Supporting Information

Stereoselective *Cis*-Vinylcyclopropanation via Gold(I)-Catalyzed Retro-Buchner Reaction under Mild Conditions

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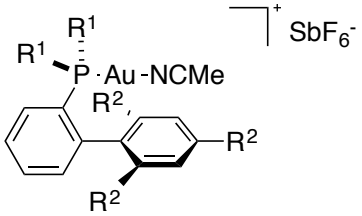
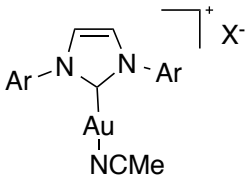
1. General information

All reactions were carried out under argon in anhydrous solvents obtained by passing them through an activated alumina column on a PureSolv^{TM} solvent purification system (Innovative Technologies, Inc., MA), unless noted otherwise. All gold-catalyzed reactions were performed in HPLC-grade solvents, without a protective atmosphere. The diastereoselectivity of the cyclopropanation reactions depends in some cases on the reaction time and temperature. The exact reaction times and temperatures are given for each example and have to be respected when reproducing this work. Tropylium tetrafluoroborate was purchased from Fluorochem. Thin layer chromatography was carried out using TLC aluminum sheets coated with 0.2 mm of silica gel (Merck Gf234). Chromatographic purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60 μm). NMR spectra were recorded at 23 ºC on Bruker Avance 300, 400 and 500 Ultrashield apparatus. Chemical shifts are reported in parts per million and referenced to residual solvent. Coupling constants (J) are reported in hertz (Hz). Mass spectra were recorded on a Waters LCT Premier Spectrometer (ESI and APCI) or on an Autoflex Bruker Daltonics (MALDI and LDI). Melting points were determined using a Büchi melting point apparatus.

The following gold complexes were synthesized according to literature procedures.[1]



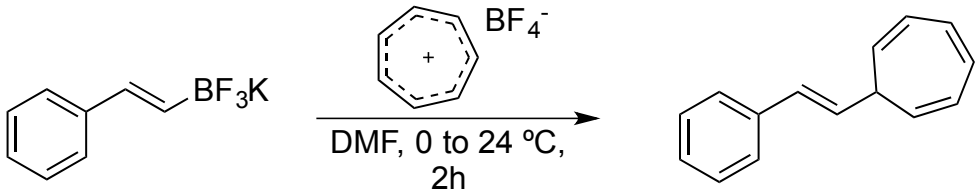
A: R^1 = *t*Bu, R^2 = H
B: R^1 = *t*Bu, R^2 = *i*Pr
C: R^1 = cyclohexyl, R^2 = H



D: Ar = mesityl, X = SbF_6
E: Ar = 2,6-diisopropylbenzene, X = BAr^F_4

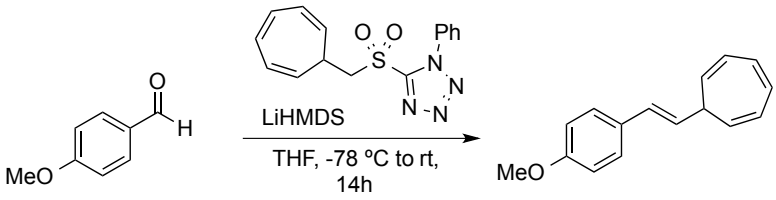
2. Preparation of vinyl cycloheptatrienes

(*E*)-7-Styrylcyclohepta-1,3,5-triene (1a)



To tropylium tetrafluoroborate (4.2 g, 23.8 mmol, 1.0 equiv) in DMF (100 mL) at 0 °C was added (*E*)-trifluoro(styryl)-λ^4-borane, potassium salt (5.0 g, 23.8 mmol, 1.0 equiv) in one portion. The solution was allowed to warm up slowly to 23 °C and quenched after 2 h by adding water and Et_2O. The phases were separated and the aq. phase was two times extracted with Et_2O. The combined organic phase was washed three times with a diluted solution of NaCl, followed by one washing with brine. The organic phase was dried over $MgSO_4$ and concentrated *in vacuo*. The crude residue was purified by filtering over a big silica plug (100 g SiO_2, eluent: pentane), affording 4.1 g (21.1 mmol, 89%) of a colorless to faint green oil.
The characterization data matched our previously reported ones.[2]

(*E*)-7-(4-Methoxystyryl)cyclohepta-1,3,5-triene (1b)



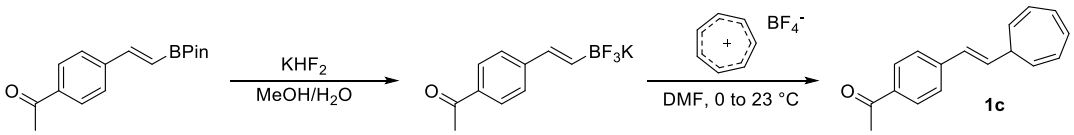
A solution of lithium bis(trimethylsilyl)amide in THF (1.0M, 1.5 mL, 1.5 mmol, 1.0 equiv) was added to a solution of **4a** (472 mg, 1.5 mmol, 1.0 equiv) in dry THF (15 mL, 0.1 M) at -78 ºC under an argon atmosphere. After stirring for 5 minutes, *p*-anisaldehyde (365 µL, 3.0 mmol, 2.0 equiv) was added neat over the glass and stirring at -78 ºC was continued for another hour before the solution was allowed to warm to room temperature over 13 hours. The reaction was quenched by the addition of water and the mixture was extracted with Et_2O, dried over Na_2SO_4 and flash chromatography (110 g, SiO_2, eluent: pentane) yielded **1b** (258 mg, 1.15 mmol, 77%) as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 2H), 6.91 – 6.87 (m, 2H), 6.74 – 6.71 (m, 2H), 6.51 (d, *J* = 16.0 Hz, 1H), 6.41 (dd, *J* = 15.9, 7.5 Hz, 1H), 5.36 (dd, *J* = 8.9, 5.7 Hz, 2H), 3.84 (s, 3H), 2.46 – 2.41 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.01, 131.04, 130.19, 129.92, 128.86, 127.30, 124.73, 124.45, 113.98, 55.31, 42.13.

M.p.: 47-48 ºC.

HRMS-APCI: calculated for $C_{16}H_{17}O$ $[M+H]^+$: 225.1274; found: 225.1271



Potassium (*E*)- 4-(acetyl)styryl trifluoroborate

To (*E*)-1-(4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)phenyl)ethan-1-one (2.720 g, 10.0 mmol, 1.0 equiv, prepared by hydroboration of the corresponding alkyne[3]) in MeOH (54 mL) at 0 °C was added KHF_2 (3.440 g, 44.0 mmol, 4.4 equiv) in water (12 mL). The reaction mixture was stirred for 1h at 23 °C. Then the reaction mixture was evaporated to dryness and the residue was placed in a Soxhlett cartridge and extracted with refluxing acetone for 3 h. After evaporating acetone, the residue was triturated with Et_2O and filtered affording 1.825 g (7.2 mmol, 72%) of a white powder.
NMR data are in agreement with literature.[4]

^{1}H NMR (500 MHz, DMSO-d^6) δ 7.88 – 7.81 (m, 2H), 7.47 – 7.41 (m, 2H), 6.54 (d, J = 18.3 Hz, 1H), 6.40 (dq, J = 18.2, 3.5 Hz, 1H), 2.53 (s, J = 4.5 Hz, 3H).

^{13}C NMR (101 MHz, DMSO-d^6) δ 197.2, 145.0, 134.4, 132.3 (q, J = 4.4 Hz), 128.5, 125.4, 26.6.

^{19}F NMR(376 MHz, DMSO-d^6) δ 138.3.

M.p.: >280 ºC (decomp.).

HRMS-ESI: calculated for $C_{10}H_9BF_3O$ $[M-K]^-$: 213.0704; found: 213.0697.

(*E*)-1-(4-(2-(Cyclohepta-2,4,6-trien-1-yl)vinyl)phenyl)ethan-1-one (1c)

To potassium (*E*)- 4-(acetyl)styryl trifluoroborate (1.300 g, 5.16 mmol, 1.05 equiv) in DMF (20 mL) at 0 °C was added tropylium tetrafluoroborate (0.875 g, 4.92 mmol, 1.00 equiv) in one portion. The solution was allowed to warm slowly up to 23 °C and quenched after 3 h by adding water and EtOAc. The phases were separated and the aq. phase was two times extracted with EtOAc. The combined organic phase was washed three times with a diluted solution of NaCl, followed by one washing with brine. The organic phase was dried over $MgSO_4$ and concentrated *in vacuo*. The crude residue was purified by flash chromatography (220 g SiO_2, eluent: pentane to 50% Et_2O) affording **1c** (823 mg, 4.92 mmol, 71%) as a yellow solid.

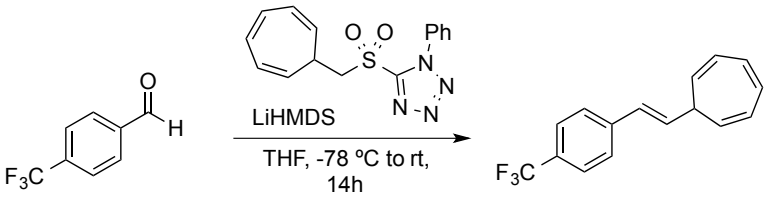
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 – 7.89 (m, 2H), 7.49 – 7.44 (m, 2H), 6.74 – 6.68 (m, 2H), 6.65 (dd, J = 15.9, 7.1 Hz, 1H), 6.58 (d, J = 16.0 Hz, 1H), 6.28 – 6.23 (m, 2H), 5.34 (dd, J = 8.9, 5.8 Hz, 2H), 2.59 (s, 3H), 2.55 – 2.47 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 197.7, 142.2, 136.0, 134.1, 131.2, 129.8, 128.9, 126.4, 125.0, 123.7, 42.2, 26.7.

M.p.: 52-53 ºC.

HRMS-ESI: calculated for $C_{17}H_{17}O$ $[M+H]^+$: 237.1274; found: 237.1277.

(*E*)-7-(4-(Trifluoromethyl)styryl)cyclohepta-1,3,5-triene (1d)



A solution of lithium bis(trimethylsilyl)amide in THF (1.0M, 1.0 mL, 1.0 mmol, 1.0 equiv) was added to a solution of **4a** (314 mg, 1.0 mmol, 1.0 equiv) in dry THF (10 mL, 0.1M) at -78 ºC under an argon atmosphere. After stirring for 5 minutes, 4-(trifluoromethyl)benzaldehyde (273 µL, 2.0 mmol, 2.0 equiv) was added neat over the glass and stirring at -78 ºC was continued for another hour before the solution was allowed to warm to room temperature over 13 hours. The reaction was quenched by the addition of water and the mixture was extracted with Et_2O, dried over Na_2SO_4 and flash chromatography (80 g, SiO_2, eluent: pentane) yielded **1d** (127 mg, 0.48 mmol, 49%) as a colorless oil.

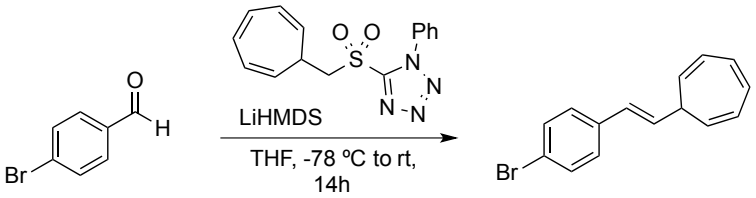
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 2H), 6.74 – 6.72 (m, 2H), 6.66 – 6.56 (m, 2H), 6.32 – 6.25 (m, 2H), 5.37 (dd, *J* = 8.9, 5.8 Hz, 2H), 2.54 (q, *J* = 5.9 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 133.59, 131.10, 129.29, 126.33, 125.52, 125.49, 124.90, 123.65, 99.99, 42.01.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.56.

HRMS-APCI: calculated for $C_{16}H_{14}F_3$ $[M+H]^+$: 263.1035; found: 263.1042

(*E*)-7-(4-Bromostyryl)cyclohepta-1,3,5-triene (1e)



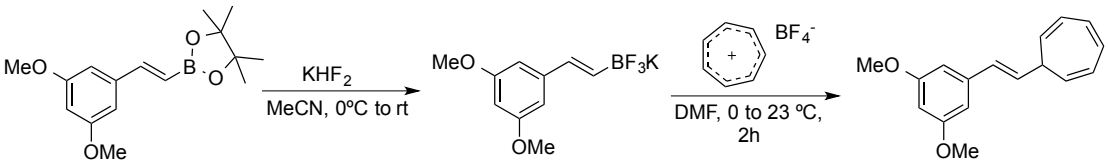
A solution of lithium bis(trimethylsilyl)amide in THF (1.0M, 2.0 mL, 2.0 mmol, 1.0 equiv) was added to a solution of **4a** (629 mg, 2.0 mmol, 1.0 equiv) in dry THF (8 mL, 0.25M) at -78 ºC under an argon atmosphere. After stirring for 5 minutes, 4-bromobenzaldehyde (740 mg, 4.0 mmol, 2.0 equiv) was added in one portion and stirring at -78 ºC was continued for another hour before the solution was allowed to warm to room temperature over 13 hours. The reaction was quenched by the addition of water and the mixture was extracted with Et_2O, dried over Na_2SO_4 and flash chromatography (80 g, SiO_2, eluent: pentane) yielded **1e** (465 mg, 1.7 mmol, 85%) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.30 – 7.26 (m, 2H), 6.74 – 6.72 (m, 2H), 6.57 – 6.46 (m, 2H), 6.29 – 6.24 (m, 2H), 5.35 (dd, *J* = 9.0, 5.8 Hz, 2H), 2.48 (q, *J* = 5.8 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.33, 131.73, 131.63, 131.08, 129.40, 127.74, 124.74, 123.98, 120.98, 42.04.

M.p.: 55-57 ºC.

HRMS-APCI: calculated for $C_{15}H_{14}Br$ $[M+H]^+$: 273.0273; found: 273.0281



Potassium (E)-(3,5-dimethoxystyryl)trifluoro-λ^4-borane

The compound was synthesized according the literature procedure.[5]

To a solution of (*E*)-2-(3,5-dimethoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1g, 3.44 mmol, 1.0 equiv) in acetonitrile (5.4 mL, 0.64M) at 0 ºC, was added a saturated aqueous solution of KHF_2 (2.3 mL, 10.3 mmol, 3.0 equiv) over 5 minutes. The reaction was left to stir over night at room whilst warming to room temperature. Then the reaction mixture was evaporated to dryness and the residue was placed in a Soxhlett cartridge and extracted with refluxing acetone for 72 h. The long extraction time is necessary for obtaining good yields because of the low solubility of the product. Acetone was evaporated and the residue was triturated in Et_2O and filtered affording 834 mg (3.09 mmol, 90%) of a white solid.

NMR data are in agreement with the literature.[5]

(*E*)-7-(3,5-Dimethoxystyryl)cyclohepta-1,3,5-triene (1f)

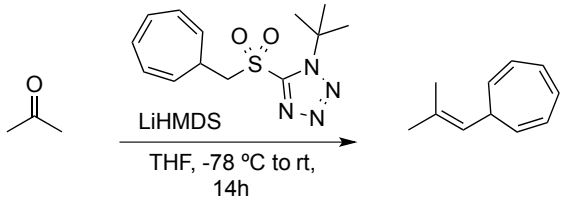
To Potassium (E)-(3,5-dimethoxystyryl)trifluoro-λ^4-borane (834 mg, 3.1 mmol, 1.0 equiv) in DMF (12.5 mL) at 0 °C was added tropylium tetrafluoroborate (550 mg, 3.1 mmol, 1.0 equiv) in one portion. The solution was allowed to warm slowly up to 23 °C and quenched after 2 h by adding water and EtOAc. The phases were separated and the aq. phase was two times extracted with EtOAc. The combined organic phase was washed three times with a diluted solution of NaCl, followed by one washing with brine. The organic phase was dried over $NaSO_4$ and concentrated *in vacuo*. The crude residue was purified by flash chromatography (220 g SiO_2, eluent: 1% Et_2O in pentane) affording **1f** (0.95 g, 4.10 mmol, 86%) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.74 – 6.71 (m, 2H), 6.59 (d, *J* = 2.2 Hz, 2H), 6.57 – 6.47 (m, 2H), 6.40 (t, *J* = 2.2 Hz, 1H), 6.29 – 6.24 (m, 2H), 5.36 (dd, *J* = 8.9, 5.7 Hz, 2H), 3.84 (s, 3H), 2.47 (q, *J* = 5.8 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.93, 139.44, 131.53, 131.07, 130.52, 124.63, 124.25, 104.33, 99.60, 55.35, 42.01.

HRMS-APCI: calculated for C17H19O2 $[M+H]^+$: 255.1380; found: 255.1379.

7-(2-Methylprop-1-en-1-yl)cycloheptа-1,3,5-triene (1g)



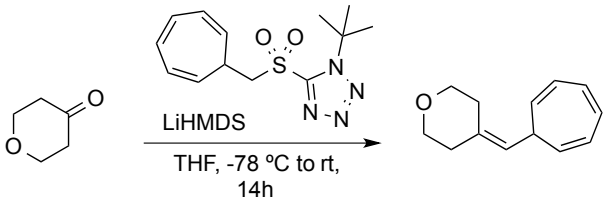
A solution of lithium bis(trimethylsilyl)amide in THF (1.0M, 4.5 mL, 4.5 mmol, 3.0 equiv) was added to a solution of **4b** (883 mg, 3.0 mmol, 2.0 equiv) and acetone (110 μL, 1.5 mmol, 1.0 equiv) in dry THF (15 mL, 0.1M) at -78 ºC under an argon atmosphere, and stirred for 1 h before the solution was allowed to warm to room temperature over 13 hours. The reaction was quenched by the addition of water and the mixture was extracted with Et_2O, dried over Na_2SO_4 and flash chromatography (40 g, SiO_2, eluent: pentane) yielded **1g** (165 mg, 1.13 mmol, 75%) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.72 – 6.69 (m, 2H), 6.22 – 6.17 (m, 2H), 5.57 (dt, *J* = 8.6, 1.4 Hz, 1H), 5.17 (dd, *J* = 8.9, 5.4 Hz, 2H), 2.34 (dt, *J* = 9.4, 5.6 Hz, 1H), 1.80 (s, 3H), 1.58 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 133.67, 130.92, 126.81, 126.31, 124.07, 38.58, 25.67, 18.04.

HRMS-APCI: calculated for $C_{11}H_{15}$ $[M+H]^+$: 147.1168; found: 147.1166

4-(Cyclohepta-2,4,6-trien-1-ylmethylene)tetrahydro-2*H*-pyran (1h)

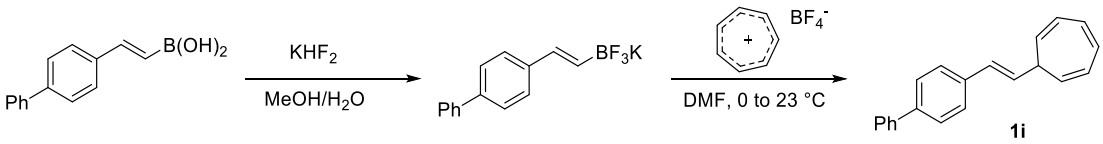


A solution of lithium bis(trimethylsilyl)amide in THF (1.0 M, 4.5 mL, 4.5 mmol, 3.0 equiv) was added to a solution of **4b** (883 mg, 3.0 mmol, 2.0 equiv) and tetrahydro-4*H*-pyran-4-one (139 μL, 1.5 mmol, 1.0 equiv) in dry THF (15 mL, 0.1M) at -78 ºC under an argon atmosphere, and stirred for 1 h before the solution was allowed to warm to room temperature over 13 hours. The reaction was quenched by the addition of water and the mixture was extracted with Et_2O, dried over Na_2SO_4 and flash chromatography (80 g, SiO_2, eluent: pentane) yielded **1h** (242 mg, 1.28 mmol, 86%) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.73 – 6.69 (m, 2H), 6.25 – 6.18 (m, 2H), 5.65 (d, *J* = 8.5 Hz, 1H), 3.77 – 3.72 (m, 2H), 3.68 – 3.64 (m, 2H), 2.37 (dt, *J* = 8.8, 5.4 Hz, 1H), 2.33 – 2.29 (m, 2H), 2.22 – 2.18 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 136.48, 131.02, 125.96, 125.56, 124.24, 69.60, 68.74, 37.52, 36.72, 30.13.

HRMS-APCI: calculated for $C_{13}H_{17}O$ $[M+H]^+$: 189.1274; found: 189.1274



Potassium (*E*)-(2-([1,1'-biphenyl]-4-yl)vinyl)trifluoroborate

The product was synthesized using a modified literature procedure4:

To *trans*-2-(4-Biphenyl)vinylboronic acid (1.066 g, 4.76 mmol, 1.0 equiv) in MeOH(95 mL) was added a solution of KHF_2 (1.635 g, 20.93 mmol, 4.4 equiv) in water (21 mL) and stirred for 3 h at 23 °C. Then the reaction mixture was evaporated to dryness and the residue was placed in a Soxhlett cartridge and extracted with refluxing acetone for 72 h. The long extraction time is necessary for obtaining good yields because of the low solubility of the product. Acetone was evaporated and the residue was triturated in Et_2O and filtered affording 1.129 g (4.76 mmol, 83%) of a white solid.

The characterization data corresponds to literature data[4]

^{1}H NMR (500 MHz, DMSO-d^6) δ 7.68 – 7.62 (m, 2H), 7.59 – 7.54 (m, 2H), 7.47 – 7.43 (m, 2H), 7.41 (d, J = 8.3 Hz, 2H), 7.35 – 7.30 (m, 1H), 6.53 (d, J = 18.2 Hz, 1H), 6.26 (dq, J = 18.2, 3.5 Hz, 1H).

(*E*)-4-(2-(Cyclohepta-2,4,6-trien-1-yl)vinyl)-1,1'-biphenyl (1i)

To potassium (*E*)-(2-([1,1'-biphenyl]-4-yl)vinyl)trifluoroborate (1.23 g, 4.3 mmol, 1.05 equiv) in DMF (16.5 mL) at 0 °C was added tropylium tetrafluoroborate (0.73 g, 4.1 mmol, 1.00 equiv) in one portion. The solution was allowed to warm slowly up to 23 °C and quenched after 2 h by adding water and EtOAc. The phases were separated and the aq. phase was two times extracted with EtOAc. The combined organic phase was washed three times with a diluted solution of NaCl, followed by one washing with brine. The organic phase was dried over $MgSO_4$ and concentrated *in vacuo*. The crude residue was purified by flash chromatography (220 g SiO_2, eluent: pentane) affording **1i** (0.95 g, 4.10 mmol, 86%) as a white solid.

