
C	2.47120100	0.67107200	0.72175000
H	0.45077100	-2.49561000	-1.97513900
H	1.78593700	-0.52463500	-1.58897000
H	1.26063500	2.52951700	-0.82799000
H	2.64747100	2.80410700	-2.03235800
H	0.61981600	-3.04049500	-0.21110800
H	1.44521700	1.05235100	0.88343200
C	2.22919300	-1.77974500	1.66736100
H	2.30696400	-1.34639300	2.66166900
H	1.53567000	-2.61683200	1.61040800
C	3.45649300	-1.80723600	0.82260500
H	3.59736400	-2.64664200	0.14322200
H	4.37804800	-1.39161000	1.22675100
Au	-0.73652100	-0.62430600	-0.35609800
P	-2.53643300	0.74449600	0.27517100
C	3.28484200	1.05530000	1.95585500
H	4.30643500	0.65475600	1.93313100
H	3.36392900	2.14788700	2.01136000
H	2.80781200	0.71524800	2.88231000
C	4.38949600	1.80616000	-0.96843000
H	4.45441800	0.86021400	-1.23074800
H	4.68295800	1.58970700	-1.84858200
H	5.13934400	1.17788800	-0.18323600
C	-1.98785800	2.26701900	1.10831100
H	-2.85804900	2.87025200	1.39746800
H	-1.40990000	2.00779100	2.00239500
H	-1.35040100	2.84903100	0.43333800
C	-3.57796600	1.29704700	-1.11008500
H	-4.01019300	0.42806900	-1.61789500
H	-4.38630800	1.93854900	-0.73652800
H	-2.97043400	1.85935500	-1.82730700
C	-3.67193100	-0.06330900	1.44552700
H	-4.48268700	0.62477000	1.71636900
H	-4.09677000	-0.96348200	0.98838600
H	-3.12282100	-0.35192700	2.34838200



Gtot(B3LYP)=-1221.309281
Gtot(M06-2X)=-1220.734439
Gtot(M06)=-1220.62633

XYZ Coordinates

C	0.78828900	1.15113500	0.41310500
C	0.85962100	0.25424200	-0.60766100
C	1.22446400	-1.18822800	-0.41995500
C	2.73192700	-1.37357500	-0.69159800
C	3.59159700	-0.70318400	0.34641000
C	4.16596300	0.48028200	0.08983400
H	0.64798800	-1.82081100	-1.10838500
H	0.87792300	0.64424800	-1.63111300
H	2.96016400	-0.97785000	-1.69291300
H	2.93931400	-2.45457100	-0.71991400
H	0.97921800	-1.50775400	0.60367100
H	4.01839100	0.90104300	-0.91302800
C	0.96413600	2.54413400	0.82497600
H	1.87197300	3.04417100	0.48527100
H	0.09478000	3.19370200	0.92031800
C	1.08813000	1.39824300	1.82521300
H	0.29104500	1.30296500	2.56233300
H	2.08010000	1.11686700	2.18191500
Au	-1.41229400	0.51018500	-0.08272300
P	-3.75051500	0.29792300	-0.02373000
C	3.72588900	-1.45305400	1.63593500
H	4.40740900	-0.97269700	2.34691500
H	2.75300800	-1.58839700	2.13442600
H	4.11723900	-2.46370200	1.44167700
C	5.00781000	1.32794300	0.99212800
H	4.56897600	2.33924600	1.01845700
H	4.97959600	0.96282000	2.02978500
C	-4.42442800	-0.49078600	-1.51908700
H	-5.51657700	-0.56461000	-1.44057500
H	-4.16218400	0.10316000	-2.40127500
H	-3.99908600	-1.49410200	-1.62990300
C	-4.35035300	-0.71489800	1.36350100
H	-5.44497000	-0.78364400	1.32811900
H	-3.92023100	-1.72017900	1.29717300
H	-4.04433700	-0.26227300	2.31276900
C	-4.62665400	1.88610600	0.11971800
H	-5.70993700	1.71125800	0.13777300
H	-4.32467200	2.39435200	1.04175100
H	-4.37554800	2.52459500	-0.73415000
C	6.46870800	1.45451300	0.54596400
H	6.50331000	1.65272200	-0.53868600
H	6.91203500	2.33603500	1.03140500
C	7.33561900	0.23742500	0.87074800
H	8.38439600	0.50557300	0.65486800
H	7.29432300	0.05021600	1.95531200
C	6.97522300	-0.99411300	0.09864000
H	6.72835800	-0.81312400	-0.95397500
C	6.93748300	-2.26347200	0.52453100
C	7.25691900	-2.71068700	1.91927100
H	7.42812100	-1.88257500	2.61591400
H	6.44342400	-3.33118300	2.32598000
H	8.15726500	-3.34440700	1.92777300
C	6.56436400	-3.37613900	-0.41001500
H	6.31923600	-3.00617300	-1.41379300
H	7.37872300	-4.11122300	-0.50600100
H	5.69348600	-3.93537900	-0.03238600

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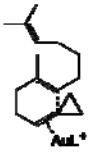
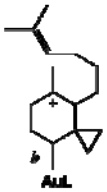


TS-1

Gtot(B3LYP)=-1221.277133
Gtot(M06-2X)=-1220.707799
Gtot(M06)=-1220.605024

XYZ Coordinates

C	1.33473700	-0.24870800	1.34827500
C	1.02726300	0.67804100	0.31149200
C	1.60445300	0.28107800	-1.02027100
C	3.16389900	0.22203200	-0.90605100
C	3.54314900	-0.65712800	0.22627100
C	3.54501900	-0.13293600	1.49812600
H	1.33911500	0.98940600	-1.81476200
H	1.27396600	1.71341300	0.59154300
H	3.53806400	1.24311900	-0.75156100
H	3.57008600	-0.15478000	-1.85390500
H	1.23415200	-0.70898000	-1.32755900
H	3.49872700	0.95852600	1.56656400
C	0.85051000	-0.51697700	2.71151400
H	1.55287000	-0.59742200	3.53834200
H	-0.10590700	-0.07279200	2.98612900
C	0.90752200	-1.62301800	1.67227300
H	-0.01059200	-1.98523100	1.20808100
H	1.65687900	-2.39576500	1.84116100
Au	-1.14400200	0.73411200	0.16192000
P	-3.48351200	0.89060000	-0.09669500
C	3.72994900	-2.09900200	-0.08700500
H	2.80471500	-2.51669800	-0.51574800
H	4.50545300	-2.20902800	-0.85759100
H	4.01821600	-2.70846100	0.77465300
C	4.09173700	-0.78846300	2.72889000
H	3.47900400	-0.50044800	3.59535400
H	4.04899100	-1.88545000	2.66591900
C	-4.01357800	1.14378600	-1.82239900
H	-5.10737000	1.21763200	-1.87444500
H	-3.56954200	2.06591800	-2.21348100
H	-3.67751500	0.30312000	-2.43934300
C	-4.40975600	-0.58031500	0.45348400
H	-5.48672700	-0.42112400	0.31237800
H	-4.09429500	-1.45458900	-0.12662000
H	-4.20735900	-0.77041300	1.51327000
C	-4.23865500	2.27427600	0.81947700
H	-5.32321100	2.29133000	0.65071100
H	-4.04038800	2.16026800	1.89090400
H	-3.80465200	3.22158500	0.48074500
C	5.53132100	-0.34970000	3.03421100
H	5.57301800	0.75151400	3.06710800
H	5.77440100	-0.69347400	4.04908800
C	6.59745500	-0.87060600	2.07091900
H	7.58066700	-0.68308200	2.53489300
H	6.51426600	-1.96668300	1.99742700
C	6.56774800	-0.23305300	0.71329000
H	6.26699000	0.82161900	0.70583800
C	6.90370300	-0.78284100	-0.46225900
C	7.37747500	-2.19414700	-0.63594900
H	7.27102800	-2.80563300	0.26697600
H	6.83439800	-2.69457800	-1.45271100
H	8.43953300	-2.21014600	-0.92483500
C	6.83804400	0.00878200	-1.73328100
H	6.52215700	1.04521000	-1.56034300
H	7.81341300	0.02856900	-2.24307700
H	6.13218600	-0.44985200	-2.44535400

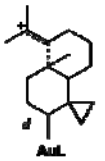


Au

Gtot(B3LYP)=-1221.279329
Gtot(M06-2X)=-1220.716232
Gtot(M06)=-1220.617252

XYZ Coordinates

C	1.87112400	0.78384900	0.54176200
C	1.08538300	-0.13664600	-0.35683500
C	1.45756600	-1.57106800	-0.07406300
C	3.02563800	-1.78800300	-0.20327600
C	3.61265600	-0.82094400	0.71695000
C	3.44832000	0.59914700	0.33926900
H	1.00026400	-2.27501700	-0.78170600
H	1.35612500	0.09563800	-1.40281600
H	3.28995000	-1.57938100	-1.24763100
H	3.26883300	-2.82569900	0.05018200
H	1.15296200	-1.88037200	0.93742600
H	3.59610200	0.70279600	-0.74736700
C	1.35015600	2.15941800	0.84916700
H	2.03472800	2.99579000	0.96159400
H	0.40217800	2.42230000	0.38116100
C	1.36303500	1.10662600	1.91817800
H	0.42282300	0.64456700	2.22221800
H	2.07732900	1.25302000	2.72905700
Au	-1.03850500	0.06342000	-0.28171600
P	-3.41470000	0.28934900	-0.23179000
C	3.77824400	-1.21562900	2.13119300
H	2.83717300	-0.96407600	2.65094600
H	3.93988600	-2.29256500	2.24272400
H	4.56798600	-0.66303400	2.64998900
C	4.33397400	1.61734300	1.05280700
H	3.91582400	2.61523000	0.87813900
H	4.31615600	1.46616300	2.14297800
C	-4.23095500	0.23391900	-1.86430000
H	-5.31476000	0.36934500	-1.75408000
H	-3.83123100	1.02738000	-2.50567900
H	-4.03517200	-0.73267300	-2.34208300
C	-4.29659400	-0.98252700	0.73828600
H	-5.37742000	-0.79041400	0.72544900
H	-4.10129300	-1.97376700	0.31382200
H	-3.93969200	-0.96993600	1.77425000
C	-3.99445200	1.86310300	0.49206200
H	-5.09152800	1.90399900	0.49293500
H	-3.62868400	1.95162600	1.52128000
H	-3.60191000	2.70441200	-0.09023400
C	5.77383000	1.63951200	0.55105300
H	5.77433200	1.85719100	-0.52991700
H	6.28628500	2.48446000	1.03018300
C	6.57985100	0.37105700	0.80757900
H	7.63241000	0.57453400	0.55124500
H	6.58448300	0.14451700	1.88491300
C	6.12296500	-0.80613900	-0.00078200
H	5.80050500	-0.57156300	-1.02150900
C	6.25907500	-2.11581600	0.31171900
C	6.78078100	-2.61672100	1.61890800
H	6.90759400	-1.83672100	2.37593000
H	6.12242600	-3.39794900	2.02762800
H	7.75990100	-3.09532500	1.46750400
C	5.93769700	-3.18571000	-0.67922700
H	5.53815500	-2.78651900	-1.61866000
H	6.84252200	-3.76599000	-0.91366400
H	5.21657500	-3.90835200	-0.26566600