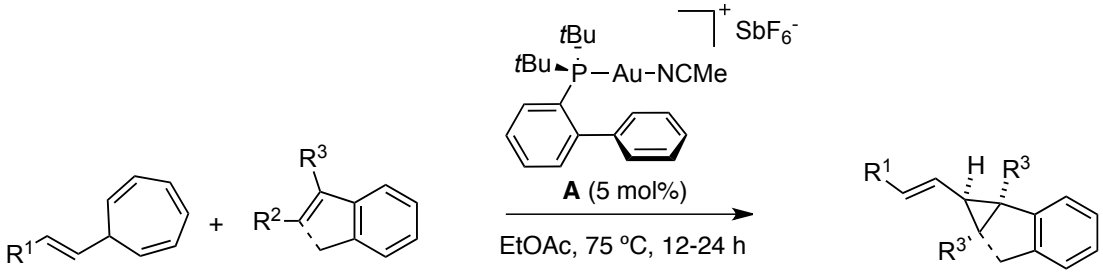
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.59 (m, 2H), 7.58 – 7.55 (m, 2H), 7.49 – 7.42 (m, 4H), 7.37 – 7.32 (m, 1H), 6.76 – 6.66 (m, 2H), 6.62 – 6.53 (m, 2H), 6.29 – 6.21 (m, 2H), 5.36 (dd, J = 9.0, 5.7 Hz, 2H), 2.52 – 2.43 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 136.6, 131.3, 131.2, 130.2, 128.9, 127.4 (two signals), 127.1, 126.8, 124.8, 124.5, 42.3.

M.p.: 101-103 ºC.

HRMS-ESI: calculated for $C_{21}H_{19}$ $[M+H]^+$: 271.1481; found: 271.1491.

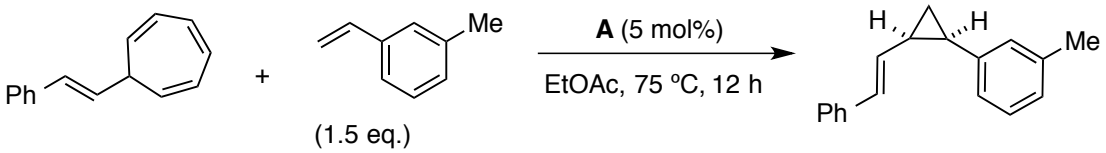
3. General procedure for the gold(I)-catalyzed cyclopropanation



A solution of vinylcycloheptatriene (1.0 equiv), olefin (1.5-2.0 equiv) and gold catalyst **A** (5 mol%) in EtOAc (10 mL/mmol) was heated in a closed screw-cap tube/vial at 75 ºC for 12-24 h. The reaction mixture was cooled to room temperature, the solvent removed *in vacuo* and the crude residue was purified by column chromatography.

4. Cyclopropanation of different olefin substrates

***Cis*-(*E*)-1-methyl-3-(2-styrylcyclopropyl)benzene (3a)**



This compound (colorless crystals, 43.7 mg, 75%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 1-methyl-3-vinylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

Suitable crystals for X-ray diffraction were obtained by slow evaporation of a solution in Chloroform.

The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.12 (m, 7H), 7.08 – 7.03 (m, 2H), 6.54 (d, *J* = 15.7 Hz, 1H), 5.57 (dd, *J* = 15.7, 9.5 Hz, 1H), 2.49 – 2.42 (m, 1H), 2.36 (s, 3H), 2.04 (qd, *J* = 8.9, 5.5 Hz, 1H), 1.38 (td, *J* = 8.4, 5.2 Hz, 1H), 1.15 (dt, *J* = 6.3, 5.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.59, 137.80, 137.61, 130.75, 130.11, 129.42, 128.36, 127.96, 126.83, 126.52, 126.01, 125.66, 23.84, 22.73, 21.46, 12.56.

M.p.: 28-30 ºC.

HRMS-APCI: calculated for $C_{18}H_{19}$ $[M+H]^+$: 235.1481; found: 235.1475.

***Cis*-((*E*)-2-(2-phenylcyclopropyl)vinyl)benzene (3b)**

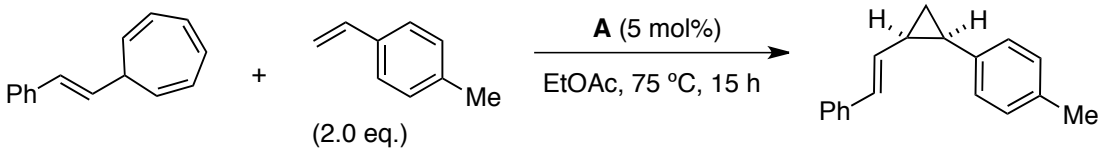
This compound (colorless oil, 37 mg, 65%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), styrene (53.6 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.11 (m, 10H), 6.53 (d, J = 15.7 Hz, 1H), 5.55 (dd, J = 15.7, 9.5 Hz, 1H), 2.48 (m, 1H), 2.05 (m, 1H), 1.39 (m, 1H), 1.16 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9 , 137.9 , 130.7 , 129.7 , 129.3 , 128.5 , 128.2 , 126.7 , 126.2 , 125.8 , 24.0 , 22.8 , 12.7 .

HRMS-APCI: calculated for $C_{17}H_{17}$ $[M+H]^+$: 221.1325; found: 221.1322.

***Cis*-1-methyl-4-(2-((*E*)-styryl)cyclopropyl)benzene (3c)**



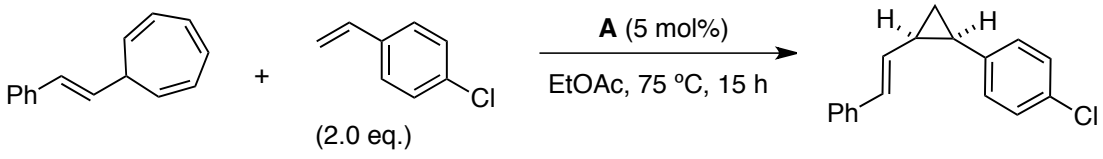
This compound (colorless oil, 41.5 mg, 69%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-methyl-4-vinylbenzene (60.8 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 6.96 (m, 9H), 6.59 (d, J = 15.7 Hz, 1H), 5.63 (dd, J = 15.7, 9.5 Hz, 1H), 2.48 (m, 1H), 2.40 (s, 3H), 2.06 (m, 1H), 1.42 (m, 1H), 1.17 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.9 , 135.7 , 135.6 , 130.9 , 129.5 , 129.2 , 128.9 , 128.5 , 126.6 , 125.8 , 23.7 , 22.8 , 21.2 , 12.8 .

HRMS-APCI: calculated for $C_{18}H_{19}$ $[M+H]^+$: 235.1481; found: 235.1477.

***Cis*-1-chloro-4-(2-((*E*)-styryl)cyclopropyl)benzene (3d)**



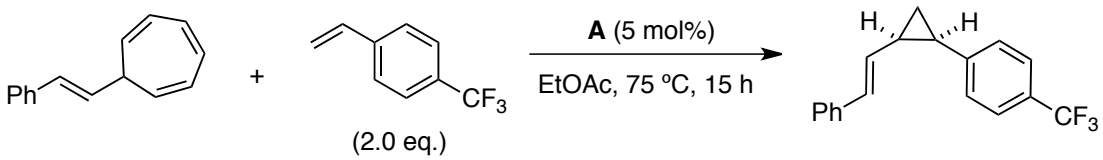
This compound (colorless oil, 49 mg, 75%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-chloro-4-vinylbenzene (71.3 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 - 7.32 (m, 9 H), 6.56 (d, J=15.8 Hz, 1 H), 5.52 (dd, J=15.8, 9.4 Hz, 1 H), 2.38 - 2.49 (m, 1 H), 2.01 - 2.13 (m, 1 H), 1.37 - 1.46 (m, 1 H), 1.08 - 1.19 (m, 1 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6 , 137.4 , 131.9 , 130.7 , 130.1 , 130.0 , 128.6 , 128.3 , 126.9 , 125.8 , 23.3 , 22.8 , 12.8 .

HRMS-APCI: calculated for $C_{17}H_{16}Cl$ $[M+H]^+$: 255.0935; found: 255.0923.

***Cis*-1-(2-((*E*)-styryl)cyclopropyl)-4-(trifluoromethyl)benzene (3e)**



This compound (colorless oil, 44 mg, 59%, d.r. 19:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-(trifluoromethyl)-4-vinylbenzene (89.0 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

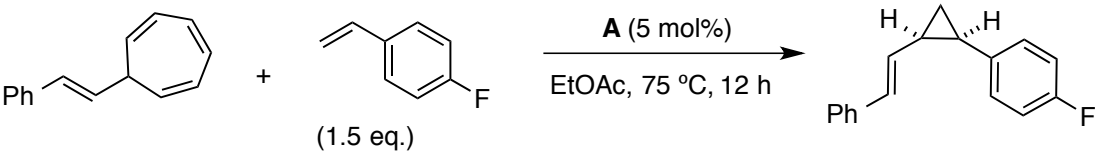
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J=8.2 Hz, 2H), 7.39 (d, J=8.2 Hz, 2H), 7.27 (m, 2H), 7.18 (m, 3H), 6.58 (d, J=15.8 Hz, 1H), 5.53 (dd, J=15.6, 9.2 Hz, 1H), 2.50 (m, 1H), 2.14 (m, 1H), 1.47 (m, 1H), 1.22 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 143.2 , 137.5 , 130.6 , 129.5 , 129.4 , 128.6 , 128.4 (q, J=32.3 Hz), 127.0 , 125.8 , 125.2 (q, J = 3.7 Hz), 124.5 (q, J= 272.6 Hz), 23.8 , 23.3 , 13.0 .

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.2 .

HRMS-APCI: calculated for $C_{18}H_{16}F_3$ $[M+H]^+$: 289.1199; found: 289.1192.

***Cis*-(*E*)-1-fluoro-4-(2-styrylcyclopropyl)benzene (3f)**



This compound (colorless oil, 38.8 mg, 65%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 1-fluoro-4-vinylbenzene (45.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

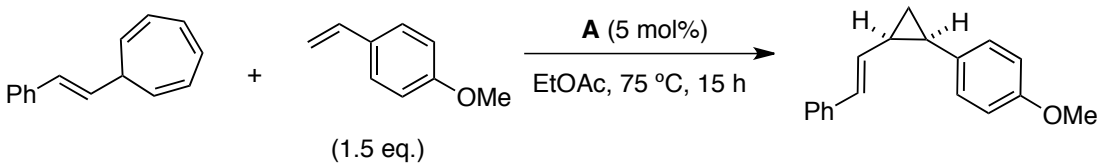
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 – 7.23 (m, 4H), 7.17 – 7.15 (m, 3H), 7.03 – 6.98 (m, 2H), 6.54 (d, *J* = 15.8 Hz, 1H), 5.49 (dd, *J* = 15.7, 9.4 Hz, 1H), 2.43 (q, *J* = 8.3 Hz, 1H), 2.03 (qd, *J* = 8.8, 5.5 Hz, 1H), 1.40 (td, *J* = 8.4, 5.2 Hz, 1H), 1.12 – 1.07 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.40 (d, *J* = 244.0 Hz), 137.62 , 134.38 (d, *J* = 3.2 Hz), 130.70 (d, *J* = 7.9 Hz), 130.32 , 129.71 , 128.42 , 126.68 , 125.63 , 114.91 (d, *J* = 21.2 Hz), 23.03 , 22.37 , 12.73.

^{19}F NMR (376 MHz, $CDCl_3$) δ -117.17 (ddd, *J* = 13.9, 8.9, 5.4 Hz).

HRMS-APCI: calculated for $C_{17}H_{14}F$ $[M-H]^+$: 237.1074; found: 237.1068.

***Cis*-1-methoxy-4-(2-((*E*)-styryl)cyclopropyl)benzene (3g)**



This compound (yellow oil that solidifies in the freezer, 45 mg, 70%, d.r. 15:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-methoxy-4-vinylbenzene (51.8 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: gradient from pentane to 1% Et_2O in pentane).

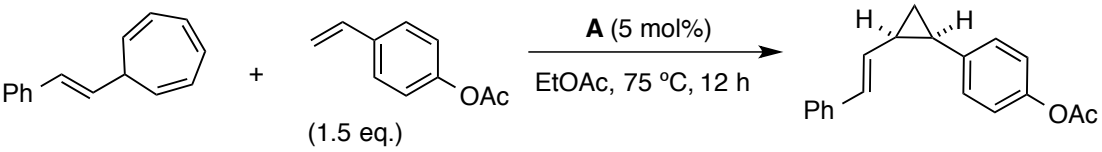
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (m, 7 H), 6.89 (m, 2 H), 6.56 (d, J=15.8 Hz, 1 H), 5.56 (dd, J=15.8, 9.4 Hz, 1 H), 3.84 (s, 3 H), 2.44 (m, 1 H), 2.02 (m, 1 H), 1.39 (m, 1 H), 1.11 (m, 1 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 137.9, 131.1, 130.9, 130.4, 129.4, 128.5, 126.6, 125.7, 113.9, 55.3, 23.2, 22.5, 12.8.

HRMS-APCI: calculated for $C_{18}H_{19}O$ $[M+H]^+$: 251.1430; found: 251.1425.

***Cis*-(*E*)-4-(2-styrylcyclopropyl)phenyl acetate (3h)**



This compound (colorless solid, 47.1 mg, 68%, d.r. 19:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 4-vinylphenyl acetate (57.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: 99:1 pentane/Et_2O).

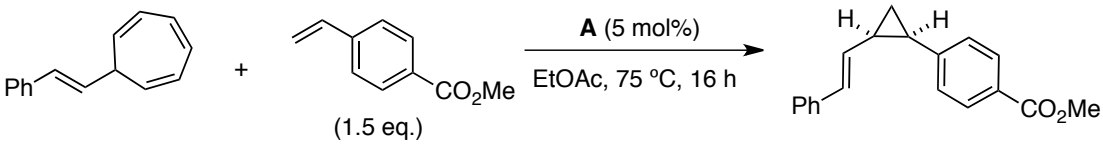
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.27 (m, 2H), 7.25 – 7.22 (m, 2H), 7.17 – 7.12 (m, 3H), 7.05 – 7.02 (m, 2H), 6.54 (d, *J* = 15.8 Hz, 1H), 5.53 (dd, *J* = 15.7, 9.5 Hz, 1H), 2.47 – 2.41 (m, 1H), 2.31 (s, 3H), 2.08 – 2.00 (m, 1H), 1.40 (td, *J* = 8.4, 5.2 Hz, 1H), 1.13 – 1.08 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.51, 148.96, 137.61, 136.38, 130.34, 130.23, 129.75, 128.40, 126.64, 125.67, 121.12, 23.25, 22.54, 21.16, 12.86.

M.p.: 61-63 ºC.

HRMS-APCI: calculated for $C_{19}H_{18}NaO_2$ $[M+Na]^+$: 301.1199; found: 301.1187.

***Cis*-methyl 4-(2-((*E*)-styryl)cyclopropyl)benzoate (3i)**



This compound (white solid, 38.5 mg, 54%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), methyl 4-vinylbenzoate (62.6 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: gradient from pentane to 6% Et_2O in pentane).

The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

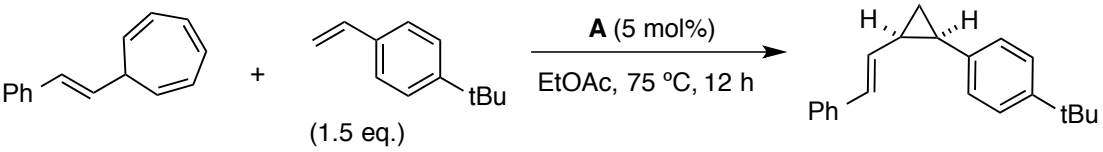
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J=8.2 Hz, 2 H), 7.31 (d, J=8.2 Hz, 2 H), 7.21 (m, 2 H), 7.13 (m, 3 H), 6.53 (d, J=15.8 Hz, 1 H), 5.51 (dd, J=15.6, 9.2 Hz, 1 H), 3.91 (s, 3 H), 2.48 (m, 1 H), 2.10 (m, 1 H), 1.43 (m, 1 H), 1.23 (m, 1 H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 167.2 , 144.6 , 137.5 , 130.5 , 129.5 , 129.5 , 129.1 , 128.5 , 128.0 , 126.9 , 125.8 , 52.1 , 24.1 , 23.5 , 13.0 .

M.p.: 60-61 ºC.

HRMS-ESI: calculated for $C_{19}H_{18}NaO_2$ $[M+Na]^+$: 301.1199; found: 301.1210.

***Cis*-(*E*)-1-(*tert*-butyl)-4-(2-styrylcyclopropyl)benzene (3j)**



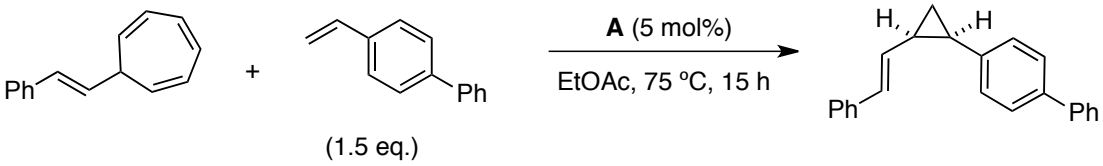
This compound (colorless oil, 48.4 mg, 70%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 1-(*tert*-butyl)-4-vinylbenzene (69.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.31 (m, 2H), 7.26 – 7.13 (m, 7H), 6.54 (d, *J* = 15.7 Hz, 1H), 5.60 (dd, *J* = 15.7, 9.5 Hz, 1H), 2.47 – 2.39 (m, 1H), 2.08 – 1.98 (m, 1H), 1.38 (td, *J* = 8.5, 5.2 Hz, 1H), 1.34 (s, 9H), 1.13 (dt, *J* = 6.4, 5.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 148.83, 137.86, 135.62, 130.95, 129.33, 128.78, 128.35, 126.49, 125.69, 125.01, 34.40, 31.40, 23.47, 22.74, 12.76.

HRMS-APCI: calculated for $C_{21}H_{23}$ $[M-H]^+$: 275.1794; found: 275.1792.

***Cis*-4-(2-((*E*)-styryl)cyclopropyl)-1,1'-biphenyl (3k)**



This compound (yellow viscous oil, 63 mg, 83%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 4-vinyl-1,1'-biphenyl (69.6 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

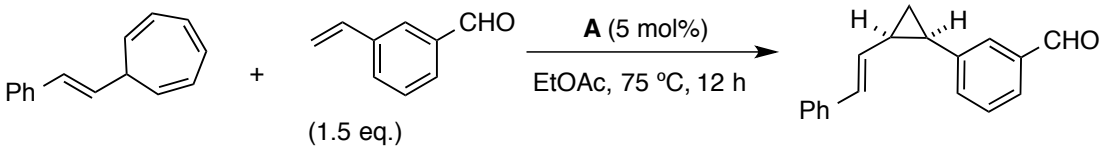
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J=7.6 Hz, 2 H), 7.49 (d, J=7.9 Hz, 2 H), 7.39 (m, 2 H), 7.29 (m, 3 H), 7.12 (m, 5 H), 6.51 (d, J=15.8 Hz, 1 H), 5.57 (dd, J=15.6, 9.5 Hz, 1 H), 2.43 (m, 1 H), 2.01 (m, 1 H), 1.36 (m, 1 H), 1.13 (m, 1 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1 , 139.0 , 138.1 , 137.8 , 130.6 , 129.9 , 129.7 , 128.9 , 128.5 , 127.2 , 127.1 , 126.9 , 126.7 , 125.8 , 23.7 , 23.1 , 12.9 .

HRMS-APCI: calculated for $C_{23}H_{21}$ $[M+H]^+$: 297.1641; found: 297.1638.

M.p.: 74-75 ºC.

***Cis*-(*E*)-3-(2-styrylcyclopropyl)benzaldehyde (3l)**



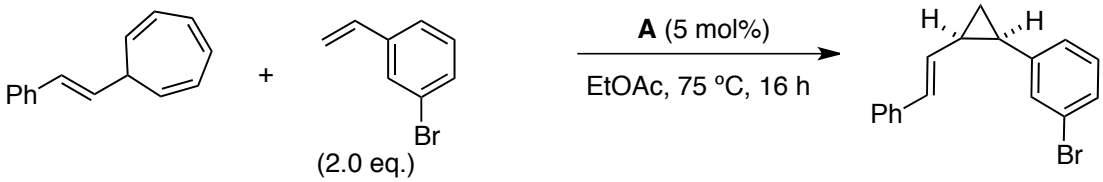
This compound (colorless oil, 44.7 mg, 72%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 3-vinylbenzaldehyde (48.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: 99:1 to 80:20 pentane/ Et_2O).

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.83 – 7.78 (m, 1H), 7.74 (dt, *J* = 7.5, 1.5 Hz, 1H), 7.55 (ddt, *J* = 7.7, 2.0, 0.8 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.18 (m, 2H), 7.18 – 7.10 (m, 3H), 6.55 (d, *J* = 15.8 Hz, 1H), 5.48 (dd, *J* = 15.7, 9.3 Hz, 1H), 2.53 (td, *J* = 8.6, 6.6 Hz, 1H), 2.17 – 2.07 (m, 1H), 1.49 – 1.44 (m, 1H), 1.25 (dt, *J* = 6.5, 5.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 192.50, 140.10, 137.41, 136.37, 135.42, 130.41, 130.02, 129.42, 128.78, 128.42, 127.83, 126.80, 125.66, 23.52, 22.85, 12.56.

HRMS-APCI: calculated for $C_{18}H_{16}NaO$ $[M+Na]^+$: 271.1093; found: 271.1089.

***Cis*-1-bromo-3-(2-((*E*)-styryl)cyclopropyl)benzene (3m)**



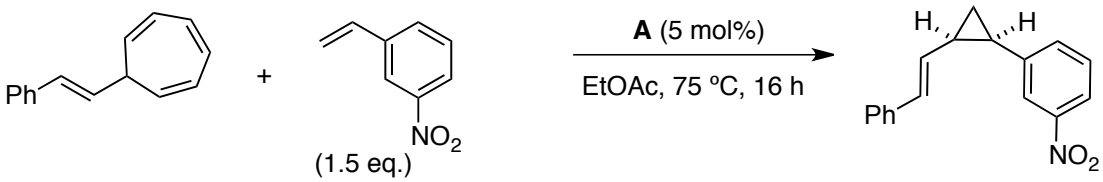
This compound (colorless oil, 43 mg, 56%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-bromo-3-vinylbenzene (94 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (br. s, 1H), 7.33 (m, 1H), 7.22 (m, 2H), 7.19 – 7.10 (m, 5H), 6.52 (d, J = 15.7 Hz, 1H), 5.49 (dd, J = 15.7, 9.4 Hz, 1H), 2.41 (m, 1H), 2.04 (m, 1H), 1.38 (m, 1H), 1.12 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.4 , 137.7 , 132.4 , 130.3 , 129.8 , 129.7 , 129.3 , 128.6 , 127.9 , 126.9 , 125.8 , 122.4 , 23.7 , 23.0 , 12.7 .