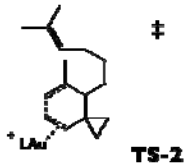
Au

TS-3

Gtot(B3LYP)=-1221.275451
Gtot(M06-2X)=-1220.714576
Gtot(M06)=-1220.61719

XYZ Coordinates

C	1.92592100	0.68278900	0.90635500
C	1.18543500	0.14420500	-0.29766800
C	1.61787600	-1.28207600	-0.56959500
C	3.17182200	-1.39102600	-0.72454400
C	3.76802600	-0.83348500	0.50576700
C	3.49351900	0.62830800	0.70739400
H	1.18383400	-1.67406300	-1.49962200
H	1.47839800	0.76047200	-1.16842400
H	3.45548400	-0.80341000	-1.60819400
H	3.44504900	-2.44078400	-0.88292500
H	1.29772900	-1.95761100	0.23931600
H	3.66825300	1.14525600	-0.25090700
C	1.33441300	1.83327400	1.67113500
H	1.97290700	2.59383200	2.11353300
H	0.38702600	2.21693300	1.29280900
C	1.36371400	0.46341800	2.28283800
H	0.43546600	-0.10507400	2.35809700
H	2.04829200	0.32286300	3.12000100
Au	-0.94094400	0.24136000	-0.24359200
P	-3.33226100	0.33505400	-0.25124800
C	3.81239200	-1.73307600	1.68784000
H	2.80514600	-1.72200400	2.13543200
H	4.03559400	-2.76873900	1.41050300
H	4.50022600	-1.40452100	2.47308700
C	4.31620700	1.33532200	1.78092400
H	3.88720400	2.33081400	1.94166600
H	4.24769200	0.81134900	2.74649800
C	-4.17736200	-1.28159700	-0.35089500
H	-5.26651800	-1.14387300	-0.34596400
H	-3.88259200	-1.79780300	-1.27151700
H	-3.88843500	-1.90264500	0.50451200
C	-4.06885800	1.11251200	1.22925700
H	-5.16346400	1.13126400	1.14741000
H	-3.78291700	0.54673200	2.12323000
H	-3.69559100	2.13769200	1.33186500
C	-4.04911700	1.28364200	-1.63843500
H	-5.14512400	1.28812900	-1.57598600
H	-3.68177400	2.31575400	-1.60717000
H	-3.74264700	0.83444800	-2.58990500
C	5.77526900	1.51698500	1.39077100
H	5.83247900	2.13149800	0.47730000
H	6.28522600	2.08823800	2.17740100
C	6.51720300	0.20968100	1.16579800
H	7.58223900	0.42506200	0.98517800
H	6.49294200	-0.39494300	2.08483000
C	6.00200400	-0.56396100	-0.01523700
H	5.73606000	0.04114000	-0.88867700
C	6.24152000	-1.88908300	-0.25456700
C	6.78816600	-2.82639400	0.76428300
H	6.83528200	-2.41205900	1.77494500
H	6.21043300	-3.76186500	0.78531300
H	7.81110000	-3.11019700	0.47354300
C	6.01148200	-2.48595100	-1.59772000
H	5.59784900	-1.77423700	-2.31932600
H	6.96995400	-2.85377300	-1.99386700
H	5.35667100	-3.36841900	-1.53847500

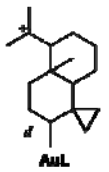


TS-2

Gtot(B3LYP)=-1221.275884
Gtot(M06-2X)=-1220.710392
Gtot(M06)=-1220.609525

XYZ Coordinates

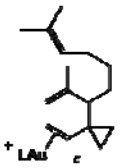
C	1.78663000	0.85263500	0.59000600
C	1.01508200	0.16107400	-0.48851600
C	1.11029400	-1.25192500	-0.47953500
C	3.20919500	-1.64704200	-0.72179600
C	3.45183600	-0.94048200	0.42266800
C	3.32741300	0.55249900	0.39436100
H	0.85242100	-1.82885400	-1.36906900
H	1.18377700	0.60601300	-1.48001600
H	3.27109300	-1.16390100	-1.69724200
H	3.24716900	-2.73689300	-0.72077700
H	0.99644300	-1.79221500	0.46188500
H	3.56190200	0.89885500	-0.62651700
C	1.30160900	2.18144900	1.08565300
H	2.01073900	2.96593700	1.33982000
H	0.37692400	2.55321900	0.64505800
C	1.23049400	0.97794200	1.98075200
H	0.25947900	0.52864200	2.19262600
H	1.92707700	0.95230100	2.81843900
Au	-1.17362100	0.18769300	-0.33688100
P	-3.52469500	0.36360300	-0.18879700
C	3.52831000	-1.64378300	1.73410700
H	2.70962900	-1.32711200	2.39828100
H	3.47842200	-2.73192500	1.60821400
H	4.46470800	-1.40589100	2.25570300
C	4.23913400	1.31442100	1.36483100
H	3.80451500	2.30843800	1.52470300
H	4.24979700	0.83269800	2.35477600
C	-4.42917400	-0.64446200	-1.40972100
H	-5.51082500	-0.50702100	-1.28332400
H	-4.14134200	-0.34380500	-2.42315100
H	-4.17965200	-1.70235700	-1.27269200
C	-4.20626000	-0.14534700	1.42416200
H	-5.29798800	-0.03155500	1.42485000
H	-3.95016900	-1.19247400	1.61952400
H	-3.77629500	0.47513600	2.21820000
C	-4.15211500	2.05758900	-0.43661600
H	-5.24649400	2.06953800	-0.35330900
H	-3.72357500	2.72420500	0.31987200
H	-3.86005000	2.41897900	-1.42872700
C	5.67635700	1.54336300	0.88809700
H	5.66119600	1.85838100	-0.16896900
H	6.07105800	2.40327100	1.44795700
C	6.66494700	0.39012100	1.06047400
H	7.67663700	0.80285300	0.90580900
H	6.64505600	0.05274200	2.10863700
C	6.46001500	-0.75398200	0.11605700
H	6.16123000	-0.46342000	-0.89841500
C	6.64181100	-2.06172400	0.34993000
C	7.07565900	-2.64485300	1.66045200
H	7.18650000	-1.90278300	2.45861300
H	6.35986400	-3.40947100	2.00117300
H	8.04184200	-3.16030500	1.55062100
C	6.40670600	-3.07863100	-0.72475300
H	6.11412800	-2.61757000	-1.67644000
H	7.30647700	-3.68749100	-0.90129000
H	5.61400400	-3.78480600	-0.42710000



Gtot(B3LYP)=-1221.2788
Gtot(M06-2X)=-1220.724755
Gtot(M06)=-1220.628519

XYZ Coordinates

C	2.01247800	0.82891400	0.10340400
C	1.13462600	-0.32881800	-0.34861300
C	1.55768400	-1.60940100	0.36476600
C	3.04536800	-1.90472400	0.17545000
C	3.93454100	-0.74906600	0.64006000
C	3.51253500	0.55115600	-0.10994500
H	0.98596700	-2.47042000	-0.01247000
H	1.33928600	-0.47641200	-1.42801400
H	3.22314900	-2.09048400	-0.89768500
H	3.30596700	-2.83020700	0.71316800
H	1.32609300	-1.54403500	1.44101200
H	3.61731400	0.31726700	-1.18787500
C	1.48769100	2.22136300	-0.11309400
H	2.16525100	3.03432500	-0.36527200
H	0.50880300	2.29785000	-0.58772700
C	1.56338300	1.65953300	1.27598900
H	0.63877400	1.35956400	1.77260500
H	2.31003900	2.09093700	1.94290900
Au	-0.96871600	-0.06608700	-0.20209900
P	-3.35930500	0.15844500	-0.05358000
C	3.86266200	-0.60953300	2.15607000
H	2.87616400	-0.22984800	2.44216700
H	3.98935900	-1.57936700	2.65689800
H	4.59815000	0.09098700	2.56924100
C	4.44732100	1.72569600	0.17213300
H	4.10450200	2.60793300	-0.38169500
H	4.42416500	1.99837800	1.23926800
C	-3.98653400	1.86901000	-0.21340000
H	-5.08117500	1.88707400	-0.13048500
H	-3.55419600	2.49524500	0.57533000
H	-3.69133100	2.28106000	-1.18509000
C	-4.30684000	-0.76027000	-1.31995400
H	-5.38492900	-0.60304700	-1.18399200
H	-4.01532700	-0.41792000	-2.31943100
H	-4.08541700	-1.83073700	-1.24085200
C	-4.09340000	-0.41488400	1.52065300
H	-5.18244800	-0.27571000	1.51158500
H	-3.86618000	-1.47688900	1.66782100
H	-3.66398200	0.15105300	2.35518300
C	5.87605700	1.41496600	-0.24285300
H	5.91813700	1.26984600	-1.33469500
H	6.53600600	2.26219000	-0.01472000
C	6.39542000	0.16964900	0.44968000
H	7.41182100	-0.06519700	0.10320500
H	6.46857000	0.34789400	1.53136200
C	5.48512800	-1.02629800	0.14890600
H	5.36745400	-1.14648400	-0.94017700
C	5.94484800	-2.28299600	0.69865400
C	6.68546900	-2.33805700	1.96102000
H	6.32589000	-1.61233200	2.69944000
H	6.74044700	-3.34433600	2.38482500
H	7.71653600	-2.01493700	1.72245600
C	5.74948700	-3.54121100	-0.02079000
H	5.16867800	-3.45128400	-0.94056200
H	6.75993900	-3.91144200	-0.27397400
H	5.33556700	-4.31357800	0.64357700