HRMS-APCI: calculated for $C_{17}H_{16}Br$ $[M+H]^+$: 299.0418; found: 299.0430.

***Cis*-1-nitro-3-(2-((*E*)-styryl)cyclopropyl)benzene (3n)**



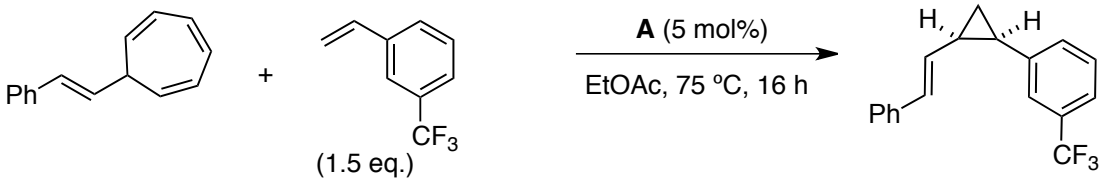
This compound (yellow oil, 31.1 mg, 47%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49. mg, 250 μmol), 1-nitro-3-vinylbenzene (52 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (24 g SiO_2, eluent: gradient from pentane to 1% Et_2O in pentane).

The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (m, 1H), 8.06 (m, 1H), 7.57 (m, 1H), 7.44 (m, 1H), 7.24 – 7.18 (m, 2H), 7.17 – 7.10 (m, 3H), 6.54 (d, J = 15.8 Hz, 1H), 5.45 (dd, J = 15.7, 9.1 Hz, 1H), 2.51 (m, 1H), 2.29 – 1.97 (m, 1H), 1.48 (m, 1H), 1.24 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3 , 141.3 , 137.3 , 135.5 , 131.2 , 129.1 , 128.7 , 128.6 , 127.1 , 125.8 , 123.9 , 121.4 , 23.6 , 23.2 , 12.9 .

***Cis*-1-(2-((*E*)-styryl)cyclopropyl)-3-(trifluoromethyl)benzene (3o)**



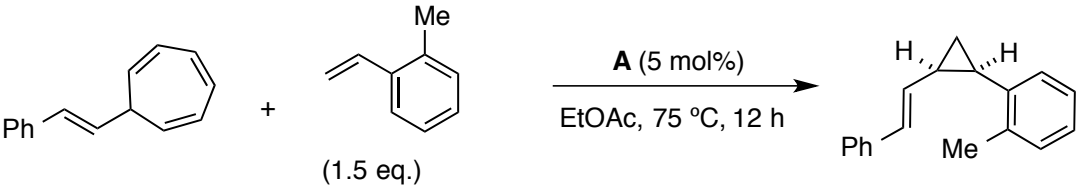
This compound (colorless oil, 37.8 mg, 52%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-(trifluoromethyl)-3-vinylbenzene (66.5 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (br. s, 1H), 7.50 – 7.36 (m, 3H), 7.22 (m, 2H), 7.15 (m, 3H), 6.54 (d, J = 15.7 Hz, 1H), 5.48 (dd, J = 15.7, 9.3 Hz, 1H), 2.48 (m, 1H), 2.10 (m, 1H), 1.44 (m, 1H), 1.18 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0 , 137.6 , 132.7 (q, J = 1.2 Hz), 130.6 (q, J = 31.9 Hz), 130.6 , 129.5 , 128.6 , 128.6 , 127.0 , 126.0 (q, J = 3.7 Hz), 125.8 , 123.1 (q, J = 3.9 Hz), 23.7 , 22.9 , 12.8 .

HRMS-APCI: calculated for $C_{18}H_{15}F_3$ $[M+H]^+$: 289.1186; found: 289.1199.

***Cis*-(*E*)-1-methyl-2-(2-styrylcyclopropyl)benzene (3p)**



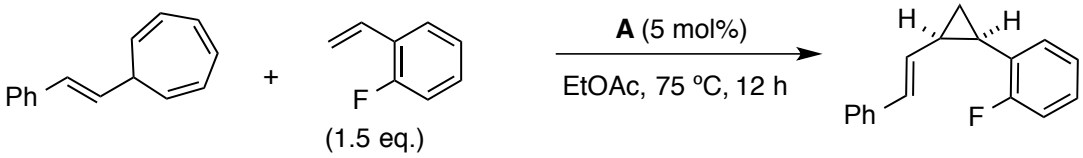
This compound (colorless oil, 38.2 mg, 65%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 1-methyl-2-vinylbenzene (49.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 – 7.10 (m, 9H), 6.53 (d, J = 15.8 Hz, 1H), 5.37 (dd, J = 15.8, 9.8 Hz, 1H), 2.37 (m, 1H),, 2.36 (s, 3H), 2.12 (qd, J = 8.5, 5.1 Hz, 1H), 1.41 (td, J = 8.4, 5.2 Hz, 1H), 1.18 (dt, J = 6.7, 5.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.85, 137.77, 137.06, 130.77, 129.61, 129.17, 128.45, 128.35, 126.49, 126.35, 125.61, 125.47, 22.90, 22.10, 19.71, 12.37.

HRMS-APCI: calculated for $C_{18}H_{19}$ $[M+H]^+$: 235.1481; found: 235.1471.

***Cis*-(*E*)-1-fluoro-2-(2-styrylcyclopropyl)benzene (3q)**



This compound (colorless oil, 36.0 mg, 60%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), 1-fluoro-2-vinylbenzene (45.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

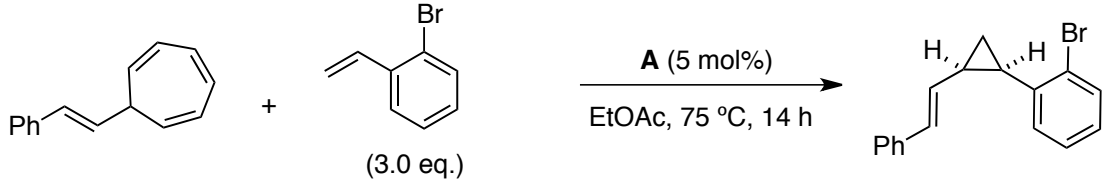
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 – 7.18 (m, 4H), 7.16 – 7.12 (m, 3H), 7.12 – 7.08 (m, 1H), 7.05 – 7.00 (m, 1H), 6.54 (d, *J* = 15.7 Hz, 1H), 5.52 (dd, *J* = 15.7, 9.3 Hz, 1H), 2.48 (q, *J* = 8.3 Hz, 1H), 2.13 (qd, *J* = 8.8, 5.6 Hz, 1H), 1.42 (td, *J* = 8.4, 5.3 Hz, 1H), 1.22 – 1.15 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.73 (d, *J* = 246.2 Hz), 137.65 , 129.94 , 129.86 (d, *J* = 4.2 Hz), 129.78 , 128.37 , 127.72 (d, *J* = 8.1 Hz), 126.63 , 126.00 (d, *J* = 14.8 Hz), 125.68 , 123.52 (d, *J* = 3.6 Hz), 115.10 (d, *J* = 21.8 Hz), 22.12 , 18.06 (d, *J* = 3.6 Hz), 11.78

^{19}F NMR (376 MHz, $CDCl_3$) δ -116.71 (dt, *J* = 10.3, 6.6 Hz).

HRMS-APCI: calculated for $C_{17}H_{16}F$ $[M+H]^+$: 239.1231; found: 239.1227.

***Cis*-1-bromo-2-(2-((*E*)-styryl)cyclopropyl)benzene (3r)**



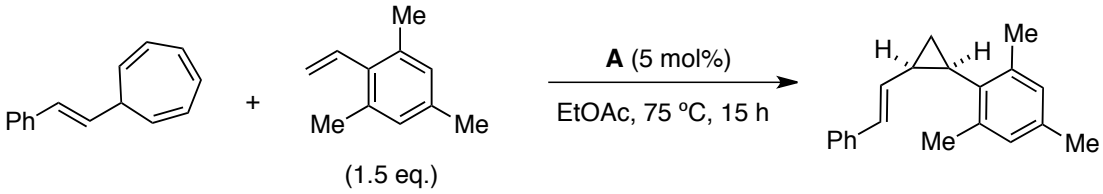
This compound (colorless oil, 51 mg, 66%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1-bromo-2-vinylbenzene (141 mg, 772 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, J = 7.9, 1.1 Hz, 1H), 7.33 – 7.19 (m, 4H), 7.19 – 7.08 (m, 4H), 6.54 (d, J = 15.7 Hz, 1H), 5.43 (dd, J = 15.7, 9.2 Hz, 1H), 2.52 (m, 1H), 2.21 (m, 1H), 1.46 (m, 1H), 1.22 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5 , 137.9 , 132.6 , 130.2 , 130.0 , 129.7 , 128.5 , 127.9 , 127.3 , 127.0 , 126.7 , 125.8 , 25.6 , 22.9 , 12.9 .

HRMS-APCI: calculated for $C_{17}H_{16}Br$ $[M+H]^+$: 299.0422; found: 299.0430.

***Cis*-1,3,5-trimethyl-2-(2-((*E*)-styryl)cyclopropyl)benzene (3s)**



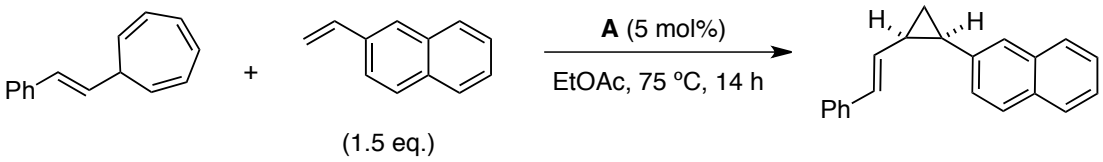
This compound (colorless oil, 31.5 mg, 37%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1,3,5-trimethyl-2-vinylbenzene (56.6 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.19 (m, 2H), 7.18 – 7.08 (m, 3H), 6.83 (m, 2H), 6.54 (d, J = 15.8 Hz, 1H), 5.41 (dd, J = 15.8, 9.8 Hz, 1H), 2.39 (s, 6H), 2.29 (s, 3H), 2.19 (m, 1H), 2.09 (m, 1H), 1.63 – 1.51 (m, 1H), 0.92 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.1 , 135.7 , 132.4 , 132.2 , 129.0 (two signals), 128.9 , 128.5 , 126.6 , 125.8 , 22.75 , 21.0 , 20.9 (two signals), 16.5 .

HRMS-APCI: calculated for $C_{20}H_{23}$ $[M+H]^+$: 263.1789; found: 263.1794.

***Cis*-2-(2-((*E*)-styryl)cyclopropyl)naphthalene (3t)**



This compound (white solid, 50.5 mg, 73%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 2-vinylnaphthalene (60 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

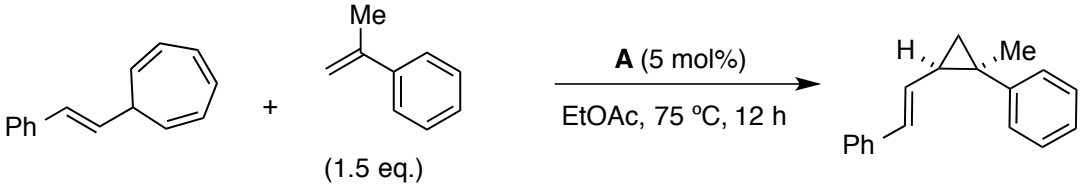
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.82 (m, 2H), 7.80 (m, 1H), 7.77 – 7.74 (m, 1H), 7.59 – 7.37 (m, 3H), 7.25 – 7.03 (m, 5H), 6.59 (d, J = 15.7 Hz, 1H), 5.58 (dd, J = 15.7, 9.5 Hz, 1H), 2.81 – 2.52 (m, 1H), 2.28 – 2.04 (m, 1H), 1.49 (, 1H), 1.32 (, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.7 , 136.6 , 133.6 , 132.3 , 130.6 , 129.8 , 128.5 , 128.3 , 127.8 (two signals) , 127.7 , 127.4 , 126.7 , 126.0 , 125.8, 125.4 , 24.3 , 23.1 , 12.9.

M.p.: 73-74 ºC.

HRMS-APCI: calculated for $C_{21}H_{19}$ $[M+H]^+$: 271.1492; found: 271.1481.

***Cis*-(1-methyl-2-((*E*)-styryl)cyclopropyl)benzene (3u)**



This compound (colorless oil, 42.9 mg, 73%, d.r. 5:1) was prepared according to the general procedure from (E)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), α-methylstyrene (49.0 μL, 375 μmol) and gold catalyst A (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

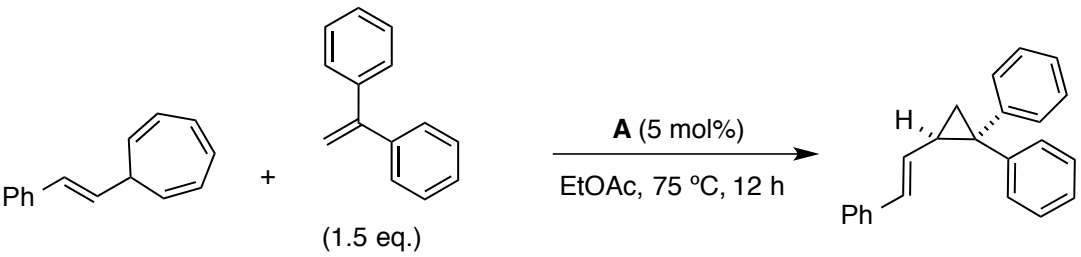
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 5H), 7.24 – 7.21 (m, 3H), 7.15 – 7.12 (m, 2H), 6.49 (d, J = 15.8 Hz, 1H), 5.33 (dd, J = 15.8, 9.8 Hz, 1H), 1.85 (ddd, J = 5.9, 7.6, 9.8 Hz, 1H), 1.48 (s, 3H), 1.21 – 1.18 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 143.5, 137.9, 132.7, 129.6, 128.4, 128.3, 128.1, 126.4, 126.2, 125.6, 29.7, 28.8, 22.3, 21.1.

HRMS-APCI: calculated for $C_{18}H_{19}$ $[M+H]^+$: 235.1481; found: 235.1483.

***Cis*-(*E*)-(2-styrylcyclopropane-1,1-diyl)dibenzene (3v)**



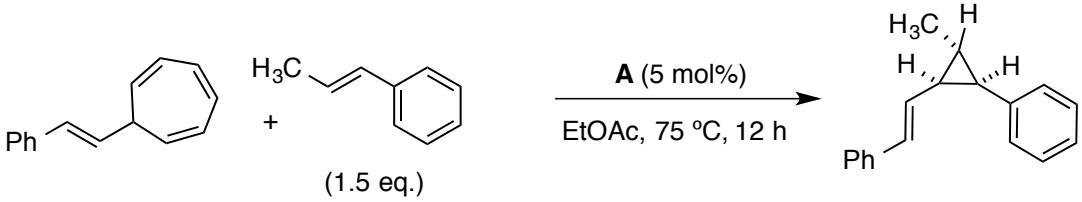
This compound (colorless oil, 54.4 mg, 73%) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), ethene-1,1-diyldibenzene (66.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.42 (m, 2H), 7.35 (td, *J* = 7.6, 1.8 Hz, 2H), 7.31 – 7.23 (m, 7H), 7.21 – 7.16 (m, 4H), 6.60 (dd, *J* = 15.7, 2.0 Hz, 1H), 5.51 (ddd, *J* = 15.7, 9.7, 2.2 Hz, 1H), 2.45 (tdd, *J* = 8.5, 5.9, 1.8 Hz, 1H), 1.78 (ddd, *J* = 8.6, 5.0, 1.8 Hz, 1H), 1.66 – 1.62 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.48, 141.35, 137.69, 131.67, 131.02, 129.16, 128.45, 128.37, 128.33, 127.15, 126.71, 126.67, 125.88, 125.77, 37.64, 31.13, 22.92.

HRMS-APCI: calculated for $C_{23}H_{20}Na$ $[M+Na]^+$: 319.1457; found: 319.1463.

***Cis*-(E)-(2-(2-methyl-3-phenylcyclopropyl)vinyl)benzene (3w)**



This compound (colorless oil, 26.6 mg, 45%, d.r. 3:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), (E)-prop-1-en-1-ylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (24 g SiO_2, eluent: pentane).

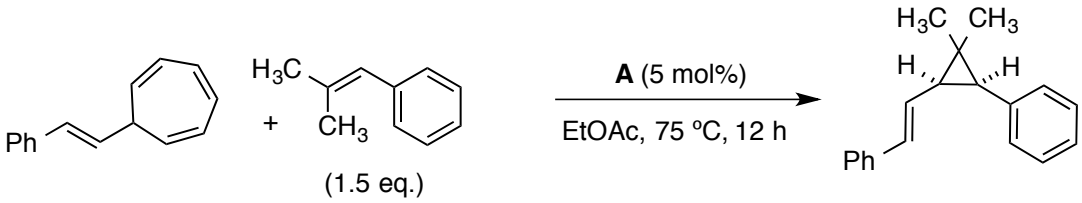
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.29 (m, 2H), 7.23 (m, 4H), 7.18 – 7.10 (m, 4H), 6.50 (d, *J* = 15.7 Hz, 1H), 5.62 (dd, *J* = 15.7, 9.6 Hz, 1H), 2.21 – 2.17 (dd, *J* = 6.27, 8.83 1H), 1.78 (td, *J* = 9.2, 4.9 Hz, 1H), 1.53 (dq, *J* = 11.6, 5.9 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 139.02, 137.80, 130.34, 129.17, 128.94, 128.36, 128.09, 126.48, 125.88, 125.60, 32.56, 31.75, 20.94, 18.55.

HRMS-APCI: calculated for $C_{18}H_{19}$ $[M+H]^+$: 235.1481; found: 235.1487.

***Cis*-(E)-(2-(2,2-dimethyl-3-phenylcyclopropyl)vinyl)benzene (3x)**



This compound (colorless oil, 21.5 mg, 35%, d.r 8:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), (2-methylprop-1-en-1-yl)benzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (24 g SiO_2, eluent: pentane).

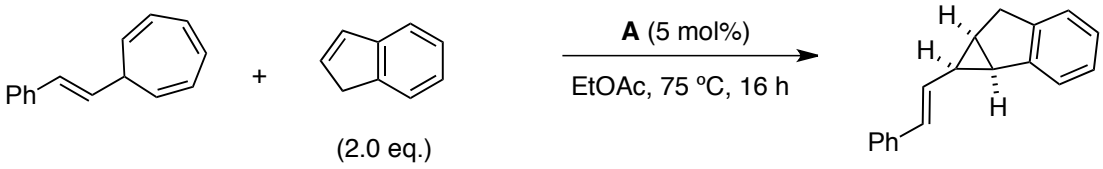
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.14 (m, 10H), 6.59 (d, *J* = 15.7 Hz, 1H), 5.79 (dd, *J* = 15.7, 10.3 Hz, 1H), 2.24 (d, *J* = 8.8 Hz, 1H), 1.87 (dd, *J* = 10.2, 9.0 Hz, 1H), 1.35 (s, 3H), 1.07 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 138.09, 137.64, 131.13, 129.58, 129.33, 128.47, 128.04, 126.50, 126.04, 125.66, 34.95, 32.81, 28.93, 23.61, 17.83.

HRMS-APCI: calculated for $C_{19}H_{21}$ $[M-H]^+$: 249.1638; found: 249.1643.

1-((*E*)-Styryl)-1,1a,6,6a-tetrahydrocyclopropa[*a*]indene (3y)



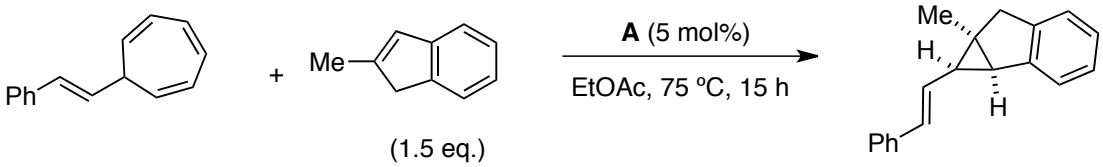
This compound (colorless oil, 51 mg, 85%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), indene (59.8 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.33 (m, 1H), 7.29 – 7.20 (m, 5H), 7.20 – 7.10 (m, 3H), 6.67 (d, J = 15.8 Hz, 1H), 5.41 (dd, J = 15.8, 9.3 Hz, 1H), 3.30 (dd, J = 17.4, 7.1 Hz, 1H), 3.02 (d, J = 17.4 Hz, 1H), 2.95 – 2.87 (m, 1H), 2.30 – 2.23 (m, 1H), 2.09 (dd, J = 17.1, 8.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 143.7, 142.4, 137.9, 132.0, 128.5, 126.8, 126.5, 126.1, 125.9, 125.8, 124.7, 124.2, 32.3, 32.0, 26.2, 24.3.

HRMS-APCI: calculated for $C_{18}H_{17}$ $[M+H]^+$: 233.1322; found: 232.1325.

***Endo*-6a-methyl-1-((*E*)-styryl)-1,1a,6,6a-tetrahydrocyclopropa[*a*]indene (3z)**



This compound (white solid, 41.5 mg, 66%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 2-methyl-1H-indene (50.3 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

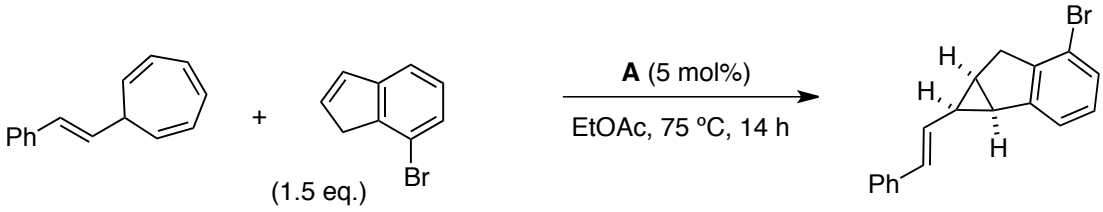
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 1H), 7.30 – 7.10 (m, 8H), 6.67 (d, J = 15.8 Hz, 1H), 5.45 (dd, J = 15.8, 9.4 Hz, 1H), 3.18 – 3.04 (m, 2H), 2.66 (dd, J = 7.9, 0.7 Hz, 1H), 2.01 (dd, J = 9.2, 8.2 Hz, 1H), 1.56 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 143.1, 137.8, 131.5, 128.4, 126.6, 126.4, 126.3, 125.8, 125.6, 124.3, 124.0, 38.6, 38.5, 33.7, 31.9, 22.8.