Gtot(B3LYP)=-1221.309557
Gtot(M06-2X)=-1220.724755
Gtot(M06)=-1220.637616

XYZ Coordinates

C	1.73460100	-0.08602000	-0.03051600
C	0.76982400	-0.50399300	-1.08179100
C	0.05471300	-1.66957700	-1.11900200
C	3.53730800	-0.91440700	-2.88099500
C	3.47562600	-1.05167300	-1.55418900
C	3.12671900	0.12548200	-0.66209400
H	-0.43512200	-1.98384800	-2.04195600
H	0.75264900	0.13501800	-1.97136200
H	3.36002200	0.04681100	-3.36498900
H	3.77374700	-1.75578000	-3.53232400
H	0.16119300	-2.41944800	-0.33325400
H	3.04030100	1.01702000	-1.31032800
C	1.26414000	0.85721800	1.04803800
H	1.95380300	1.62893300	1.38475000
H	0.22033000	1.17618200	1.03438100
C	1.56490800	-0.57318600	1.37807500
H	0.72671100	-1.23139200	1.60580100
H	2.46085500	-0.78578300	1.95918000
Au	-1.60969800	-0.27246700	-0.39332800
P	-3.54936100	0.79816300	0.38260800
C	3.73706500	-2.36574800	-0.88138400
H	2.93054000	-2.62618000	-0.17958300
H	3.83238400	-3.17545300	-1.61400200
H	4.66639700	-2.33699200	-0.29047800
C	4.23939000	0.38692300	0.35348000
H	3.94300000	1.18123900	1.05605500
H	4.40311500	-0.51622500	0.96032500
C	-4.67832900	1.33632600	-0.93835800
H	-5.55972800	1.82307700	-0.50179900
H	-4.16292200	2.04189200	-1.59880100
H	-4.99693400	0.46956100	-1.52737400
C	-4.55209300	-0.24123200	1.48880100
H	-5.43647200	0.31653200	1.82236000
H	-4.87058400	-1.14608800	0.96014400
H	-3.95561000	-0.53258200	2.36007400
C	-3.16818400	2.29604000	1.34355000
H	-4.09625000	2.76025500	1.70096000
H	-2.54136400	2.02902600	2.20185400
H	-2.62126000	3.00811700	0.71591300
C	5.55713100	0.78500900	-0.29742300
H	5.78783600	0.09738200	-1.12765100
H	5.45818000	1.78544600	-0.74694900
C	6.71843000	0.76479700	0.70232100
H	7.59612100	1.23888400	0.23725000
H	6.46047400	1.38504700	1.57386800
C	7.06808200	-0.63496900	1.10436100
H	7.56010400	-1.22020700	0.31896800
C	6.80339300	-1.26309600	2.25865000
C	6.11637500	-0.63768300	3.43508200
H	5.87258900	0.42008100	3.28835700
H	5.17802500	-1.16953900	3.65878900
H	6.73777400	-0.72094600	4.33941700
C	7.18251800	-2.69987800	2.46104600
H	7.66349200	-3.12933800	1.57360500
H	7.87072800	-2.81337300	3.31264100
H	6.29777200	-3.31025500	2.69952300

A1-TS

Gtot(M06)=-986.283095

XYZ Coordinates

C	1.41579000	0.77977400	-0.51111700
C	0.82125200	-0.60356300	-0.16401300
C	1.22421100	-0.95422700	1.27202000
C	2.73709200	-1.09182100	1.43893900
C	3.49494800	-0.08368700	0.69691500
C	2.91714200	0.83017200	-0.17562000
H	0.74927100	-1.89115200	1.59379000
H	3.10931500	-2.05985400	1.05072500
H	3.06944200	-1.09308100	2.48847000
H	4.57937400	-0.05879800	0.83187000
H	0.86624700	-0.17220700	1.96097500
Au	-1.31257400	-0.52886300	-0.25739100
P	-3.71243300	-0.49608000	-0.37638700
C	3.50948100	2.15105900	0.62527300
H	2.66090700	2.78267300	0.88068300
H	4.25705600	2.04521600	1.40759000
C	3.85456900	1.87037300	-0.76192100
H	4.87565600	1.55467900	-0.96974500
H	3.39636200	2.48112900	-1.53452300
H	0.91650000	1.51994400	0.13689900
C	1.31667800	-1.68149200	-1.13290000
H	0.90322300	-1.55421300	-2.14160800
H	2.41726400	-1.70588600	-1.24867300
H	1.00962600	-2.67814000	-0.78290400
C	1.17164500	1.18744300	-1.96100000
H	0.11950000	1.00292200	-2.21682900
H	1.36677500	2.25265100	-2.13563700
H	1.79396100	0.60874600	-2.65684200
C	-4.40798800	0.89474300	-1.33666500
H	-5.50390700	0.83598900	-1.36216400
H	-4.10722700	1.84527800	-0.88163900
H	-4.02154900	0.86300400	-2.36183700
C	-4.44660600	-1.97084500	-1.16883100
H	-5.54060600	-1.88486900	-1.20202700
H	-4.06062000	-2.07189600	-2.18954300
H	-4.17181700	-2.86833500	-0.60298600
C	-4.58982900	-0.39425600	1.22370500
H	-5.67595600	-0.39199600	1.06370600
H	-4.31959200	-1.25310200	1.84854400
H	-4.30046900	0.52303500	1.74882900

A2

Gtot(M06)=-986.289013

XYZ Coordinates

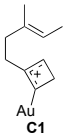
C	1.57014400	-0.64122700	-0.45651600
C	0.71253700	0.25460500	0.45617700
C	1.07054800	1.71867200	0.16947100
C	2.52682000	2.04789000	0.50648000
C	3.48061500	1.03664700	-0.04681000
C	3.02872800	-0.23940800	-0.47899800
H	0.42023700	2.39080400	0.74664200
H	2.67932500	2.08038400	1.59507300
H	2.81731300	3.04162000	0.13839600
H	4.53410600	1.14335100	0.21830900
H	0.87893800	1.95178700	-0.89152600
Au	-1.35445000	-0.03780100	0.00796900
P	-3.69096900	-0.31346500	-0.48201400
C	3.58827400	0.76044200	-1.73239500
H	2.73087000	1.02129600	-2.34982400
H	4.48375700	1.34210400	-1.94443400
C	3.93294400	-0.73906900	-1.49904500
H	4.99012900	-0.85779500	-1.26521100
H	3.52956100	-1.47764900	-2.18985000
H	1.21157400	-0.54787300	-1.49797700
C	0.95714500	-0.06266100	1.93354000
H	0.55745600	-1.04337400	2.22189300
H	2.02722300	-0.06557900	2.21712600
H	0.46051800	0.68579000	2.56795600
C	1.52197400	-2.12985500	-0.09883900
H	0.47139700	-2.44359500	-0.03858100
H	2.02138900	-2.74901300	-0.85320200
H	1.99017200	-2.33397900	0.87212500
C	-4.07061700	-1.48278200	-1.83444700
H	-5.15530500	-1.54917900	-1.99004300
H	-3.59360300	-1.14385700	-2.76110700
H	-3.68077400	-2.47626700	-1.58565100
C	-4.69946500	-0.92866100	0.91230500
H	-5.74982200	-1.03351000	0.61067700
H	-4.31897200	-1.90197700	1.24255800
H	-4.63347300	-0.22697200	1.75155100
C	-4.55215000	1.21627200	-0.99152800
H	-5.61433800	1.01347800	-1.18163000
H	-4.46403200	1.97229200	-0.20303400
H	-4.09194500	1.61096400	-1.90457700

C

Gtot(M06)=-986.279359

XYZ Coordinates

C	1.33304800	-1.36707200	2.71848600
C	2.57190100	-1.29410900	3.32416600
C	3.71984200	-0.40941200	3.05820400
H	4.60575300	-1.06192100	2.95540400
H	2.76368800	-1.97386000	4.16820400
H	3.90931300	0.08277000	4.03037300
C	0.71043800	-2.84208100	2.96046400
H	0.11858700	-3.13378600	2.09630000
H	1.40230900	-3.59735800	3.32833700
C	0.25056800	-1.82288200	3.84268300
H	0.59109800	-1.80763700	4.87587500
H	-0.68858500	-1.30782400	3.65473600
Au	0.62659100	-0.33269700	1.02658800
P	-0.25801700	0.74202200	-0.88750200
C	3.66196600	0.63791100	1.96318700
H	2.73046700	1.22323200	2.06986100
H	4.46805200	1.36339300	2.15895400
C	3.77888600	0.17935000	0.53266500
C	3.87352300	-1.11017600	0.18024800
H	3.87988300	-1.85984200	0.97614000
C	3.75972300	1.32629100	-0.43265500
H	2.79395200	1.85613600	-0.37937900
H	4.52834500	2.06865700	-0.17212800
H	3.92661700	1.03012100	-1.47323800
C	3.94695400	-1.68558700	-1.19532200
H	3.93117600	-0.92701700	-1.98594600
H	4.85741600	-2.28706900	-1.32698200
H	3.09949500	-2.36462500	-1.37259400
C	-0.27747600	2.56601500	-0.81714000
H	-0.70610700	2.97651000	-1.74054700
H	-0.87864100	2.89311100	0.03858900
H	0.74168600	2.95061600	-0.69254500
C	-1.99017700	0.29636200	-1.24669200
H	-2.62626400	0.57751000	-0.39988600
H	-2.33705300	0.81598100	-2.14922100
H	-2.06776300	-0.78586000	-1.39868100
C	0.62898700	0.35876100	-2.43622900
H	0.63950200	-0.72579700	-2.59379800
H	0.13667900	0.84603000	-3.28782300
H	1.66466300	0.71311300	-2.36960000