M.p.: 65-67 ºC.

HRMS-APCI: calculated for $C_{19}H_{19}$ $[M+H]^+$: 247.1481; found: 247.1483.

***Endo*-5-bromo-6a-methyl-1-((*E*)-styryl)-1,1a,6,6a-tetrahydrocyclopropa[*a*]indene (3aa)**



This compound (yellow solid, 56.5 mg, 71%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 7-bromo-1H-indene (75 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

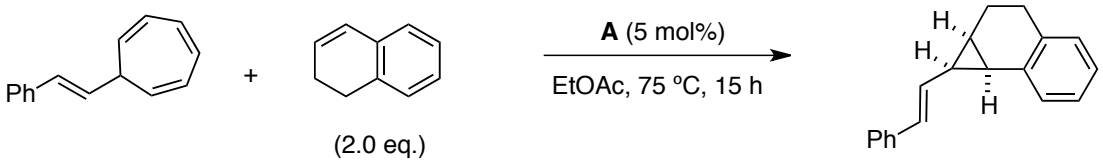
^{1}H NMR (400 MHz, $CDCl_3$) δ7.35 – 7.30 (m, 1H), 7.25 – 7.20 (m, 3H), 7.17 – 7.09 (m, 3H), 7.07 – 7.02 (m, 1H), 6.63 (d, J = 15.8 Hz, 1H), 5.34 (dd, J = 15.8, 9.3 Hz, 1H), 3.21 (dd, J = 18.1, 7.0 Hz, 1H), 3.00 (d, J = 18.1 Hz, 1H), 2.91 (ddd, J = 7.9, 6.1, 1.8 Hz, 1H), 2.25 (dddd, J = 8.1, 7.0, 6.1, 0.9 Hz, 1H), 2.06 (dd, J = 17.2, 8.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 144.1, 137.6, 132.7, 129.2, 128.6, 128.5, 127.0, 125.8, 124.8, 123.6, 119.3, 34.1, 32.8, 26.1, 23.7.

M.p.: 75-76 ºC.

HRMS-APCI: calculated for $C_{19}H_{19}$ $[M+H]^+$: 247.1483; found: 247.1481.

***Endo*-1-((*E*)-styryl)-1a,2,3,7b-tetrahydro-1*H*-cyclopropa[*a*]naphthalene (3ab)**



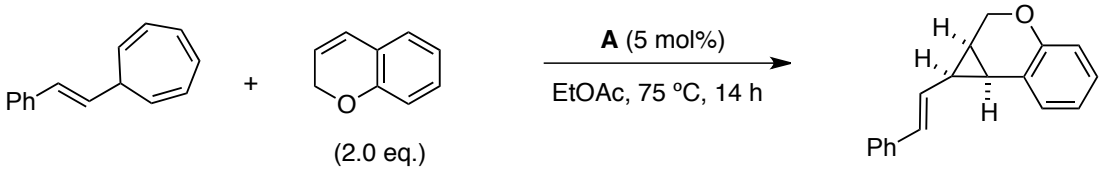
This compound (viscous colorless solid, 31.5 mg, 50%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 1,2-dihydronaphthalene (67 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.26 (m, 1H), 7.24 – 7.08 (m, 8H), 6.55 (d, J = 15.8 Hz, 1H), 5.64 (dd, J = 15.8, 8.9 Hz, 1H), 2.81 (m, 1H), 2.57 – 2.47 (m, 1H), 2.36 (m, 1H), 2.14 – 2.04 (m, 2H), 2.02 – 1.93 (m, 1H), 1.81 (ddd, J = 15.0, 8.8, 3.7 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.0, 136.6, 135.0, 131.5, 130.2, 128.5 (two signals), 127.6, 126.8, 126.3, 125.80, 125.77, 28.6, 27.9, 21.0, 20.0, 19.2.

HRMS-APCI: calculated for $C_{19}H_{19}$ $[M+H]^+$: 247.1489 found: 247.1481.

***Endo*-1-((*E*)-styryl)-1,1a,2,7b-tetrahydrocyclopropa[*c*]chromene (3ac)**



This compound (white solid, 36 mg, 56%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol), 2H-chromene (68 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: gradient from 0.5% Et_2O in pentane to 1.5% Et_2O in pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.21 (m, 5H), 7.21 – 7.11 (m, 2H), 6.99 – 6.88 (m, 2H), 6.60 (d, J = 15.8 Hz, 1H), 6.05 (dd, J = 15.8, 9.6 Hz, 1H), 4.45 (dd, J = 11.2, 0.8 Hz, 1H), 4.24 (dd, J = 11.2, 3.0 Hz, 1H), 2.48 – 2.42 (m, 1H), 2.26 (dd, J = 17.7, 8.6 Hz, 1H), 2.00 – 1.92 (m, 1H).

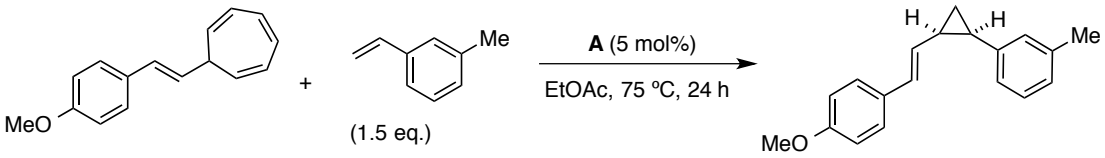
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.3, 137.7, 132.5, 129.8, 128.5, 127.2, 126.9, 126.4, 126.0, 122.6, 121.5, 117.1, 62.0, 28.4, 22.9, 18.6.

M.p.: 88-90 ºC.

HRMS-APCI: calculated for $C_{18}H_{17}O$ $[M+H]^+$: 249.1269; found: 249.1274.

5. Cyclopropanation with different cycloheptatriene derivatives

***Cis*-(*E*)-1-(2-(4-methoxystyryl)cyclopropyl)-3-methylbenzene (3ad)**



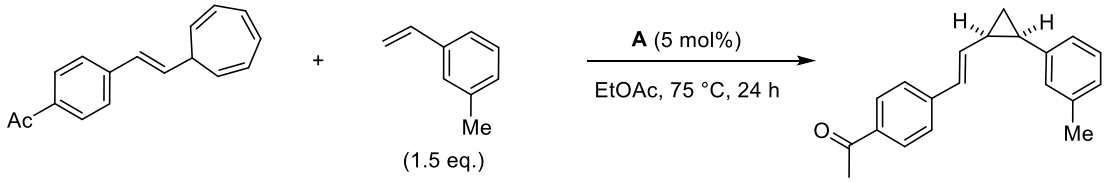
This compound (colorless oil, 31.8 mg, 48%, d.r. 12:1) was prepared according to the general procedure from (*E*)-7-(4-methoxystyryl)cyclohepta-1,3,5-triene (56.0 mg, 25 μmol), 1-methyl-3-vinylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (80 g SiO_2, eluent: pentane).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27 (dd, *J* = 6.3, 2.3 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H), 6.92 (dd, *J* = 9.3, 1.8 Hz, 2H), 6.88 – 6.82 (m, 2H), 6.44 (d, *J* = 15.8 Hz, 1H), 5.79 (dd, *J* = 15.8, 8.6 Hz, 1H), 3.82 (s, 3H), 2.35 (s, 3H), 2.00 (ddd, *J* = 8.6, 5.8, 4.2 Hz, 1H), 1.87 – 1.75 (m, 1H), 1.34 – 1.27 (m, 1H), 1.20 (dt, *J* = 8.7, 5.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.63, 142.24, 137.93, 130.73, 130.43, 128.27, 127.62, 126.77, 126.51, 126.40, 122.67, 113.96, 55.29, 27.29, 25.57, 21.43, 16.94.

HRMS-APCI: calculated for $C_{19}H_{21}O$ $[M+H]^+$: 265.1587; found: 265.1575.

***cis*-1-(4-((*E*)-2-(2-(m-tolyl)cyclopropyl)vinyl)phenyl)ethanone (3ae)**



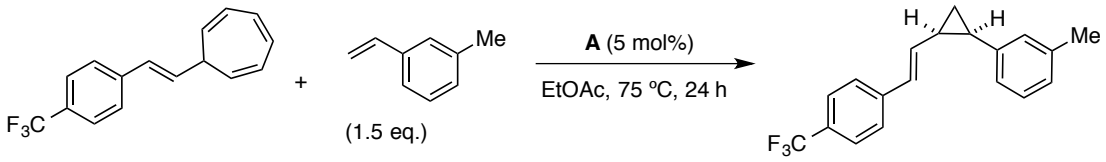
This compound (colorless oil, 61.5 mg, 87%, d.r. >20:1) was prepared according to the general procedure from (*E*)-1-(4-(2-(cyclohepta-2,4,6-trien-1-yl)vinyl)phenyl)ethan-1-one (60.7 mg, 257 μmol), 1-methyl-3-vinylbenzene (45.6 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, gradient: pentane to 50% Et_2O).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 – 7.77 (m, 2H), 7.23 – 7.16 (m, 3H), 7.11 – 7.08 (m, 1H), 7.07 – 7.01 (m, 2H), 6.54 (d, J = 15.7 Hz, 1H), 5.69 (dd, J = 15.7, 9.7 Hz, 1H), 2.54 (s, 3H), 2.48 (ddd, J = 8.5, 6.5 Hz, 1H), 2.34 (s, 3H), 2.08 – 1.99 (m, 1H), 1.40 (ddd, J = 8.4, 5.2 Hz, 1H), 1.19 (ddd, J = 6.4, 5.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 197.6, 142.6, 138.4, 137.9, 135.3, 134.6, 130.2, 128.8, 128.6, 128.2, 127.2, 126.1, 125.7, 26.6, 24.5, 23.1, 21.6, 13.1.

HRMS-ESI: calculated for $C_{20}H_{20}O$ $[M+H]^+$: 277.1587; found: 277.1587.

***Cis*-(*E*)-1-methyl-3-(2-(4-(trifluoromethyl)styryl)cyclopropyl)benzene (3af)**



This compound (colorless oil, 59.6 mg, 79%, d.r. 17:1) was prepared according to the general procedure from (*E*)-7-(4-(trifluoromethyl)styryl)cyclohepta-1,3,5-triene (66.0 mg, 25 μmol), 1-methyl-3-vinylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

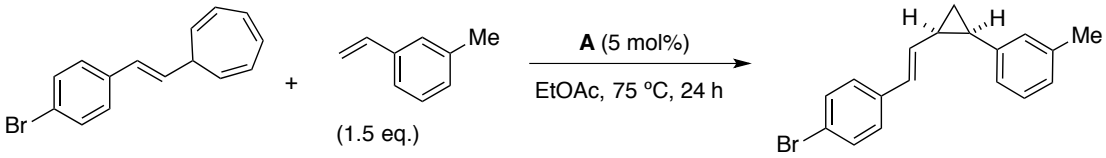
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.45 (m, 2H), 7.25 – 7.18 (m, 3H), 7.13 – 7.03 (m, 3H), 6.55 (d, *J* = 15.8 Hz, 1H), 5.65 (dd, *J* = 15.8, 9.6 Hz, 1H), 2.49 (td, *J* = 8.5, 6.5 Hz, 1H), 2.36 (d, *J* = 0.8 Hz, 3H), 2.10 – 2.00 (m, 1H), 1.41 (td, *J* = 8.4, 5.2 Hz, 1H), 1.19 (dt, *J* = 6.5, 5.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.18 , 138.26 , 137.73 , 133.89 , 130.10 , 128.06 , 128.03 , 127.01 , 126.00 , 125.68 , 125.32 (q, *J* = 3.8 Hz), 24.17 , 22.71 , 21.44 , 12.76 .

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.50.

HRMS-APCI: calculated for $C_{19}H_{18}F_3$ $[M+H]^+$: 303.1355; found: 303.1341.

***Cis*-(*E*)-1-(2-(4-bromostyryl)cyclopropyl)-3-methylbenzene (3ag)**



This compound (white solid, 66.4 mg, 85%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-(4-bromostyryl)cyclohepta-1,3,5-triene (68.0 mg, 250 μmol), 1-methyl-3-vinylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: 2 to 10% Et_2O in pentane).

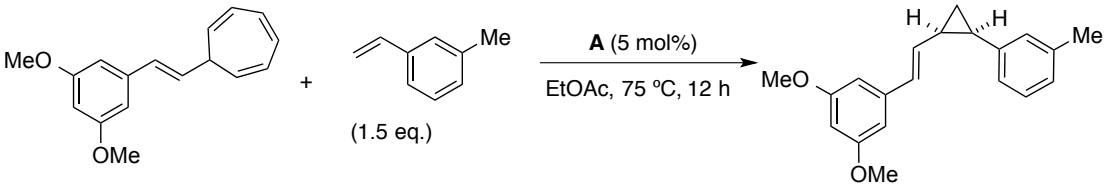
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.32 (m, 2H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.10 (bs, 1H), 7.05 (bt, *J* = 7.9 Hz, 2H), 7.03 – 7.00 (m, 2H), 6.46 (d, *J* = 15.7 Hz, 1H), 5.55 (dd, *J* = 15.7, 9.6 Hz, 1H), 2.46 (q, *J* = 8.6 Hz, 1H), 2.02 (qd, *J* = 8.8, 5.5 Hz, 1H), 1.38 (td, *J* = 8.4, 5.2 Hz, 1H), 1.18 ? 1.13 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.41, 137.66, 136.70, 131.73, 131.41, 130.10, 128.23, 127.98, 127.17, 126.91, 125.99, 120.07, 23.94, 22.67, 21.45, 12.61.

M.p.: 56-60 ºC.

HRMS-APCI: calculated for $C_{18}H_{18}Br$ $[M+H]^+$: 313.0586; found: 313.0592.

***Cis*-(*E*)-1,3-dimethoxy-5-(2-(2-(*m*-tolyl)cyclopropyl)vinyl)benzene (3ah)**



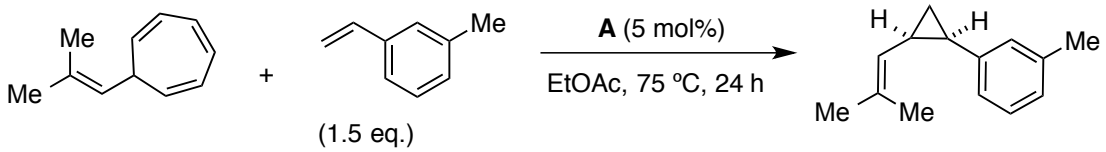
This compound (colorless oil, 50.8 mg, 69%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-(3,5-dimethoxystyryl)cyclohepta-1,3,5-triene (63.6 mg, 25 μmol), 1-methyl-3-vinylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (80 g SiO_2, eluent: 1% Et_2O in pentane).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (t, *J* = 7.6 Hz, 1H), 7.10 (s, 1H), 7.04 (dd, *J* = 14.9, 7.8 Hz, 2H), 6.47 (d, *J* = 15.7 Hz, 1H), 6.31 (dd, *J* = 12.8, 2.2 Hz, 3H), 5.55 (dd, *J* = 15.7, 9.5 Hz, 1H), 3.75 (s, 6H), 2.44 (q, *J* = 8.5 Hz, 1H), 2.35 (s, 3H), 2.01 (qd, *J* = 8.8, 5.6 Hz, 1H), 1.37 (td, *J* = 8.4, 5.2 Hz, 1H), 1.15 (q, *J* = 5.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.73, 139.91, 138.51, 137.58, 131.56, 130.06, 129.32, 127.95, 126.86, 126.02, 103.88, 98.73, 77.34, 55.22, 23.91, 22.60, 21.45, 12.61.

HRMS-APCI: calculated for $C_{20}H_{23}O_2$ $[M+H]^+$: 295.1693; found: 295.1698.

***Cis*-1-methyl-3-(2-(2-methylprop-1-en-1-yl)cyclopropyl)benzene (3ai)**



This compound (white crystals, 31.9 mg, 69%, d.r. 9:1) was prepared according to the general procedure from 7-(2-methylprop-1-en-1-yl)cyclohepta-1,3,5-triene (37.0 mg, 25 μmol), 1-methyl-3-vinylbenzene (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

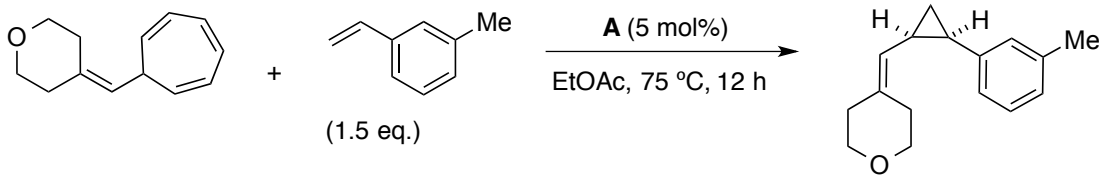
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (t, J = 7.5 Hz, 1H), 7.04 – 6.96 (m, 4H), 4.55 (dt, J = 8.9, 1.3 Hz, 1H), 2.36 (s, 3H), 2.26 (td, J = 8.6, 6.5 Hz, 1H), 1.89 (qd, J = 8.8, 5.8 Hz, 1H), 1.74 (d, J = 1.0 Hz, 4H), 1.61 – 1.60 (m, 4H), 1.25 (td, J = 8.5, 4.9 Hz, 1H), 0.90 – 0.85 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 139.30, 137.31, 132.61, 129.86, 127.71, 126.37, 125.86, 123.10, 25.64, 22.71, 21.46, 18.31, 18.26, 12.32.

HRMS-APCI: calculated for $C_{14}H_{19}$ $[M+H]^+$: 187.1481; found: 187.1480.

***Cis*-4-((2-(*m*-tolyl)cyclopropyl)methylene)tetrahydro-2*H*-pyran (3aj)**



This compound (colorless oil, 40.2 mg, 70%, d.r. 6:1) was prepared according to the general procedure from 4-(cyclohepta-2,4,6-trien-1-ylmethylene)tetrahydro-2*H*-pyran (47.0 mg, 250 μmol), 1-methyl-3-vinylbenzenee (50.0 μL, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: 2 to 10% Et_2O in pentane).

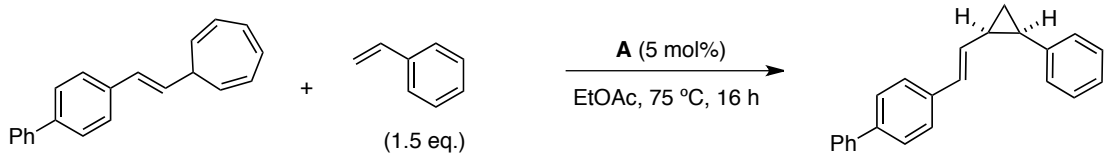
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (t, *J* = 7.8 Hz, 1H), 7.05 – 6.95 (m, 3H), 4.61 (d, *J* = 8.5 Hz, 1H), 3.71 (dt, *J* = 10.7, 5.3 Hz, 2H), 3.64 (ddd, *J* = 10.6, 6.2, 4.3 Hz, 1H), 3.49 (ddd, *J* = 11.0, 6.9, 4.4 Hz, 2H), 2.38 (td, *J* = 5.6, 1.1 Hz, 2H), 2.35 (s, 3H), 2.27 (td, *J* = 8.6, 6.5 Hz, 1H), 2.07 (dtt, *J* = 9.4, 7.2, 5.1 Hz, 2H), 1.89 (qd, *J* = 8.6, 5.8 Hz, 1H), 1.28 (td, *J* = 8.5, 5.0 Hz, 1H), 0.94 – 0.89 (m, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 138.97, 137.33, 135.59, 129.85, 127.74, 126.51, 125.90, 121.98, 69.58, 68.66, 36.65, 30.28, 22.97, 21.46, 17.15, 12.57.

HRMS-APCI: calculated for $C_{16}H_{20}NaO$ $[M+Na]^+$: 251.1406; found: 251.1405.

***Cis*-4-((*E*)-2-(2-phenylcyclopropyl)vinyl)-1,1'-biphenyl (3ak)**



This compound (white solid, 48.5 mg, 64%, d.r. >20:1) was prepared according to the general procedure from (*E*)-4-(2-(cyclohepta-2,4,6-trien-1-yl)vinyl)-1,1'-biphenyl (69.5 mg, 257 μmol), styrene (40.2 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

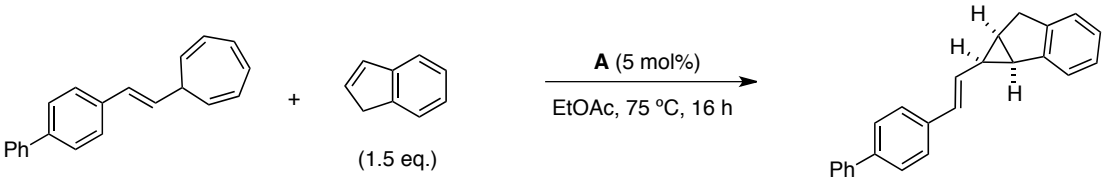
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (m, 2H), 7.45 – 7.35 (m, 4H), 7.32 – 7.23 (m, 5H), 7.22 – 7.15 (m, 3H), 6.53 (d, J = 15.7 Hz, 1H), 5.56 (dd, J = 15.7, 9.5 Hz, 1H), 2.45 (ddd, J = 8.6, 6.8 Hz, 1H), 2.02 (dddd, J = 8.8, 5.5 Hz, 1H), 1.36 (ddd, J = 8.4, 5.2 Hz, 1H), 1.14 (dd, J = 11.8, 5.4 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 141.0, 139.4, 138.8, 136.9, 131.0, 129.3, 129.2, 128.8, 128.3, 127.2 (two signals), 126.9, 126.2, 126.2, 24.1, 22.9, 12.8.

HRMS-APCI: calculated for $C_{23}H_{20}$ $[M+H]^+$: 297.1635; found: 297.1638.

M.p.: 75-76 ºC.

***Endo*-1-((*E*)-2-([1,1'-biphenyl]-4-yl)vinyl)-1,1a,6,6a-tetrahydrocyclopropa[a]indene (3al)**



This compound (white solid, 60 mg, 76%, d.r. >20:1) was prepared according to the general procedure from (*E*)-4-(2-(cyclohepta-2,4,6-trien-1-yl)vinyl)-1,1'-biphenyl (69.5 mg, 257 μmol), indene (44.8 mg, 386 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

Suitable crystals for X-ray diffraction were obtained by slow evaporation of a solution in chloroform.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.55 (m, 2H), 7.48 – 7.41 (m, 4H), 7.37 – 7.31 (m, 2H), 7.23 – 7.16 (m, 5H), 6.67 (d, J = 15.8 Hz, 1H), 5.42 (dd, J = 15.8, 9.4 Hz, 1H), 3.28 (dd, J = 17.5, 7.0 Hz, 1H), 3.01 (d, J = 17.5 Hz, 1H), 2.89 (ddd, J = 7.7, 6.2, 1.5 Hz, 1H), 2.26 (dddd, J = 7.8, 6.9, 0.7 Hz, 1H), 2.08 (dd, J = 17.2, 8.3 Hz, 1H).