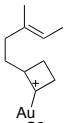


C1

Gtot(M06)=-986.285649

XYZ Coordinates

C	0.74051000	-1.45591700	0.39593100
C	1.90534700	-0.83962500	0.92661800
C	1.94449500	0.59060100	1.37768300
H	1.45331800	0.64257500	2.36157500
H	2.68074100	-1.48183000	1.36566800
H	1.33393700	1.20511300	0.69886900
C	1.99672100	-1.27713100	-0.70867000
H	1.67452800	-0.58210400	-1.48065500
H	3.06280300	-1.50244900	-0.74886500
C	1.18707800	-2.58284300	-0.40408400
H	1.85866600	-3.32861200	0.02860100
H	0.50463100	-2.96822500	-1.15864200
Au	-1.06545000	-0.44588300	0.07677800
P	-3.13681800	0.67488100	-0.20531700
C	3.37075700	1.13774100	1.49237000
H	3.30682200	2.16898000	1.87360800
H	3.91431800	0.55379700	2.25045700
C	4.12696000	1.11512200	0.19171100
C	5.16627400	0.28764000	0.01567100
H	5.45576600	-0.34508700	0.85971000
C	3.63139100	2.05084300	-0.86959000
H	4.25346500	2.03707600	-1.77103900
H	2.60097200	1.81378700	-1.17782100
H	3.60407700	3.08439500	-0.49296200
C	5.97687000	0.14462000	-1.23887200
H	6.48215600	1.08106400	-1.51542500
H	6.75266000	-0.61976700	-1.12297900
H	5.35790000	-0.14735200	-2.10017800
C	-2.96794500	2.43654600	-0.64415800
H	-3.95907400	2.89325700	-0.76285900
H	-2.41870000	2.96231900	0.14471300
H	-2.41084000	2.53176800	-1.58267500
C	-4.18102300	0.67390000	1.28917400
H	-3.64870200	1.16348800	2.11221800
H	-5.11971600	1.20867600	1.09532800
H	-4.40596000	-0.35777200	1.58154300
C	-4.20546400	-0.01874600	-1.50959600
H	-4.44511700	-1.06187000	-1.27550900
H	-5.13526000	0.56020800	-1.58187600
H	-3.68242700	0.01357100	-2.47160200



C2

Gtot(M06)=-986.278299

XYZ Coordinates

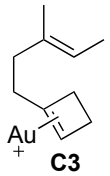
C	0.33292500	0.92492000	-0.93308600
C	1.68755000	0.52122500	-1.37384000
C	2.52122500	-0.39408300	-0.49145100
H	1.88501400	-1.22717500	-0.15503300
H	1.53363400	0.04396300	-2.36562300
H	2.81297400	0.15914100	0.41475400
C	1.99810000	2.02657600	-1.61758900
H	2.51177900	2.47193500	-0.75918000
H	2.52404900	2.28993000	-2.53947600
C	0.47329400	2.25960200	-1.55863600
H	0.01280700	2.23526200	-2.56070100
H	0.02898900	3.10773800	-1.02379000
Au	-1.02992700	0.05265400	0.28967600
P	-2.64629200	-1.02730200	1.69016800
C	3.75138400	-0.95383300	-1.21020100
H	4.29006400	-1.60644100	-0.50431900
H	3.40907300	-1.59451100	-2.03756400
C	4.68158700	0.10531300	-1.73979300
C	4.78376100	0.30957100	-3.06078100
H	4.18161100	-0.33608800	-3.70892300
C	5.43075800	0.87285600	-0.69199000
H	6.13557400	1.59986700	-1.10778200
H	4.74839400	1.42342800	-0.02675800
H	5.99843000	0.18696200	-0.04534000
C	5.60758300	1.32448000	-3.78090200
H	6.28857200	0.84546500	-4.49874000
H	4.96772400	1.99975500	-4.36826100
H	6.21349300	1.94521400	-3.11169500
C	-4.08514500	0.00023000	2.13179700
H	-4.77651900	-0.57464100	2.76119400
H	-3.75242600	0.88937400	2.67836900
H	-4.60441900	0.32056100	1.22197300
C	-1.97893900	-1.59783300	3.28788100
H	-2.76966700	-2.08819400	3.87017500
H	-1.16304300	-2.30801500	3.11412200
H	-1.58857500	-0.74452500	3.85298300
C	-3.36319300	-2.52291500	0.93263700
H	-4.09126100	-2.97767100	1.61641600
H	-3.86266500	-2.25999800	-0.00621300
H	-2.56765900	-3.24467100	0.71762400

C-TS3

Gtot(M06)=-986.270109

XYZ Coordinates

C	0.46684800	0.36715200	0.82836000
C	1.85075300	0.13072800	0.61849600
C	2.78371600	-0.84313000	1.24926300
H	2.18864000	-1.64821100	1.70563200
H	0.98659600	-0.51206200	-0.05848900
H	3.26815100	-0.31471000	2.08574500
C	2.04886600	1.37303400	-0.22985900
H	2.70905600	2.10557800	0.24910100
H	2.39617000	1.20820300	-1.25489400
C	0.53721900	1.62601500	-0.02405200
H	-0.10555100	1.65688700	-0.90935500
H	0.31665400	2.50255300	0.59710200
Au	-0.97721800	-0.58904500	1.95987400
P	-2.63849000	-1.64470900	3.29057000
C	3.83873000	-1.41330100	0.29563100
H	4.38209500	-2.19923100	0.84428900
H	3.33183200	-1.91131800	-0.54471100
C	4.81968900	-0.39308500	-0.22133700
C	4.90459900	-0.14850600	-1.53627900
H	4.22827700	-0.71044700	-2.18887900
C	5.65723400	0.27422400	0.82934800
H	6.49053900	0.84904200	0.41305800
H	5.06364800	0.96696900	1.44579400
H	6.07672100	-0.47036500	1.52234100
C	5.80097500	0.81284700	-2.24205900
H	6.36237500	0.31144900	-3.04272900
H	5.21624500	1.60832000	-2.72754400
H	6.52554400	1.29668700	-1.57788100
C	-4.07101000	-0.58652000	3.68059800
H	-4.79709200	-1.14489500	4.28540500
H	-3.73816100	0.29575500	4.23835400
H	-4.54992600	-0.25494500	2.75277000
C	-2.04703600	-2.22222300	4.91578000
H	-2.86735800	-2.70161600	5.46534900
H	-1.23322700	-2.94276700	4.77868400
H	-1.67009200	-1.37240500	5.49532500
C	-3.36503500	-3.12861100	2.51847100
H	-4.12546000	-3.56315200	3.17996100
H	-3.82690500	-2.85971500	1.56213700
H	-2.58008600	-3.86995200	2.33308100



C3

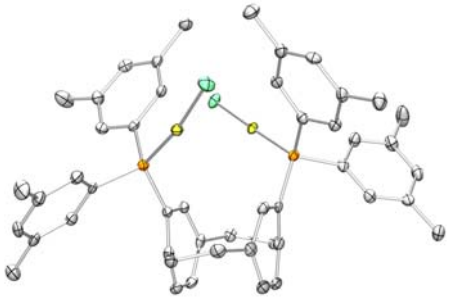
Gtot(M06)=-986.32065

XYZ Coordinates

C	1.32496900	1.16708100	-0.87953700
C	2.14929800	0.15505500	-0.42188800
C	2.58653200	-1.15267300	-0.98593900
H	1.73080500	-1.69510500	-1.41084000
H	0.78490300	1.28366100	-1.82156000
H	3.00450800	-1.78356100	-0.18901200
C	2.74793500	1.02776300	0.66573300
H	2.55715900	0.71596500	1.69987400
H	3.82731500	1.18491200	0.53484000
C	1.87099800	2.18355200	0.10909300
H	2.46223900	2.96913300	-0.37893400
H	1.16372500	2.65341100	0.80147200
Au	-0.16681900	-0.10727100	0.34580000
P	-2.02540400	-1.04405300	1.42302100
C	3.62046700	-0.93090900	-2.11164000
H	3.92768000	-1.92403500	-2.47543200
H	3.11118800	-0.42366500	-2.94421300
C	4.82054800	-0.13401200	-1.68531200
C	5.00765600	1.11310200	-2.13824700
H	4.27910300	1.50769500	-2.85247900
C	5.74504000	-0.80094100	-0.71046800
H	5.30261900	-0.86894100	0.29644500
H	5.96050000	-1.83379500	-1.02101800
H	6.70054600	-0.27449700	-0.60857400
C	6.12787900	2.02963700	-1.74629500
H	5.98737900	3.03012700	-2.16943200
H	6.20612200	2.14274300	-0.65506800
H	7.10402000	1.66393800	-2.09771900
C	-1.57950600	-2.28285100	2.67937100
H	-0.94471200	-1.82310600	3.44435500
H	-2.48846900	-2.67966300	3.14978900
H	-1.02699600	-3.10242000	2.20716800
C	-3.05647000	0.17599600	2.29392500
H	-3.90410300	-0.33077100	2.77248600
H	-2.46017200	0.68657400	3.05774300
H	-3.43230000	0.91963900	1.58294800
C	-3.15161600	-1.90268100	0.28077600
H	-2.61287600	-2.70686100	-0.23205600
H	-3.99627400	-2.32763400	0.83792600
H	-3.52864800	-1.19722400	-0.46757400

7. Crystallographic Data

(S)-3,5-xylyl-PHANEPHOS(AuCl)$_2$ (4): A suitable single crystal of **4** was selected, covered in oil, and mounted on the end of a fiber. Intensity data were collected on a Bruker-AXS SMART 1D diffractometer with CCD detector using Cu Kα radiation. Structure solution was carried out using direct methods[21] and refined by least-squares techniques on F^2. Figures were prepared using ORTEP.[22] Two benzene molecules and hydrogen atoms have been omitted for clarity.



Empirical formula	$C_{60}H_{62}Au_2Cl_2P_2$
Formula weight	1309.87
Temperature	100(2) K
Crystal system	Orthorhombic
Space group	P $2_12_12_1$
Unit cell dimensions	a = 11.4778(2) Å α = 90° b = 16.5221(3) Å β = 90° c = 27.7080(4) Å γ = 90°
Unit cell volume	5254.47(15) Å^3
Z	4
Density (calculated)	1.656 mg/m^3
Absorption coefficient	12.140 mm^{-1}

[21] Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Burla, M. C.; Polidori, G.; Camalli, M. *J. Appl. Cryst.* **1994**, *27*, 435.
[22] Farrugia, L. *J. Appl. Cryst.* **1997**, *30*, 565.

Crystal size	$0.27 \times 0.25 \times 0.068\ mm^3$
Theta range for data collection	3.11 - 70.0°
Reflections collected	48339
Independent reflections	9953
Absorption correction	Numerical
Data / restraints / parameters	9953 / 36 / 603
Flack parameter	-0.002(6)
Goodness-of-fit on F^2	1.034
Final R-indices [$I>2\sigma(I)$]	R1 = 0.0247, wR2 = 0.0621
R indices (all data)	R1 =0.0252, wR2 = 0.0625