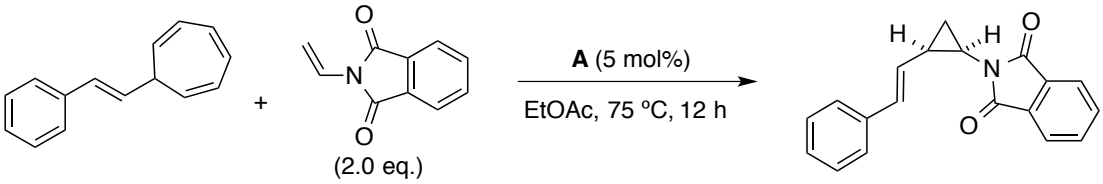
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 142.4, 140.9, 139.5, 136.9, 131.5, 128.8, 127.2, 127.2, 126.9, 126.6, 126.2 (two signals), 124.8, 124.3, 32.4, 32.1, 26.3, 24.4.

HRMS-APCI: calculated for $C_{24}H_{21}$ $[M+H]^+$: 309.1634; found: 309.1638.

M.p.: 146-148 ºC.

6. Cyclopropanation of *N*-vinylphthalimide

***Cis*-(*E*)-2-(2-styrylcyclopropyl)isoindoline-1,3-dione (6a)**



This compound (white solid, 54.1 mg, 75%, d.r. 6:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 μL, 25 μmol), *N*-vinylphthalimide (87.0 mg, 500 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (120 g SiO_2, eluent: 20% Et_2O in pentane).

Multi-gram scale: This compound (white solid, 2.14 g, 74%, d.r. 7:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (1.94 g, 10 mmol), *N*-vinylphthalimide (3.46 g, 20 mmol) and gold catalyst **A** (386 mg, 0.5 mmol). The heating was stopped and reaction was quenched after 9 hours by the addition of triethylamine. The crude residue was purified by flash chromatography (330 g SiO_2, eluent: 0 to 50% Et_2O in pentane).

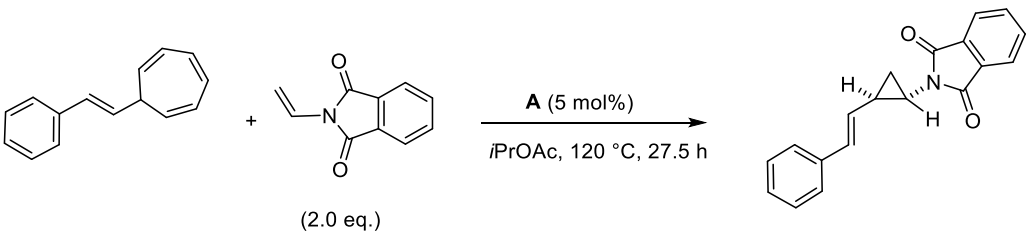
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.26 – 7.17 (m, 4H), 7.17 – 7.12 (m, 1H), 6.48 (d, *J* = 15.8 Hz, 1H), 5.89 (dd, *J* = 15.8, 7.7 Hz, 1H), 3.03 (ddd, *J* = 7.8, 7.1, 4.9 Hz, 1H), 2.18 – 2.10 (m, 1H), 1.78 (td, *J* = 6.8, 4.9 Hz, 1H), 1.55 (ddd, *J* = 8.9, 7.9, 6.7 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.05, 137.24, 134.04, 131.65, 131.23, 128.36, 126.98, 126.23, 125.95, 123.24, 28.11, 20.14, 10.70.

M.p.: 146-148 ºC.

HRMS-ESI: calculated for $C_{19}H_{15}NNaO_2$ $[M+Na]^+$: 312.0995; found: 312.0997.

***Trans*-2-(2-((*E*)-styryl)cyclopropyl)isoindoline-1,3-dione) (*trans*-6a)**



The *trans*-isomer (off-white solid, 41.0 mg, 55%) was prepared from the reaction of (*E*)-7-styrylcyclohepta-1,3,5-triene (50.0 mg, 257 μmol) with 2-vinylisoindoline-1,3-dione (89.0 mg, 515 μmol) and gold catalyst **A** (9.9 mg, 13 μmol) in the presence of diphenylmethane as internal reference (43.3 mg, 257 μmol) in *i*PrOAc at 120 °C over 27.5h. The crude was quenched with 0.5 mL Et_3N and stirred at room temperature for 1h before being charged on silica gel and purified by flash chromatography (40 g SiO_2, gradient: pentane to 30% Et_2O, the *trans*-isomer elutes first).

An NMR analysis of the crude against the internal reference shows 55% *trans*-isomer and 13% cis-isomer (ratio 4.2 : 1)

trans-isomer:

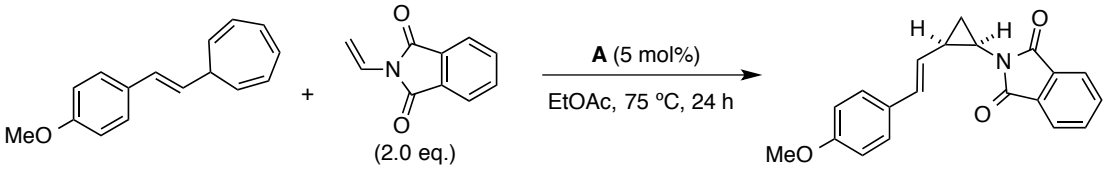
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 2H), 7.73 – 7.68 (m, 2H), 7.38 – 7.33 (m, 2H), 7.33 – 7.27 (m, 2H), 7.23 – 7.18 (m, 1H), 6.60 (d, J = 15.8 Hz, 1H), 6.03 (dd, J = 15.8, 7.9 Hz, 1H), 2.83 (ddd, J = 7.8, 4.5, 3.4 Hz, 1H), 2.25 – 2.13 (m, 1H), 1.58 (ddd, J = 9.4, 6.2, 4.5 Hz, 1H), 1.35 – 1.27 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.6, 137.3, 134.2, 131.9, 130.4, 129.5, 128.6, 127.2, 126.1, 123.3, 29.5, 21.7, 13.5.

HRMS-ESI: calculated for $C_{19}H_{15}NNaO_2$ $[M+Na]^+$: 312.0995; found: 312.0997.

M.p.: 99-100 ºC.

***Cis*-(*E*)-2-(2-(4-methoxystyryl)cyclopropyl)isoindoline-1,3-dione (6b)**



This compound (yellow waxy solid, 41.8 mg, 52%, d.r. 6:1) was prepared according to the general procedure from (*E*)-7-(4-methoxystyryl)cyclohepta-1,3,5-triene (56.0 mg, 25 μmol), *N*-vinylphthalimide (87.0 mg, 500 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (120 g SiO_2, eluent: 0 to 60% Et_2O in pentane).

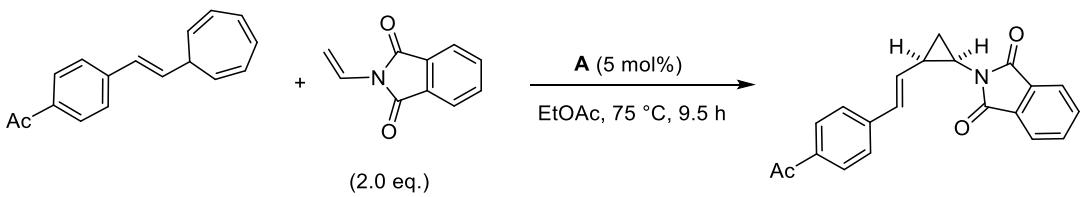
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.74 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.34 – 7.30 (m, 2H), 6.89 – 6.85 (m, 2H), 6.57 (d, *J* = 15.7 Hz, 1H), 5.92 (dd, *J* = 15.8, 7.7 Hz, 1H), 3.83 (s, 3H), 2.82 (ddd, *J* = 7.8, 4.5, 3.4 Hz, 1H), 2.22 – 2.15 (m, 1H), 1.60 – 1.55 (m, 1H), 1.34 – 1.29 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.55, 158.89, 134.04, 131.82, 130.03, 129.79, 127.10, 127.07, 123.18, 113.95, 55.29, 29.31, 21.54, 13.32.

M.p.: 92-97 ºC.

HRMS-APCI: calculated for $C_{19}H_{21}NaO$ $[M+Na]^+$: 342.1101; found: 342.1097.

***Cis*-2-(2-((*E*)-4-acetylstyryl)cyclopropyl)isoindoline-1,3-dione (6c)**



This compound (yellow solid, 54.0 mg, 63%) was prepared according to the general procedure from (*E*)-1-(4-(2-(cyclohepta-2,4,6-trien-1-yl)vinyl)phenyl)ethan-1-one (60.7 mg,

257 μmol), 2-vinylisoindoline-1,3-dione (89.0 mg, 514 μmol) and gold catalyst **A** (9.9 mg, 13 μmol). The crude was quenched with 0.5 mL Et_3N and stirred at room temperature for 1h before being charged on silica gel and purified by flash chromatography (40 g SiO_2, gradient: pentane to 75% Et_2O).

In the reaction crude, only a trace of the *trans*-diastereoisomer was detected (4%).

The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

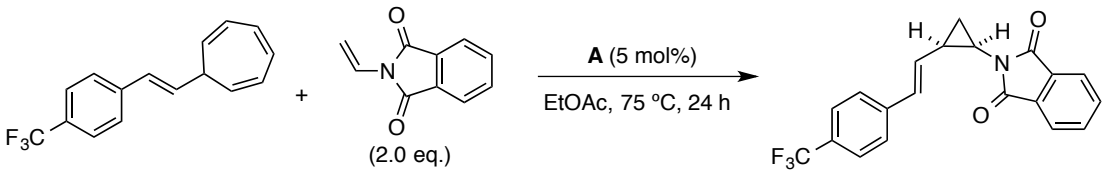
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (dd, J = 5.4, 3.0 Hz, 2H), 7.77 (d, J = 8.3 Hz, 2H), 7.68 (dd, J = 5.4, 3.1 Hz, 2H), 7.22 (d, J = 8.3 Hz, 2H), 6.49 (d, J = 15.8 Hz, 1H), 5.98 (dd, J = 15.8, 8.1 Hz, 1H), 3.09 – 2.99 (m, 1H), 2.51 (s, 3H), 2.19 – 2.08 (m, 1H), 1.81 – 1.73 (m, 1H), 1.60 – 1.51 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 197.5, 169.1, 141.9, 135.7, 134.3, 131.7, 130.2, 129.9, 128.7, 126.0, 123.4, 28.5, 26.6, 20.5, 11.3.

M.p.: 176-177 ºC.

HRMS-ESI: calculated for $C_{21}H_{17}NNaO_3$ $[M+Na]^+$: 354.1101; found: 354.1108.

***Cis*-(*E*)-2-(2-(4-(trifluoromethyl)styryl)cyclopropyl)isoindoline-1,3-dione (6d)**



This compound (white solid, 57.8 mg, 79%, d.r. 10:1) was prepared according to the general procedure from (*E*)-7-(4-(trifluoromethyl)styryl)cyclohepta-1,3,5-triene (56.0 mg, 205 μmol), *N*-vinylphthalimide (71.0 mg, 410 μmol) and gold catalyst **A** (8.0 mg, 10.3 μmol). The crude residue was purified by flash chromatography (120 g SiO_2, eluent: 0 to 45% Et_2O in pentane).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.48 – 7.43 (m, 2H), 7.30 – 7.25 (m, 3H), 6.51 (d, *J* = 15.8 Hz, 1H), 5.98 (dd, *J* = 15.8, 8.0 Hz, 1H), 3.06 (ddd, *J* = 7.8, 7.0, 4.9 Hz, 1H), 2.17 (ddtd, *J* = 8.9, 7.9, 7.0, 0.8 Hz, 1H), 1.79 (td, *J* = 6.8, 4.9 Hz, 1H), 1.63 – 1.55 (m, 2H).

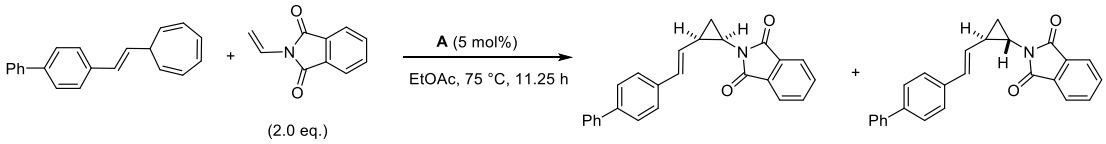
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.96 , 140.62 , 134.16 , 131.57 , 129.76 , 129.33 , 128.62 , 128.11 , 126.02 , 125.35 (q, *J* = 3.8 Hz), 123.29 , 28.33 , 20.23 , 11.07.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.60.

M.p.: 117-119 ºC.

HRMS-APCI: calculated for $C_{20}H_{14}F_3NNaO_2$ $[M+Na]^+$: 380.0869; found: 380.0864.

***Cis*-2-(2-((*E*)-2-([1,1'-biphenyl]-4-yl)vinyl)cyclopropyl)isoindoline-1,3-dione (6e)**



The *cis*-isomer (white solid, 38.5 mg, 50%) and the *trans*-isomer (white solid, 15.0 mg, 19%) were prepared according to the general procedure from (*E*)-4-(2-(cyclohepta-2,4,6-trien-1-yl)vinyl)-1,1'-biphenyl (57.2 mg, 212 μmol), 2-vinylisoindoline-1,3-dione (73.3 mg, 423 μmol) and gold catalyst **A** (8.2 mg, 11 μmol). The crude was quenched with 0.5 mL Et_3N and stirred at room temperature for 1h before being charged on silica gel and purified by flash chromatography (40 g SiO_2, gradient: pentane to 50% Et_2O, the *trans*-isomer elutes first).

Suitable crystals for X-ray diffraction of both isomers were obtained by slow evaporation of a solution in $CDCl_3$ in NMR tubes.

In addition to the structural evidence for both isomers by crystallography, their stereochemistry was independently confirmed by 1D NOESY experiments[6] (see spectra for full details).

Cis-isomer:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.78 (m, 2H), 7.73 – 7.64 (m, 2H), 7.55 – 7.50 (m, 2H), 7.46 – 7.37 (m, 4H), 7.33 – 7.28 (m, 1H), 7.27 – 7.24 (m, 2H), 6.50 (d, J = 15.8 Hz, 1H), 5.93 (dd, J = 15.8, 7.7 Hz, 1H), 3.03 (ddd, J = 7.7, 7.1, 4.9 Hz, 1H), 2.21 – 2.10 (m, 1H), 1.84 – 1.75 (m, 1H), 1.55 (ddd, J = 8.8, 7.9, 6.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.2, 140.8, 139.9, 136.4, 134.2, 131.8, 130.9, 128.8, 127.3, 127.2, 126.9, 126.5, 126.5, 123.4, 28.3, 20.4, 10.9.

M.p.: 155-156 ºC.

HRMS-ESI: calculated for $C_{25}H_{19}NNaO_2$ $[M+Na]^+$: 388.1308; found: 388.1303.

Trans-isomer:

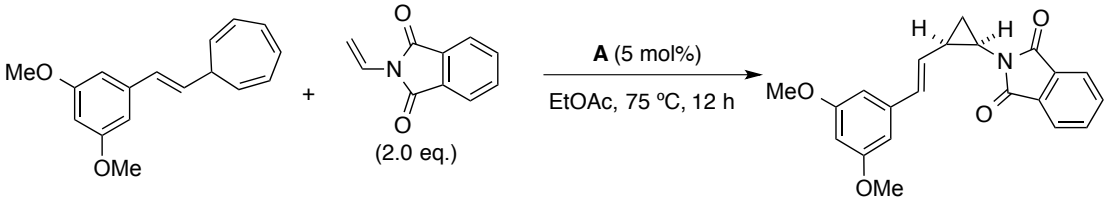
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.81 (m, 2H), 7.75 – 7.69 (m, 2H), 7.63 – 7.58 (m, 2H), 7.58 – 7.52 (m, 2H), 7.47 – 7.40 (m, 4H), 7.36 – 7.30 (m, 1H), 6.64 (d, J = 15.8 Hz, 1H), 6.07 (dd, J = 15.8, 7.9 Hz, 1H), 2.85 (ddd, J = 7.8, 4.4, 3.5 Hz, 1H), 2.26 – 2.16 (m, 1H), 1.60 (ddd, J = 9.5, 6.2, 4.6 Hz, 1H), 1.38 – 1.29 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 140.9, 140.0, 136.4, 134.2, 132.0, 130.0, 129.7, 128.9, 127.3 (two signals), 127.0, 126.5, 123.4, 29.6, 21.8, 13.6.

M.p.: 187-188 ºC.

HRMS-ESI: calculated for $C_{25}H_{19}NNaO_2$ $[M+Na]^+$: 388.1308; found: 388.1312.

***Cis*-(*E*)-2-(2-(3,5-dimethoxystyryl)cyclopropyl)isoindoline-1,3-dione (6f)**



This compound (yellow solid, 52.5 mg, 60%, d.r. 6:1) was prepared according to the general procedure from (*E*)-7-(3,5-dimethoxystyryl)cyclohepta-1,3,5-triene (56.0 mg, 25 μmol), *N*-vinylphthalimide (87.0 mg, 500 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (120 g SiO_2, eluent: 10 to 50% Et_2O in pentane).

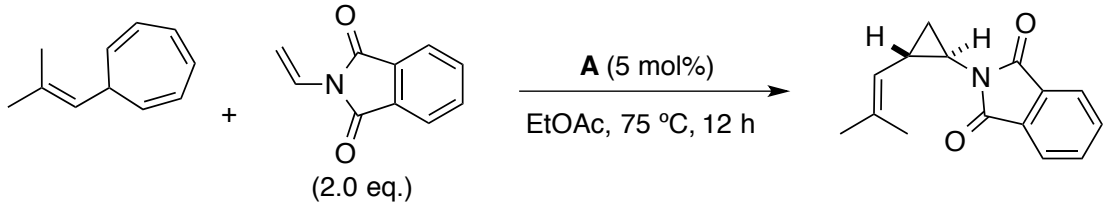
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.71 (dd, *J* = 5.5, 3.0 Hz, 2H), 6.40 (d, *J* = 15.7 Hz, 1H), 6.34 (d, *J* = 2.2 Hz, 2H), 6.28 (t, *J* = 2.3 Hz, 1H), 5.87 (dd, *J* = 15.7, 7.7 Hz, 1H), 3.72 (s, 6H), 3.05 – 2.99 (m, 1H), 2.20 – 2.07 (m, 1H), 1.78 (td, *J* = 6.8, 4.9 Hz, 1H), 1.59 – 1.49 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.01, 160.70, 139.32, 134.05, 131.64, 131.18, 126.90, 123.24, 104.13, 99.23, 55.24, 28.17, 20.05, 10.76.

M.p.: 119-121 ºC.

HRMS-APCI: calculated for $C_{21}H_{19}NNaO_4$ $[M+Na]^+$: 372.1206; found: 372.1208.

***Trans*-2-(2-(2-methylprop-1-en-1-yl)cyclopropyl)isoindoline-1,3-dione (6g)**



This compound (white solid, 35.3 mg, 59%, d.r. 4.7:1) was prepared according to the general procedure from 7-(2-methylprop-1-en-1-yl)cyclohepta-1,3,5-triene (37.0 mg, 250 μmol), *N*-vinylphthalimide (87.0 mg, 500 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (120 g SiO_2, eluent: 5 to 10% Et_2O in pentane).

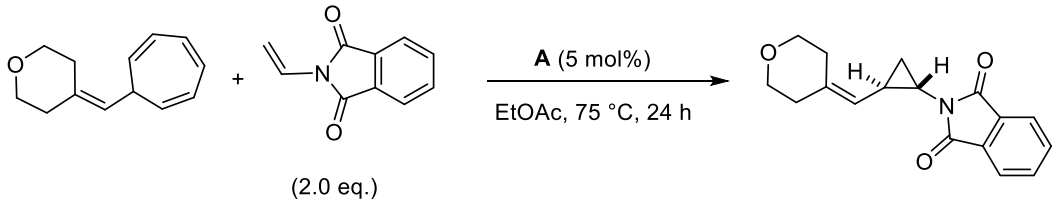
The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.82 (m, 2H), 7.74 – 7.71 (m, 2H), 4.75 (dt, *J* = 8.8, 1.3 Hz, 1H), 2.65 (ddd, *J* = 7.5, 4.1, 3.5 Hz, 1H), 2.12 (tdd, *J* = 9.4, 6.5, 3.4 Hz, 1H), 1.87 (d, *J* = 1.1 Hz, 3H), 1.77 (d, *J* = 1.1 Hz, 3H), 1.42 (ddd, *J* = 9.7, 5.9, 4.2 Hz, 1H), 1.06 (dt, *J* = 7.3, 6.2 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.64, 134.24, 133.96, 131.84, 124.13, 123.12, 28.64, 25.62, 18.33, 17.91, 13.94.

HRMS-APCI: calculated for $C_{15}H_{15}NNaO_2$ $[M+Na]^+$: 264.0995; found: 264.1004.

***Trans*-2-(2-((tetrahydro-4*H*-pyran-4-ylidene)methyl)cyclopropyl)isoindoline-1,3-dione (6h)**



This compound (colorless oil, 51.8 mg, 73%, d.r. 1.2:1) was prepared according to the general procedure from 4-(cyclohepta-2,4,6-trien-1-ylmethylene)tetrahydro-2*H*-pyran (47.0 mg, 250 μmol), *N*-vinylphthalimide (87.0 mg, 500 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (120 g SiO_2, eluent: 10 to 60% Et_2O in pentane).

The stereochemistry was confirmed for the minor *cis*-isomer by 1D NOESY experiments[6] (see spectral data for full details).

cis-Isomer: **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (td, *J* = 5.3, 3.0 Hz, 2H), 7.72 (td, *J* = 5.4, 3.1 Hz, 2H), 4.60 (d, *J* = 8.5 Hz, 1H), 3.75 – 3.70 (m, 1H), 3.62 (ddd, *J* = 10.5, 6.0, 4.3 Hz, 1H), 3.46 (ddd, *J* = 10.9, 7.6, 3.9 Hz, 1H), 2.55 – 2.48 (m, 1H), 2.42 – 2.34 (m, 1H), 2.15 (td, *J* = 6.2, 3.1 Hz, 1H), 2.04 (dd, *J* = 9.0, 3.9 Hz, 1H), 2.02 – 1.95 (m, 1H), 1.56 (td, *J* = 6.5, 4.9 Hz, 1H), 1.50 – 1.44 (m, 1H).

trans-Isomer: **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (td, *J* = 5.3, 3.0 Hz, 2H), 7.72 (td, *J* = 5.4, 3.1 Hz, 2H), 4.80 (d, *J* = 8.5 Hz, 1H),3.73 – 3.67 (m, 3H), 2.65 (ddd, *J* = 7.5, 4.2, 3.4 Hz, 1H), 2.63 – 2.56 (m, 1H), 2.50 – 2.43 (m, 1H), 2.28 – 2.23 (m, 2H), 2.12 – 2.07 (m, 1H), 1.46 – 1.41 (m, 1H), 1.09 (dt, *J* = 7.3, 6.3 Hz, 1H).

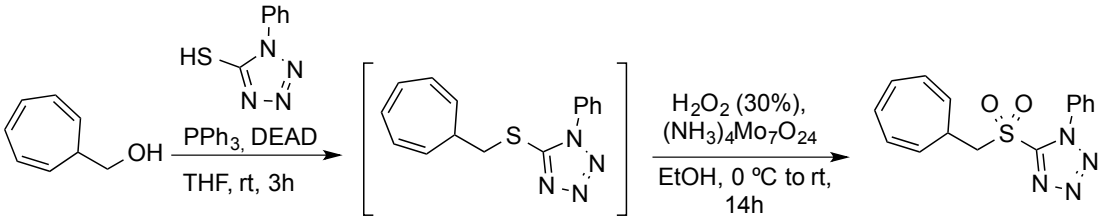
cis-Isomer: **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.60, 138.22, 134.02, 131.77, 123.13, 119.34, 69.40, 68.55, 36.68, 30.41, 27.70, 15.14, 11.82.

trans-Isomer: **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.87, 136.78, 134.00, 131.77, 123.11, 122.83, 69.36, 68.75, 36.59, 30.24, 28.84, 16.95, 14.12.

HRMS-APCI: calculated for $C_{17}H_{17}NNaO_3$ $[M+Na]^+$: 306.1101; found: 306.1090.

7. Preparation of Julia-Kocienski reagents

5-((Cyclohepta-2,4,6-trien-1-ylmethyl)sulfonyl)-1-phenyl-1H-tetrazole (4a)



This compound was synthesized according to a modified literature procedure.[7]

To a solution of cyclohepta-2,4,6-trien-1-ylmethanol[8] (5.35 g, 43.8 mmol, 1.0 equiv), 1-Phenyl-1H-tetrazole-5-thiol (7.81 g, 43.8 mmol, 1.0 equiv), triphenylphosphine (11.49 g, 43.8 mmol, 1.0 equiv) in THF (175 mL, 0.25M) was added diethyl azodicarboxylate (40% toluene, 19.1 mL, 43.8 mmol, 1.0 equiv) dropwise and the reaction was left to stir for an additional 3 hours. Then, ethanol (230 mL, 0.15M) was added and the reaction was cooled to 0 ºC, followed by the dropwise addition of a solution of ammonium molybdate tetrahydrate (4.31 g, 3.5 mmol, 0.15 equiv) in hydrogen peroxide (30%, 44 mL, 434 mmol, 12.5 equiv). The reaction was left to stir over night whilst warming to room temperature. Water (400 mL) was added and the mixture was extracted with DCM (400 mL) 3 times. The organic layers were combined, washed with brine (400 ml), dried over Na_2SO_4 and concentrated to dryness. Flash chromatography (330 g SiO_2, eluent: 1:1:8 Et_2O:CH_2Cl_2:pentane) afforded 8.25 g (26.3 mmol, 60%) of a white solid.[9]

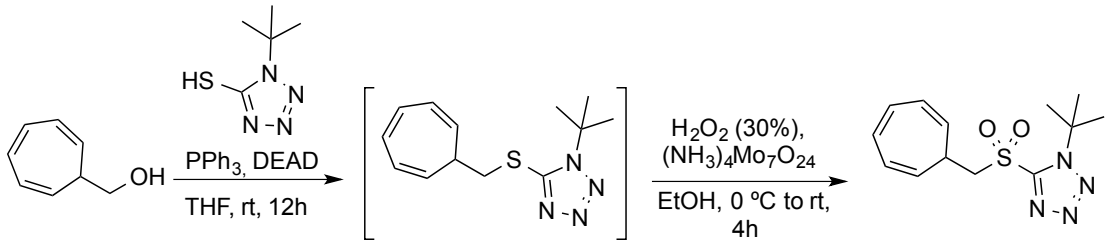
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 5H), 6.72 – 6.70 (m, 2H), 6.30 (dt, *J* = 9.2, 2.9 Hz, 2H), 5.40 (dd, *J* = 9.1, 6.7 Hz, 2H), 3.97 (d, *J* = 7.2 Hz, 2H), 2.97 (p, *J* = 6.9 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.71, 132.99, 131.42, 129.66, 126.61, 125.18, 121.18, 57.02, 32.95.

M.p.: 98-99 ºC.

HRMS-APCI: calculated for $C_{15}H_{14}N_4NaO_2S$ $[M+Na]^+$: 337.0730; found: 337.0725

1-(*Tert*-butyl)-5-((cyclohepta-2,4,6-trien-1-ylmethyl)sulfonyl)-1*H*-tetrazole (4b)



This compound was synthesized according to a modified literature procedure.[7]

To a solution of cyclohepta-2,4,6-trien-1-ylmethanol[8] (3.83 g, 31.4 mmol, 1.0 equiv), 1-tert-butyl-1H-tetrazole-5-thiol[7,10] (4.97 g, 31.4 mmol, 1.0 equiv), triphenylphosphine (8.24 g, 31.4 mmol, 1.0 equiv) in THF (125 mL, 0.25M) was added diethyl azodicarboxylate (40% toluene, 13.7 mL, 31.4 mmol, 1.0 equiv) dropwise and the reaction was left to stir for an additional 12 hours. Then, ethanol (150 mL, 0.15M) was added and the reaction was cooled to 0 ºC, followed by the dropwise addition of a solution of ammonium molybdate tetrahydrate (3.28 g, 2.65 mmol, 0.0845 equiv) in hydrogen peroxide (30%, 33 mL, 320 mmol, 12.5 equiv). The reaction was left to stir for an additional 4 hours whilst warming to room temperature. Water (200 mL) was added and the mixture was extracted with DCM (200 mL) 3 times. The organic layers were combined, washed with brine (200 ml), dried over Na2SO4 and concentrated to dryness. Flash chromatography (330 g SiO_2, eluent: 1:1:8 Et_2O:CH_2Cl_2:pentane) afforded 4.28 g (14.5 mmol, 46%) of a light yellow solid.[11]

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 – 6.71 (m, 2H), 6.32 (dt, *J* = 9.4, 3.3 Hz, 2H), 5.45 (dd, *J* = 9.0, 6.5 Hz, 2H), 4.12 (d, *J* = 7.1 Hz, 2H), 2.92 (p, *J* = 6.9 Hz, 1H), 1.86 (s, 9H).

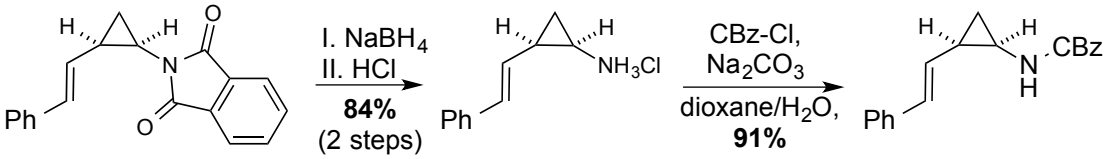
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.34, 131.41, 126.32, 121.56, 65.53, 57.98, 33.15, 29.68.

M.p.: 45-51 ºC.

HRMS-APCI: calculated for $C_{13}H_{18}N_4NaO_2S$ $[M+Na]^+$: 317.1043; found: 317.1042

8. Miscellaneous

Phthalimide deprotection and functionalization of amine.



(*E*)-2-Styrylcyclopropan-1-aminium chloride (7) was synthesized according to a modified literature procedure.[12]

(*E*)-2-(2-styrylcyclopropyl)isoindoline-1,3-dione **6a** (1.16g, 4.0 mmol, 1.0 equiv) is dissolved in dichloromethane (6 mL, 0.66M) and 2-propanol (36, 0.11M) and water (6 mL, 0.66M) is added, followed by sodium borohydride (755 mg, 20 mmol, 5.0 equiv) and the reaction is left to stir for 4 hours (checked by TLC). Ethyl acetate and silica were added carefully and the mixture was poured on a silica plug and washed with Et_2O. The solvents were evaporated on the rotovap and the crude white solid could directly be used in the next step.

The solids were dissolved in dioxane (13 mL, 0.3M) and cooled to 0 ºC before dry hydrochloric acid in dioxane (13 mL, 4M) was added and the reaction was left to stir over night, warming to room temperature. The white solid was collected on a filter and the orange byproduct was washed out with Et_2O. Drying under high vacuum yielded 656 mg (3.35 mmol, 84%) of a white powder.

^{1}H NMR (500 MHz, Methanol-d4) δ 7.43 – 7.40 (m, 2H), 7.33 – 7.28 (m, 2H), 7.25 – 7.20 (m, 1H), 6.75 (d, J = 15.7 Hz, 1H), 6.08 (dd, J = 15.7, 8.6 Hz, 1H), 2.87 (td, J = 7.6, 4.5 Hz, 1H), 2.07 (dt, J = 16.3, 8.6 Hz, 1H), 1.34 (ddd, J = 9.2, 7.6, 6.6 Hz, 1H), 1.02 (td, J = 6.7, 4.5 Hz, 1H).

^{13}C NMR (126 MHz, MeOD) δ 136.86, 134.30, 128.30, 127.34, 125.80, 123.25, 28.11, 18.37, 10.42.

M.p.: 167 ºC (decomposition)

HRMS-APCI: calculated for $C_{11}H_{14}N$ $[M\text{-}Cl]^+$: 160.1121; found: 160.1128

Benzyl (*E*)-(2-styrylcyclopropyl)carbamate (8)

(*E*)-2-Styrylcyclopropan-1-aminium chloride **7** (294 mg, 1.5 mmol, 1.0 equiv) was dissolved in a mixture of dioxane (12 mL) and water (12 mL) and cooled to 0 ºC. Na_2CO_3 (795 mg, 7.5 mmol, 5.0 equiv) was added, quickly followed by benzyl chloroformate. (236 μL, 1.65 mmol, 1.1 equiv) and the reaction was left to stir for 1 hour before being warmed to room temperature. The mixture was extracted with dichloromethane (10 mL, x3) and washed with water (20 mL) and brine (20 mL). Flash chromatography (silica, eluent: 30% Et_2O in pentane) yielded 402 mg (1.37 mmol, 91%) of a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.39 (m, 1H), 7.37 – 7.29 (m, 8H), 7.26 – 7.21 (m, 1H), 6.58 (d, J = 15.9 Hz, 2H), 5.95 (dd, J = 15.8, 8.5 Hz, 1H), 5.19 – 5.13 (m, 1H), 5.02 (d, J =

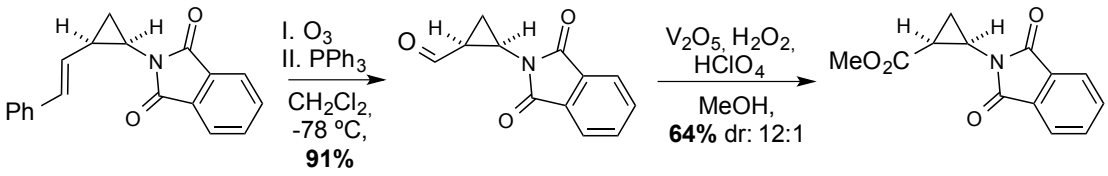
75.8 Hz, 1H), 4.73 (d, J = 5.9 Hz, 1H), 3.00 – 2.91 (bm, 1H), 1.91 – 1.83 (bm, 1H), 1.33 – 1.25 (bm, 1H), 0.81 (bs, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.27 (C=O), 136.42 (C=O), 131.68, 128.57, 128.53, 128.50, 128.12 (broad), 127.66, 127.09, 126.99, 126.96 (broad), 125.90, 66.81 (benzylic), 65.41 (benzylic), 29.72, 20.70, 14.29.

M.p.: 114-116 ºC

HRMS-APCI: calculated for $C_{19}H_{19}NNaO_2$ $[M+Na]^+$: 316.1308; found: 316.1312

Oxidative cleavage to aldehyde and esterification.



***Cis*-2-(1,3-dioxoisoindolin-2-yl)cyclopropane-1-carbaldehyde (9a)**

(E)-2-(2-styrylcyclopropyl)isoindoline-1,3-dione **6a** (723 mg, 2.5 mmol) was dissolved in dichloromethane (100 mL, 0.025M) and cooled to -78 ºC. Ozone was bubbled through the solution until a blue color appeared. Oxygen and then nitrogen gas was bubbled through the solution followed by the addition of triphenylphospine (656 mg, 2.5 mmol). The reaction was stirred at room temperature for 2 hours before it was concentrated. Flash chromatography (silica, eluent: 50 to 100% Et_2O in pentane) yielded 490 mg (2.275 mmol, 91%) of a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.67 (d, J = 2.7 Hz, 1H), 7.85 (dd, J = 5.5, 3.0 Hz, 2H), 7.74 (dd, J = 5.5, 3.0 Hz, 2H), 3.14 (td, J = 7.2, 5.8 Hz, 1H), 2.58 (dtd, J = 8.5, 6.9, 2.7 Hz, 1H), 2.16 (q, J = 6.3 Hz, 1H), 1.71 (ddd, J = 8.3, 7.4, 6.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 196.56, 168.47, 134.26, 131.41, 123.44, 29.69, 26.40, 12.82.

M.p.: 107 ºC

HRMS-APCI: calculated for $C_{12}H_9NNaO_3$ $[M+Na]^+$: 238.0475; found: 238.0477

Methyl 2-(1,3-dioxoisoindolin-2-yl)cyclopropane-1-carboxylate (10)

The oxidative esterification to 12 based on a literature procedure.[13]

2-(1,3-dioxoisoindolin-2-yl)cyclopropane-1-carbaldehyde **9a** (43 mg, 0.2 mmol, 1.0 equiv) was dissolved in methanol (4 mL, 0.05M). Meanwhile, vanadium(V)oxide (36 mg, 0.2 mmol, 1.0 equiv) was dissolved in a H_2O_2 solution (15% 1.5 mL) at 0 ºC. The solution of aldehyde **9a** is cooled to 0 ºC and once the vanadium solution turns deep red, perchloric acid (1.44 µL, 70%, 0.01 mmol, 0.05 equiv) is added to it. The oxidant mixture is carefully added to the methanolic solution and left to stir for 3 hours, whilst slowly warming. The reaction was quenched by adding a saturated sodium thiosulfate solution at 0 ºC and stirring was continued for 1 hour. The mixture was extracted with ethyl acetate (25 mL) and washed with water (20

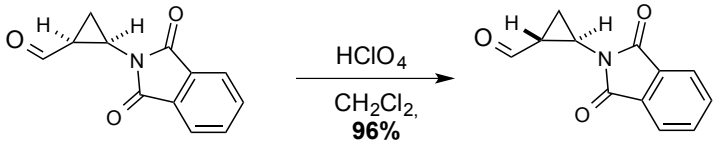
mL, x2) and brine (20 mL). Concentration followed by flash chromatography (silica 24 g, eluent: 20 to 90% Et_2O in pentane over 1 hour, fractions analyzed by GC-FID)[14] afforded 31.1 mg (0.127 mmol, 64%) of a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 2H), 7.72 (dd, J = 5.5, 3.0 Hz, 2H), 3.62 (s, 3H), 3.04 (td, J = 7.4, 5.8 Hz, 1H), 2.23 (dt, J = 8.6, 6.8 Hz, 1H), 1.96 (q, J = 6.3 Hz, 1H), 1.66 (ddd, J = 8.7, 7.7, 6.3 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.01, 168.56, 134.07, 131.62, 123.34, 52.13, 27.53, 18.60, 13.03.

HRMS-APCI: calculated for $C_{13}H_{11}NNaO_4$ $[M+Na]^+$: 268.0580; found: 268.0574

Epimerization of aldehyde.



***Trans*-2-(1,3-dioxoisoindolin-2-yl)cyclopropane-1-carbaldehyde (9b)**

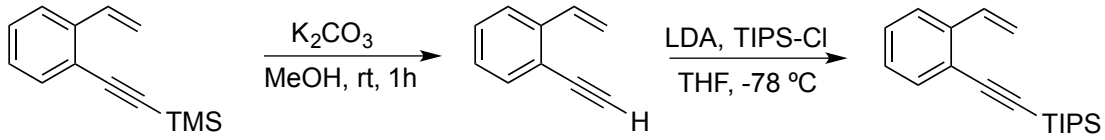
2-(1,3-dioxoisoindolin-2-yl)cyclopropane-1-carbaldehyde **9a** (43 mg, 0.2 mmol, 1.0 equiv) was dissolved in dichloromethane (1 mL) and perchloric acid (2.9 μL, 70%, 0.02 mmol, 0.1 equiv) was added. The reaction was stirred for 2 hours before it was extracted with dichloromethane (5 mL) and wash with water (5 mL, 3x) and brine (5 mL), affording 41 mg (0.192 mmol, 96%) of a yellowish solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (d, J = 2.7 Hz, 1H), 7.84 (dd, J = 5.5, 3.1 Hz, 2H), 7.74 (dd, J = 5.5, 3.1 Hz, 2H), 3.13 (td, J = 7.2, 5.8 Hz, 1H), 2.58 (dtd, J = 8.4, 6.9, 2.7 Hz, 1H), 2.15 (q, J = 6.3 Hz, 1H), 1.70 (ddd, J = 8.4, 7.4, 6.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.57, 168.47, 134.26, 131.40, 123.45, 29.69, 26.40, 12.82.

M.p.: 98 ºC

Preparation of styrenes.



1-Ethynyl-2-vinylbenzene

This compound was synthesized using a modified literature procedure [15] : Anhydrous potassium carbonate (622 mg, 4.5 mmol, 1.5 equiv) was added to a solution of trimethyl((2-vinylphenyl)ethynyl)silane[16] (600 mg, 3.0 mmol, 1.0 equiv) in methanol (4.5 mL, 0.667M) and the suspension was stirred for 1 hour at room temperature. The mixture was extracted with pentane, washed with brine and used directly in the next step.

The crude data was consistent with the literature[15].

Triisopropyl((2-vinylphenyl)ethynyl)silane (11)

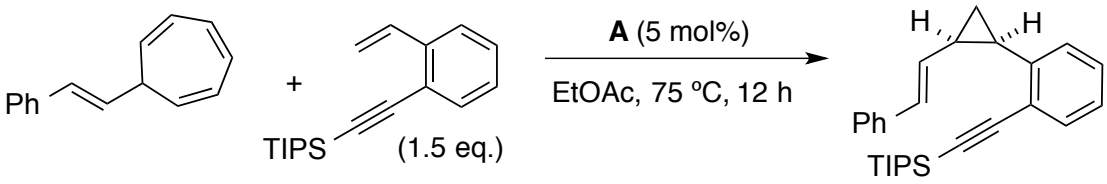
1-ethynyl-2-vinylbenzene (3.0 mmol, 1.0 equiv) was dissolved in dry THF (15 mL, 0.2M) and cooled to -78 ºC, followed by the addition of lithium diisopropylamine (0.5M THF, 8.0 mL, 4.0 mmol, 1.2 equiv) over 10 minutes, and finally the addition of triisopropylsilyl chloride (963 μL, 4.5 mmol, 1.5 equiv). The reactions was slowly warmed to room temperature, after which it was quenched with water, extracted with Et_2O, washed with brine and dried over Na_2SO_4. Flash chromatography (80 g, SiO_2, eluent: pentane) afforded 617 mg (2.17 mmol, 72%) of a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 1H), 7.51 – 7.48 (m, 1H), 7.34 – 7.25 (m, 2H), 7.21 (td, *J* = 7.5, 1.2 Hz, 1H), 5.83 (dd, *J* = 17.7, 1.1 Hz, 1H), 5.36 (dd, *J* = 11.0, 1.0 Hz, 1H), 1.17 (s, 18H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 139.34, 135.03, 133.05, 128.42, 127.31, 124.46, 122.27, 115.45, 105.14, 95.56, 18.70, 11.34.

HRMS-APCI: calculated for $C_{19}H_{29}Si$ $[M+H]^+$: 285.2033; found: 285.2046

***Cis*-(*E*)-triisopropyl((2-(2-styrylcyclopropyl)phenyl)ethynyl)silane (12a)**



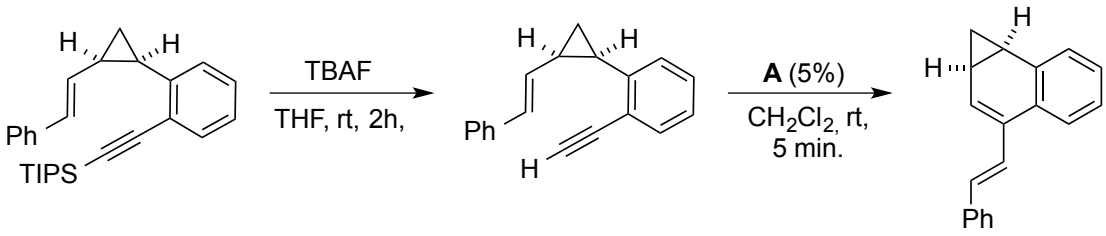
This compound (colorless oil, 64.5 mg, 64%, d.r. >20:1) was prepared according to the general procedure from (*E*)-7-styrylcyclohepta-1,3,5-triene (49.0 mg, 25 μmol), triisopropyl((2-vinylphenyl)ethynyl)silane (107 mg, 375 μmol) and gold catalyst **A** (9.7 mg, 12.5 μmol). The crude residue was purified by flash chromatography (40 g SiO_2, eluent: pentane).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 7.4, 0.9 Hz, 1H), 7.32 – 7.21 (m, 1H), 7.18 (dt, *J* = 5.0, 3.6 Hz, 4H), 7.14 – 7.08 (m, 3H), 6.46 (d, *J* = 15.7 Hz, 1H), 5.47 (dd, *J* = 15.7, 9.2 Hz, 1H), 2.70 (q, *J* = 8.4 Hz, 1H), 2.13 (qd, *J* = 8.8, 5.5 Hz, 1H), 1.47 – 1.37 (m, 1H), 1.30 – 1.21 (m, 1H), 1.16 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.96, 137.82, 132.83, 129.98, 129.78, 128.27, 127.91, 127.64, 126.43, 125.84, 125.65, 125.40, 105.82, 94.70, 23.57, 23.10, 18.74, 12.37, 11.39.

HRMS-APCI: calculated for $C_{28}H_{37}Si$ $[M+H]^+$: 401.2659; found: 401.2665.

A gold(I)-catalyzed1,7-enyne cyclizaton



(*E*)-1-ethynyl-2-(2-styrylcyclopropyl)benzene (12b)

To a solution of **12a** (46 mg, 0.115 mmol, 1.0 equiv) in THF (1.7 mL, 0.07M) was added a solution of tetrabutylammonium fluoride (1.0M THF, 575 μL, 5.0 equiv) and the reaction was stirred for 2 hours. Extracting with Et_2O, drying with Na_2SO_4 and filtration of a silica plug yielded the pure compound in 27.7 mg (0.113 mmol, 99%) as a colorless oil

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.24 – 7.17 (m, 4H), 7.15 – 7.11 (m, 3H), 6.51 (d, *J* = 15.7 Hz, 1H), 5.52 (dd, *J* = 15.7, 9.2 Hz, 1H), 3.31 (s, 1H), 2.74 – 2.66 (m, 1H), 2.18 (qd, *J* = 8.7, 5.6 Hz, 1H), 1.43 (td, *J* = 8.3, 5.4 Hz, 1H), 1.24 (dt, *J* = 6.4, 5.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 141.39, 137.78, 132.86, 129.96, 129.79, 128.37, 128.33, 127.72, 126.54, 125.91, 125.66, 123.95, 82.60, 81.15, 23.16, 22.93, 17.71, 12.51, 12.30.

HRMS-APCI: calculated for $C_{19}H_{17}$ $[M+H]^+$: 245.1325; found: 245.1334

(*E*)-3-styryl-1a,7b-dihydro-1*H*-cyclopropa[*a*]naphthalene (13)

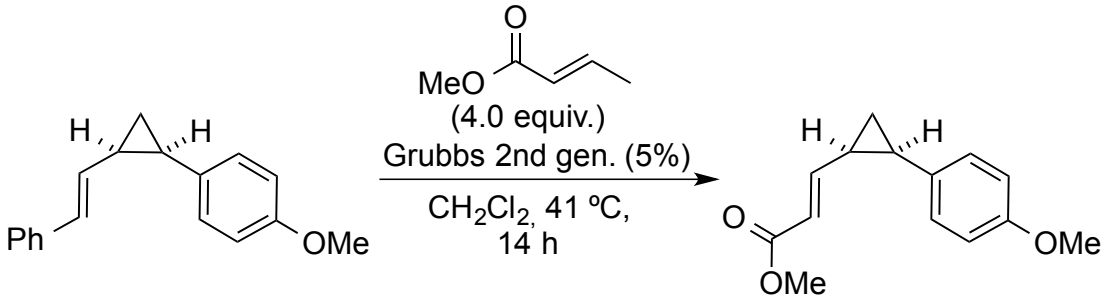
Catalyst **A** (3 mg, 0.004 mmol, 5 mol%) was added to a stirred solution of (*E*)-1-ethynyl-2-(2-styrylcyclopropyl)benzene (19.3 mg, 0.079 mmol, 1.0 equiv) in CH_2Cl_2 (1.25 mL, 0.0625M). After the disappearance of the pink color, a drop of triethylamine was added and the solution was filtered over a silica plug, providing the pure compound in 19.0 mg (0.078 mmol, 98%) as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.49 (m, 3H), 7.45 (dd, *J* = 7.3, 1.6 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 2H), 7.30 – 7.20 (m, 4H), 6.85 (d, *J* = 15.7 Hz, 1H), 6.55 (d, *J* = 5.5 Hz, 1H), 2.54 (td, *J* = 8.3, 5.1 Hz, 1H), 2.13 (tt, *J* = 7.9, 4.0 Hz, 1H), 1.62 (td, *J* = 8.8, 3.6 Hz, 1H), -0.12 – -0.16 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 137.75, 136.04, 131.14, 130.31, 130.11, 128.63, 128.39, 127.39, 127.27 (2CH), 127.05, 126.47, 125.61, 124.17, 21.23, 17.84, 10.57.

HRMS-APCI: calculated for $C_{19}H_{17}$ $[M+H]^+$: 245.1325; found: 245.1336

Cross metathesis of vinyl cyclopropanes



Methyl (*E*)-3-(2-(4-methoxyphenyl)cyclopropyl)acrylate (14)

This method is based on a literature procedure.[17]

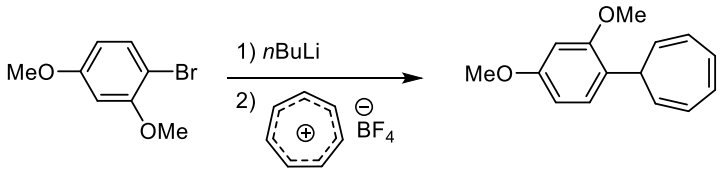
Grubbs catalyst 2nd generation (21 mg, 0.025 mmol, 5 mol%) and **3g** (125 mg, 0.5 mmol, 1.0 equiv) were mixed in a 5 mL microwave vial. After capping, the atmosphere was evacuated and backfilled with argon three times. CH_2Cl_2 (3.3 mL, 0.155M) and methyl crotonate (212 µL 2.0 mmol, 4.0 equiv) were added sequentially and the reaction mixture was stirred for 14h at 41 ºC. The mixture was cooled to room temperature and adsorbed directly on florisil. Flash chromatography (24 g SiO_2, eluent: 5 to 20% Et2O in pentane) yielded 83 mg (0.36 mmol, 72%, dr: 15:1) of a grey oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.16 (d, *J* = 8.3 Hz, 2H), 6.87 – 6.83 (m, 2H), 6.27 (dd, *J* = 15.4, 10.6 Hz, 1H), 5.93 (d, *J* = 15.4 Hz, 1H), 3.82 (s, 3H), 3.65 (s, 3H), 2.55 (q, *J* = 8.3 Hz, 1H), 2.01 – 1.93 (m, 1H), 1.45 (td, *J* = 8.6, 5.2 Hz, 1H), 1.23 (dt, *J* = 6.7, 5.2 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.70, 158.28, 150.63, 130.11, 129.38, 119.49, 113.81, 55.25, 51.22, 24.84, 22.23, 13.84.

HRMS-APCI: calculated for $C_{14}H_{16}NaO_3$ $[M+Na]^+$: 255.0992; found: 255.0980

7-(2,4-Dimethoxyphenyl)cyclohepta-1,3,5-triene (S1)



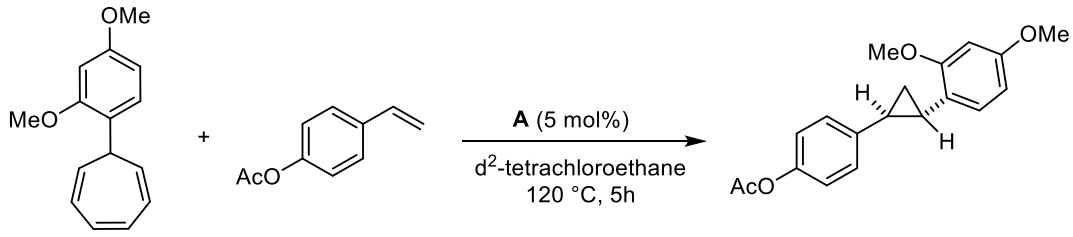
To a solution of 1-bromo-2,6-dimethoxy-benzene (6.033 g, 27.8 mmol, 1.05 equiv) in dry Et_2O (132 mL) at −78 ºC was added dropwise *n*-BuLi (15.571 mL, 1.87 M in hexanes, 29.1 mmol, 1.10 equiv) under argon. The mixture was stirred for 30 min at −78 °C, and then tropylium tetrafluoroborate (4.710 g, 26.5 mmol, 1.00 equiv) was added in one portion. The cooling bath was removed and the reaction was allowed to warm up to 23 °C and stirred for 2.5 h. The reaction was quenched by addition of brine. The aqueous phase was extracted with Et_2O, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated *in vacuo*. The crude residue was purified by flash chromatography (120 g SiO_2, eluent: gradient from CyHex to 10% EtOAc) affording 4.550 g (4.92 mmol, 71%) of a yellow oil. Dimethoxybenzene was removed from the product via Kugelrohr distillation (80 °C at 2.4 x 10^{-1} mbar) affording 4.040 g (17.7 mmol, 67%) of **S1** as a yellow oil. The product contains 6% of an impurity, presumably a regiosisomer of the cycloheptatriene.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 8.0 Hz, 1H), 6.83 – 6.75 (m, 2H), 6.63 – 6.55 (m, 2H), 6.34 – 6.27 (m, 2H), 5.50 (dd, J = 8.9, 5.6 Hz, 2H), 3.89 (s, 3H), 3.84 (s, 3H), 3.18 – 3.11 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.8, 158.4, 130.9, 129.3, 127.6, 124.4, 124.1, 104.4, 99.0, 55.4 (2 signals), 40.2.

HRMS-ESI: calculated for $C_{15}H_{17}O_2$ $[M+H]^+$: 229.1223; found: 229.1228.

***Trans*-4-((2-(2,4-dimethoxyphenyl)cyclopropyl)phenyl acetate (S2)**



A solution of the cyclohepatriene **S1** (45.9 mg, 201 µmol, 2.0 equiv), 4-vinylphenyl acetate (16.3 mg, 101 µmol, 1.0 equiv), diphenylmethane (17 µl, 101 µmol, 1.0 equiv) as internal standard(1.0 equiv) and gold catalyst **A** (3.9 mg, 5 µmol, 0.05 equiv) in d^2-1,1,2,2-tetrachloroethane (0.6 mL) was added to Young-NMR tube. The atmosphere was exchanged by three vacuum/Argon cycles and the tube was sealed. The NMR-tube was placed in a NMR machine, preheated to 120 °C. The reaction was monitored by ^{1}H NMR every 10 min for 5 h. The reaction mixture was cooled to room temperature and the solvent was removed *in vacuo*. The crude residue was purified by column chromatography (4 g SiO_2, eluent: gradient from

CyHex to 20% EtOAc) affording **S2** (28.9 mg, 92.59 µmol, 92%, d.r. 12:1) as a pale yellow oil.

The stereochemistry was confirmed by 1D NOESY experiments[6] (see spectral data for full details).

^{1}H NMR (400 MHz, CDCl3) δ 7.24 – 7.17 (m, 2H), 7.03 – 6.97 (m, 2H), 6.89 (d, J = 8.1 Hz, 1H), 6.49 – 6.41 (m, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 2.34 – 2.28 (m, 4H), 2.08 – 2.00 (m, 1H), 1.37 – 1.32 (m, 1H), 1.31 – 1.26 (m, 1H).

^{13}C NMR (101 MHz, CDCl3) δ 169.8, 159.3, 159.2, 148.7, 140.9, 127.3, 126.1, 123.2, 121.4, 104.0, 98.6, 55.6, 55.5, 25.7, 21.6, 21.3, 16.4.

HRMS-ESI: calculated for $C_{19}H_{21}O_4$ $[M+H]^+$: 313.1434; found: 313.1446.

Reaction progress monitored by ^{1}H NMR:

The reaction was monitored by ^{1}H NMR, integrations were normalized against diphenylmethane (CH2 at 4.07 ppm). For **S1** the CH at 3.22 ppm, for ***cis*-S2** the CH_3-C(O) at 2.25 ppm and ***trans*-S2** the CH at 2.39 ppm were integrated. The given concentration in Table S1 can be considered as correct within the experimental error.

The cyclopropanation reaction procedes very fast at 120 °C. Already after 10 min it is complete, full conversion of styrene and 85% conversion of **S1** is reached (Figure S1). *In situ* formed ***cis*-S2** is converted, most likely, into ***trans*-S2**. The d.r. is changing during the course of the reaction from 3.7:1 (10 min) to 10.8:1 (45 min).

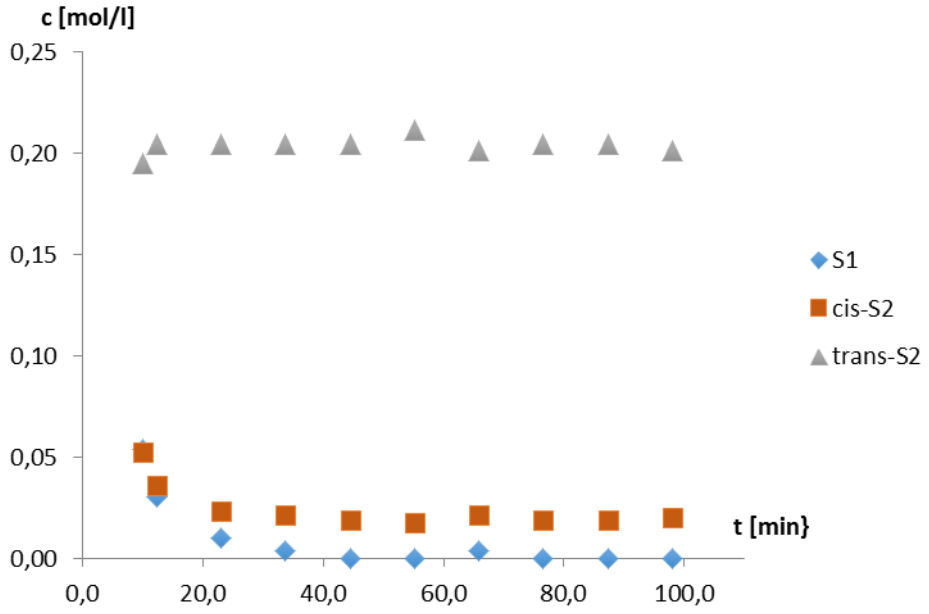
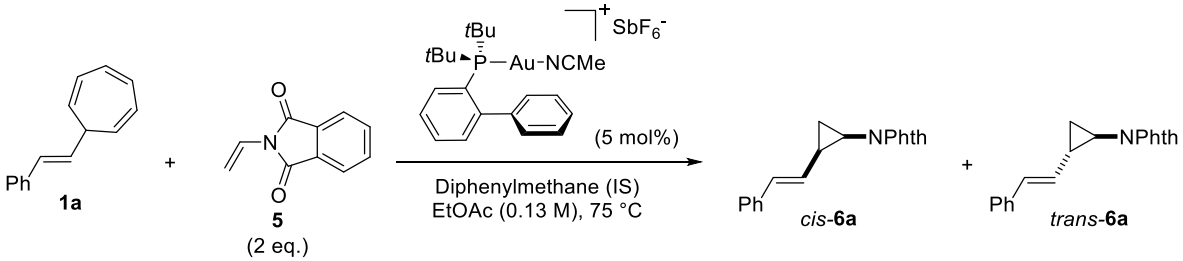


Figure S1. Reaction profile of the cyclopropanation of 4-vinylphenyl acetate using S1

Table S1. Measured concentration (^{1}H NMR) during the cyclopropanation of 4-vinylphenyl acetate using S1

Time [min]	c(S1) [mol/l]	c(*cis*-S2) [mol/l]	c(*trans*-S2) [mol/l]
10	0,05	0,05	0,19
12	0,03	0,04	0,20
23	0,01	0,02	0,20
34	0,00	0,02	0,20
45	0,00	0,02	0,20
55	0,00	0,02	0,21
66	0,00	0,02	0,20
77	0,00	0,02	0,20
87	0,00	0,02	0,20
98	0,00	0,02	0,20
109	0,00	0,02	0,22
119	0,00	0,02	0,19
130	0,00	0,02	0,20
141	0,00	0,02	0,20
152	0,00	0,02	0,19
162	0,00	0,02	0,19
173	0,00	0,02	0,19

9. Kinetic experiments for the epimerization of alkenylcyclopropanes



Initial rate studies for the gold(I)-catalyzed retro-Buchner reaction of 1a.
Cycloheptatriene **1a** (100.0 mg, 515 µmol, 1 equiv), *N*-vinyl phthalimide **5** (178.0 mg, 1.03 mmol, 2 equiv), gold catalyst **A** (19.9 mg, 26 µmol, 5 mol%) and diphenylmethane (86 µL, 515 µmol, 1 equiv) were added to a small round-bottom flask and the atmosphere was exchanged for argon with three vacuum/Argon cycles before adding EtOAc (4 mL). The round-bottom flask was placed in a preheated oil bath and stirred at 75 °C.
Aliquots of the reaction mixture were taken, filtered in a pipette over silica gel with EtOAc and were then concentrated to dryness. ^{1}H NMR spectra were recorded (8 scans, $CDCl_3$, 400 MHz) and the concentration of the products quantified by integration against the internal standard diphenylmethane.

The reaction profile shows a fast consumption of cycloheptatrienes **1a** going along with a fast formation of ***cis*-6a**. After complete conversion of **1a**, the amount ***cis*-6a** is slowly decreasing and at the same time ***trans*-6a** is forming.

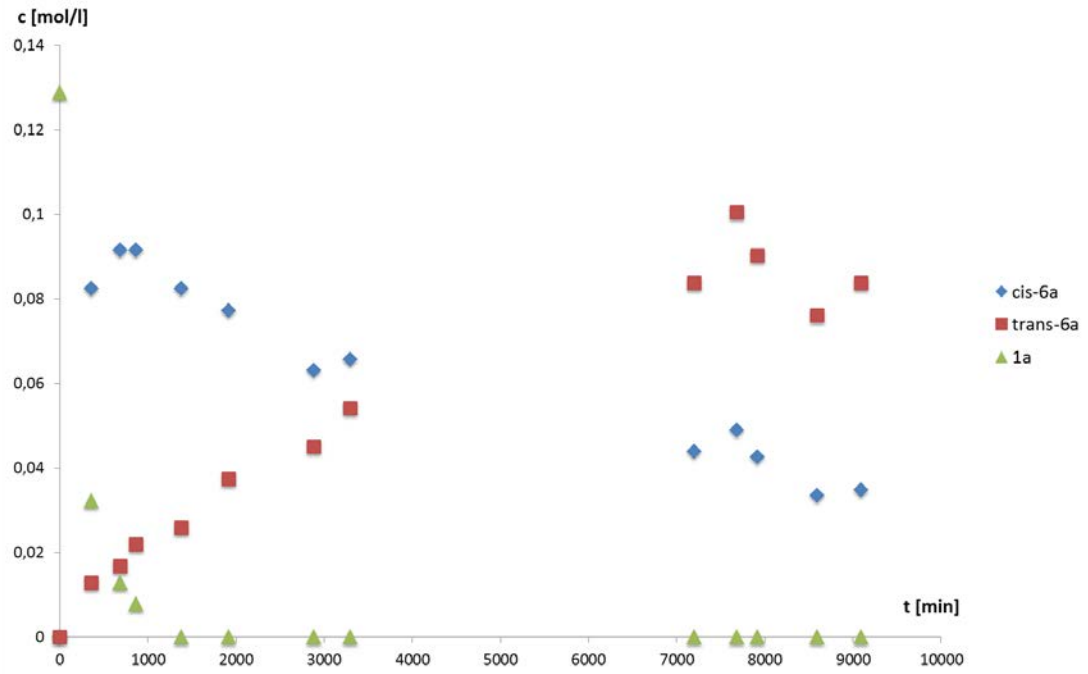


Figure S2. Reaction profile of the cyclopropanation of *N*-vinyl phthalimide using 1a

Table S2. Measured concentration (^{1}H NMR) during the cyclopropanation of *N*-vinyl phthalimide using 1a

t (min)	c(*cis*-6a)	ln (c(*cis*-6a))	c(*trans*-6a)	ln (c(*trans*-6a))	c(1a)	ln (c(1a))
0	0	-	0	-	0,13	-2,05
360	0,08	-2,49	0,01	-4,35	0,03	-3,43
690	0,09	-2,39	0,02	-4,09	0,01	-4,35
870	0,09	-2,39	0,02	-3,82	0,01	-4,86
1380	0,08	-2,49	0,03	-3,66	0,00	-
1920	0,08	-2,56	0,04	-3,29	0,00	-
2880	0,06	-2,76	0,05	-3,10	0,00	-
3300	0,07	-2,72	0,05	-2,92	0,00	-
7200	0,04	-3,13	0,08	-2,48	0,00	-
7680	0,05	-3,02	0,10	-2,30	0,00	-
7920	0,04	-3,16	0,09	-2,40	0,00	-
8595	0,03	-3,40	0,08	-2,58	0,00	-
9090	0,03	-3,36	0,08	-2,48	0,00	-

From these data we were able to obtain the initial rate by plotting the concentration (ln(mol·l^{-1})) of **1a** versus the reaction time (Figure S3). We were assuming a pseudo-first order kinetic due to the excess of substrate relative to gold catalyst **A**.

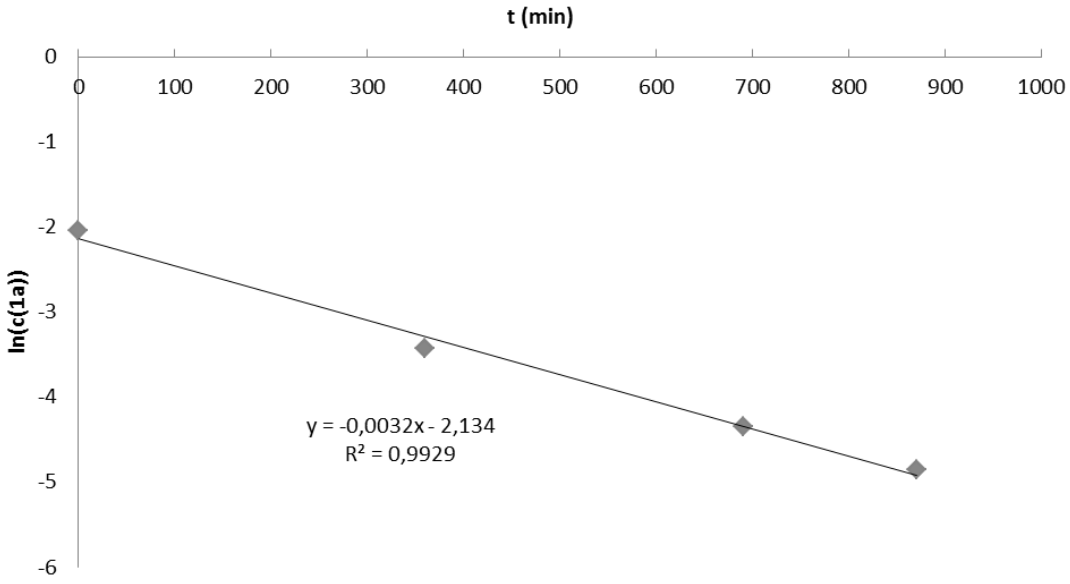


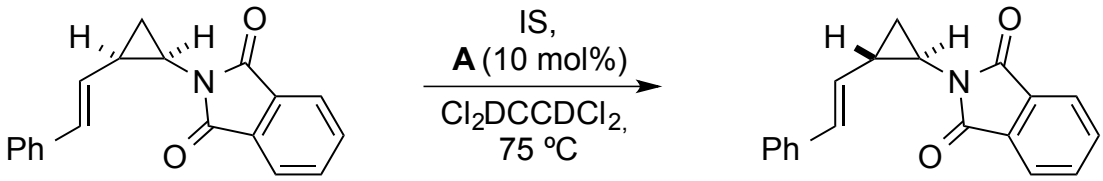
Figure S3. Initial rate plot for consumption of 1a.

A reaction rate constant of k= **-5.33 10^{-5}** /s = for the consumption of cycloheptatrienes **1a** was determined. Using the rewritten Eyring equation below, we were able to estimate the value for the energy of activation to be **27.0** kcal·mol^{-1}.

$$\Delta G^{\ddagger} = -RT\, ln\frac{-k_r h}{k_B T}$$

Where:

$\Delta G^{\ddagger}$	=	Gibbs energy of activation	120998.3	J·mol^{-1}
R	=	*Gas constant*	*8.3144598*	J·K^{-1}·mol^{-1}
T	=	Absolute temperature	348	K
k_r	=	Reaction rate constant	-5.33·10^{-5}	mol·s^{-1}
h	=	*Planck constant*	*6.626070040·10^{-34}*	J·s
k_B	=	*Boltzmann´s constant*	*1.38064852·10^{-23}*	J·K^{-1}



Initial rate studies for the gold(I) mediated epimerization of 6a.

cis-(*E*)-2-(2-styrylcyclopropyl)isoindoline-1,3-dione **6a** (4.5 mg, 0.0155 mmol), gold catalyst **A** (1.2 mg, 0.00155 mmol, 10 mol%) and diphenylmethane (2.6 μL, 0,0155 mmol) were added to a Young NMR tube and the atmosphere was flushed with argon three times before adding 1,1,2,2,-tetrachloroethane-*d2* (0.4 mL). The mixture was heated in a Bruker NMR machine to 75 ºC for 7 hours, while performing ^{1}H measurements every 20 minutes.

The corrected data, to the internal standard, is presented in Table S3:

Table S3. Measured concentration (^{1}H NMR) of *cis*-6a during its isomerization to *trans*-6a

Concentration of *cis*-6a[a] (M)	ln(concentration of *cis*-6a)[b]	Time (s)
~~0,01574~~ [c]	~~-4,133~~[c]	~~0~~[c]
~~0,01632~~ [c]	~~-4,146~~ [c]	~~1200~~[c]
~~0,02118~~ [c]	~~-4,161~~[c]	~~2400~~[c]
0,02605	-4,174	3600
0,02638	-4,184	4800
0,02729	-4,187	6000
0,02693	-4,196	7200
0,03389	-4,209	8400
0,03467	-4,212	9600
0,03572	-4,219	10800
0,03779	-4,221	12000
0,04145	-4,232	13200
0,04171	-4,240	14400
0,04197	-4,248	15600
0,05034	-4,251	16800
0,05060	-4,253	18000
0,04467	-4,266	19200
0,05675	-4,267	20400
0,05216	-4,275	21600
0,05120	-4,280	22800
0,05758	-4,284	24000

[a]The disappearance of the *cis*-isomer was used for our data set as the accuracy was better compared to the appearance of the *trans*-isomer. [b]We are assuming 1st-order kinetics; hence the concentration is presented as the natural logarithm. [c]The first three data points were omitted to reduce the experimental error.

From these data we were able to make an initial rate plot with the concentration ($\ln(mol \cdot l^{-1})$) of ***cis*-6a** versus reaction time (s) (Figure S4).

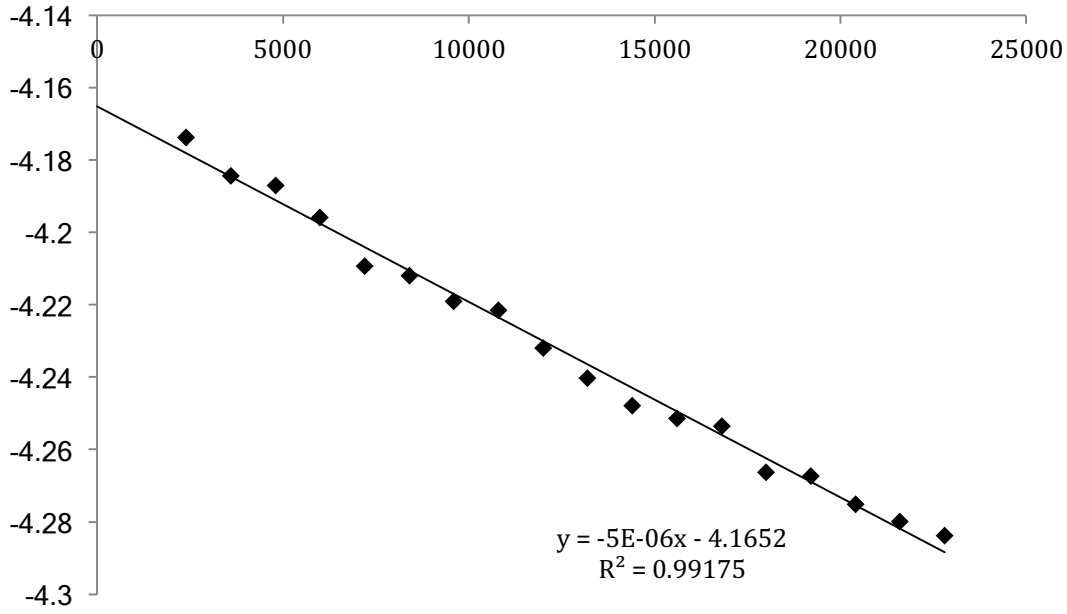


Figure S4. Initial rate plot for the epimerization of *cis*-6a.

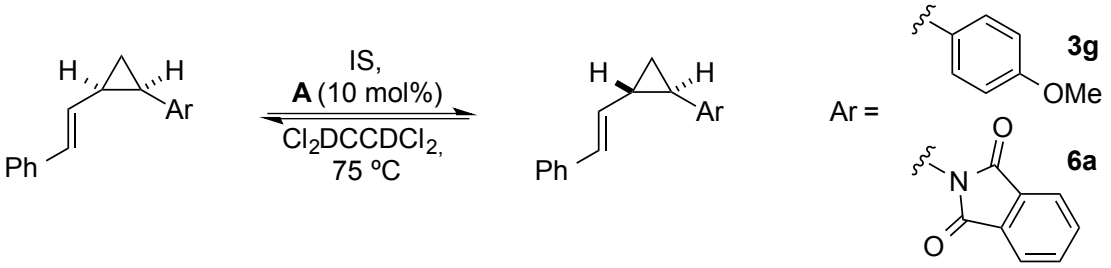
A reaction rate constant of **$-5 \cdot 10^{-6}$** for the disappearance of the *cis*-isomer was derived from this plot. Using the rewritten Eyring equation below, we were able to estimate the value for the energy of activation to be **28.9** kcal·mol^{-1}.

$$\Delta G^{\ddagger} = -RT\, ln \frac{-k_r h}{k_B T}$$

Where:

$\Delta G^{\ddagger}$	=	Gibbs energy of activation	120998.3	J·mol^{-1}
R	=	*Gas constant*	*8.3144598*	J·K^{-1}·mol^{-1}
T	=	Absolute temperature	348	K
k_r	=	Reaction rate constant	$-5 \cdot 10^{-6}$	mol·s^{-1}
h	=	*Planck constant*	$6.626070040 \cdot 10^{-34}$	J·s
k_B	=	*Boltzmann´s constant*	$1.38064852 \cdot 10^{-23}$	J·K^{-1}

Calculating the energy difference between the *cis*- and *trans*-isomers of 3g and 6a.



3g: *cis*-(E)-1-methoxy-4-(2-styrylcyclopropyl)benzene **3g** (3.8 mg, 0.03 mmol), gold catalyst **A** (2.3 mg, 0.003 mmol, 10 mol%) and diphenylmethane (4.8 μL, 0,03 mmol) were added to a Young NMR tube and the atmosphere was flushed with argon three times before adding chloroform-*d1* (0.4 mL). The mixture was heated to 75 ºC for 7 days, until equilibrium was reached, with a cis/trans ratio of 0.148:1.

6a: *cis*-(*E*)-2-(2-styrylcyclopropyl)isoindoline-1,3-dione **6a** (4.5 mg, 0.0155 mmol), gold catalyst **A** (1.2 mg, 0.00155 mmol, 10 mol%) and diphenylmethane (2.6 μL, 0,0155 mmol) were added to a Young NMR tube and the atmosphere was flushed with argon three times before adding 1,1,2,2,-tetrachloroethane-*d2* (0.4 mL). The mixture was heated to 75 ºC for 2 weeks, until equilibrium was reached, with a cis/trans ratio of 0.465:1.

Using the ratio of the as the equilibrium constant, k_{eq}, in the following equation, we estimated the difference in Gibbs free energy for the two isomers:

$$\Delta G^{\theta} = -RT \ln k_{eq}$$

Where:

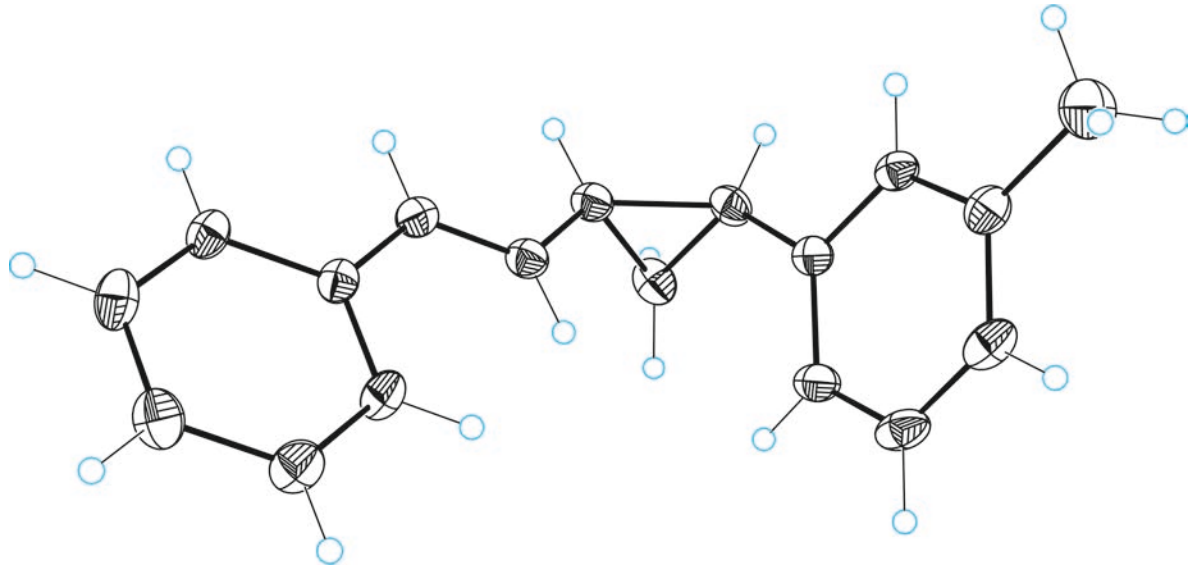
ΔG^{θ}	=	Gibbs energy of activation	5446.5 (**3g**), 2246.7 (**6a**)	$J \cdot mol^{-1}$
R	=	*Gas constant*	*8.3144598*	$J \cdot K^{-1} \cdot mol^{-1}$
T	=	Absolute temperature	348	K
k_{eq}	=	Reaction rate constant	0.148 (**3g**), 0.465 (**6a**)	$mol \cdot s^{-1}$

Signifying that ***trans*-3g** is more stable by **1.3** $kcal \cdot mol^{-1}$ and ***trans*-6a** is more stable by **0.5** $kcal \cdot mol^{-1}$.

10. X-ray crystallography

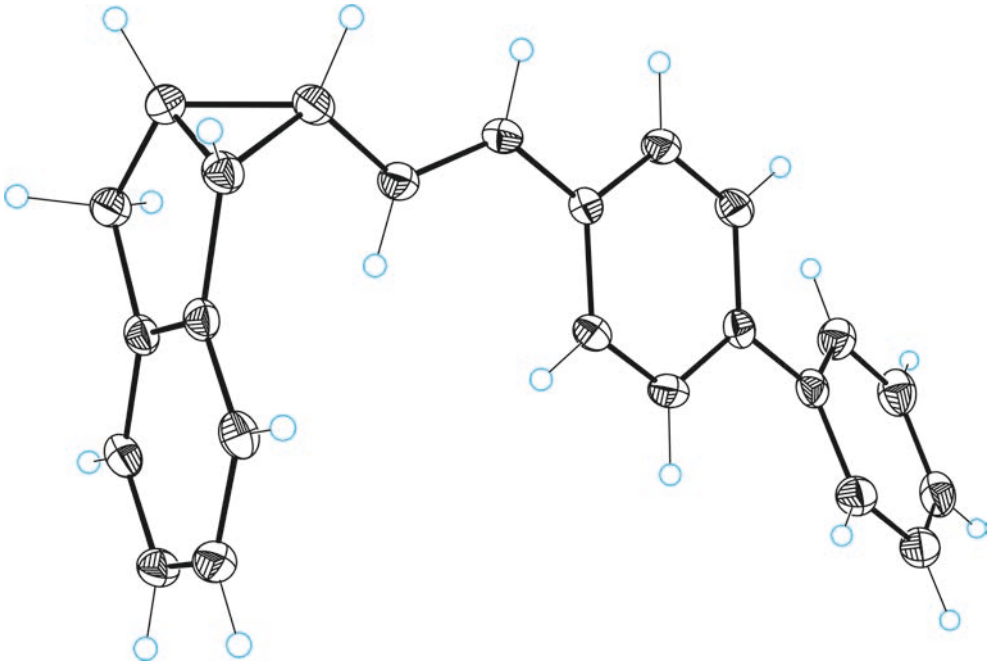
Crystal structure determinations were carried out using a Bruker-Nonius diffractometer equipped with an APPEX 24K CCD area detector, a FR591 rotating anode with MoKa radiation, Montel mirrors as monochromator and a Kryoflex low temperature device (T = – 173 °C). Full-sphere data collection was used with w and j scans. Programs used: Data collection APEX-2, data reduction Bruker Saint V/.60A and absorption correction SADABS. Structure Solution and Refinement: Crystal structure solutions were achieved using direct methods as implemented in SHELXTL and visualized using the program XP. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F2 using all measured intensities was carried out using the program SHELXTL. All non-hydrogen atoms were refined including anisotropic displacement parameters. ORTEP drawings are represented with 50% probability of the thermal ellipsoids.

Crystal data and structure refinement for *cis*-3a



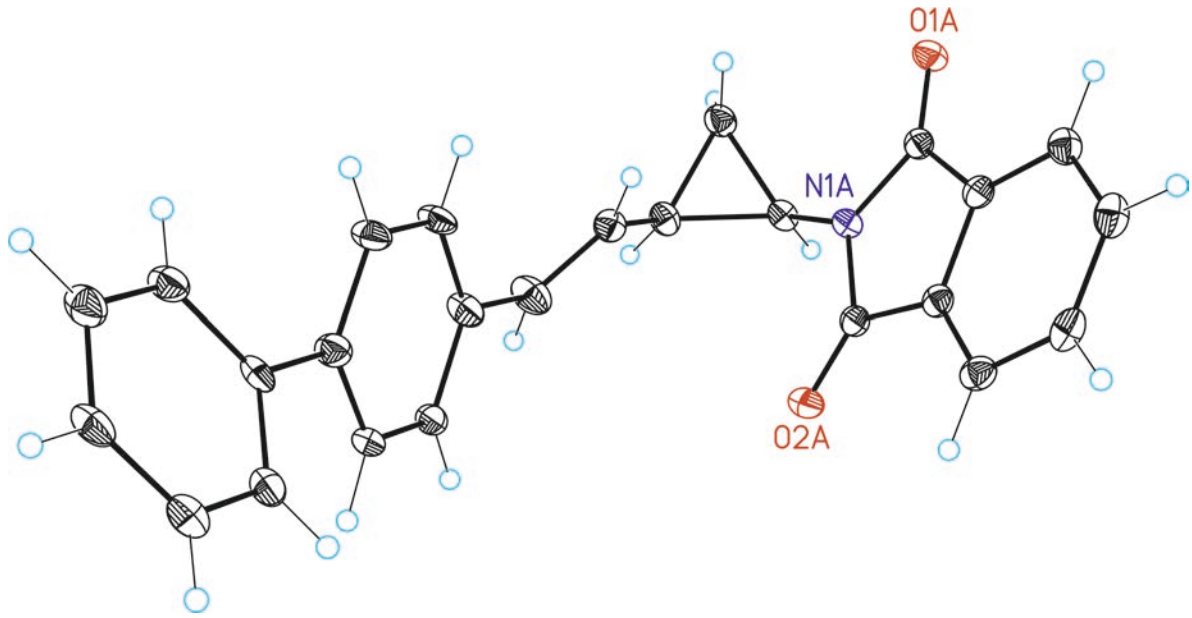
Empirical formula	C18 H18	
Formula weight	234.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.035(2)Å	α= 90°.
	b = 5.7594(15)Å	β = 100.891(7)°.
	c = 13.277(3)Å	γ = 90°.
Volume	678.5(3) $Å^3$	
Z	2	
Density (calculated)	1.147 Mg/m^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	252	
Crystal size	0.20 x 0.15 x 0.06 mm^3	
Theta range for data collection	2.295 to 32.557°.	
Index ranges	-13<=h<=12,-8<=k<=5,-19<=l<=15	
Reflections collected	9047	
Independent reflections	3680[R(int) = 0.0254]	
Completeness to theta =32.557°	92.7%	
Absorption correction	Empirical	
Max. and min. transmission	0.996 and 0.874	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3680/ 1/ 164	
Goodness-of-fit on F^2	1.050	
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.0989	
R indices (all data)	R1 = 0.0544, wR2 = 0.1056	
Flack parameter	x =0.1(10)	
Largest diff. peak and hole	0.251 and -0.211 $e.Å^{-3}$	

Crystal data and structure refinement for *endo*-3al



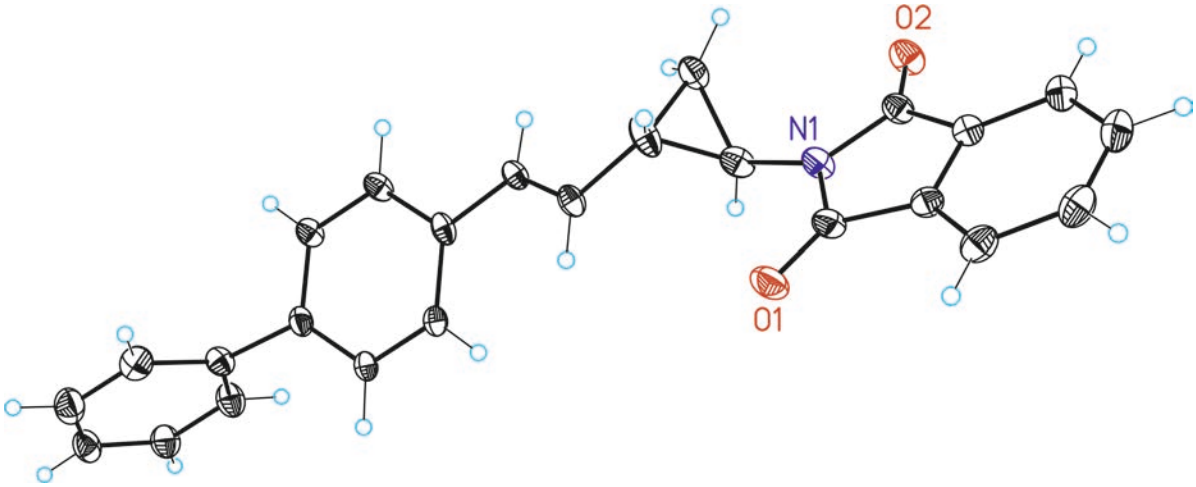
Empirical formula	C24 H20	
Formula weight	308.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2(1)	
Unit cell dimensions	a = 9.9863(13)Å	α= 90°.
	b = 18.438(2)Å	β = 90°.
	c = 8.9744(13)Å	γ = 90°.
Volume	1652.4(4) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	656	
Crystal size	0.40 x 0.40 x 0.06 mm^3	
Theta range for data collection	2.209 to 31.541°.	
Index ranges	-7<=h<=14,-17<=k<=27,-12<=l<=13	
Reflections collected	12057	
Independent reflections	5071[R(int) = 0.0401]	
Completeness to theta =31.541°	97.299995%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.996 and 0.837	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5071/ 1/ 217	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0573, wR2 = 0.1275	
R indices (all data)	R1 = 0.0810, wR2 = 0.1408	
Flack parameter	x =-0.1(10)	
Largest diff. peak and hole	0.289 and -0.233 e.$Å^{-3}$	

Crystal data and structure refinement for *cis*-6e



Empirical formula	C25 H19 N O2	
Formula weight	365.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8574(4)Å	α= 83.974(3)°.
	b = 10.5363(4)Å	β = 85.964(3)°.
	c = 19.0980(6)Å	γ = 69.875(4)°.
Volume	1850.89(13) $Å^3$	
Z	4	
Density (calculated)	1.311 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	768	
Crystal size	0.12 x 0.12 x 0.03 mm^3	
Theta range for data collection	2.202 to 28.875°.	
Index ranges	-13<=h<=12,-13<=k<=13,-23<=l<=23	
Reflections collected	30805	
Independent reflections	8327[R(int) = 0.0463]	
Completeness to theta =28.875°	85.6%	
Absorption correction	Empirical	
Max. and min. transmission	0.998 and 0.768	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8327/ 230/ 669	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1309	
R indices (all data)	R1 = 0.0795, wR2 = 0.1458	
Largest diff. peak and hole	0.377 and -0.261 $e.Å^{-3}$	

Crystal data and structure refinement for *trans*-6e



Empirical formula	C25 H19 N O2	
Formula weight	365.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 4.88608(8)Å	α= 90°.
	b = 39.9585(6)Å	β = 91.1105(15)°.
	c = 9.27521(15)Å	γ = 90°.
Volume	1810.55(5) $Å^3$	
Z	4	
Density (calculated)	1.341 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	768	
Crystal size	0.2 x 0.18 x 0.03 mm^3	
Theta range for data collection	2.039 to 60.660°.	
Index ranges	-11<=h<=11,-96<=k<=94,-22<=l<=20	
Reflections collected	106963	
Independent reflections	25432[R(int) = 0.0484]	
Completeness to theta =60.660°	91.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.998 and 0.768	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	25432/ 710/ 532	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0910, wR2 = 0.2494	
R indices (all data)	R1 = 0.1348, wR2 = 0.2737	
Largest diff. peak and hole	0.865 and -0.897 e.$Å^{-3}$	

11. DFT calculations

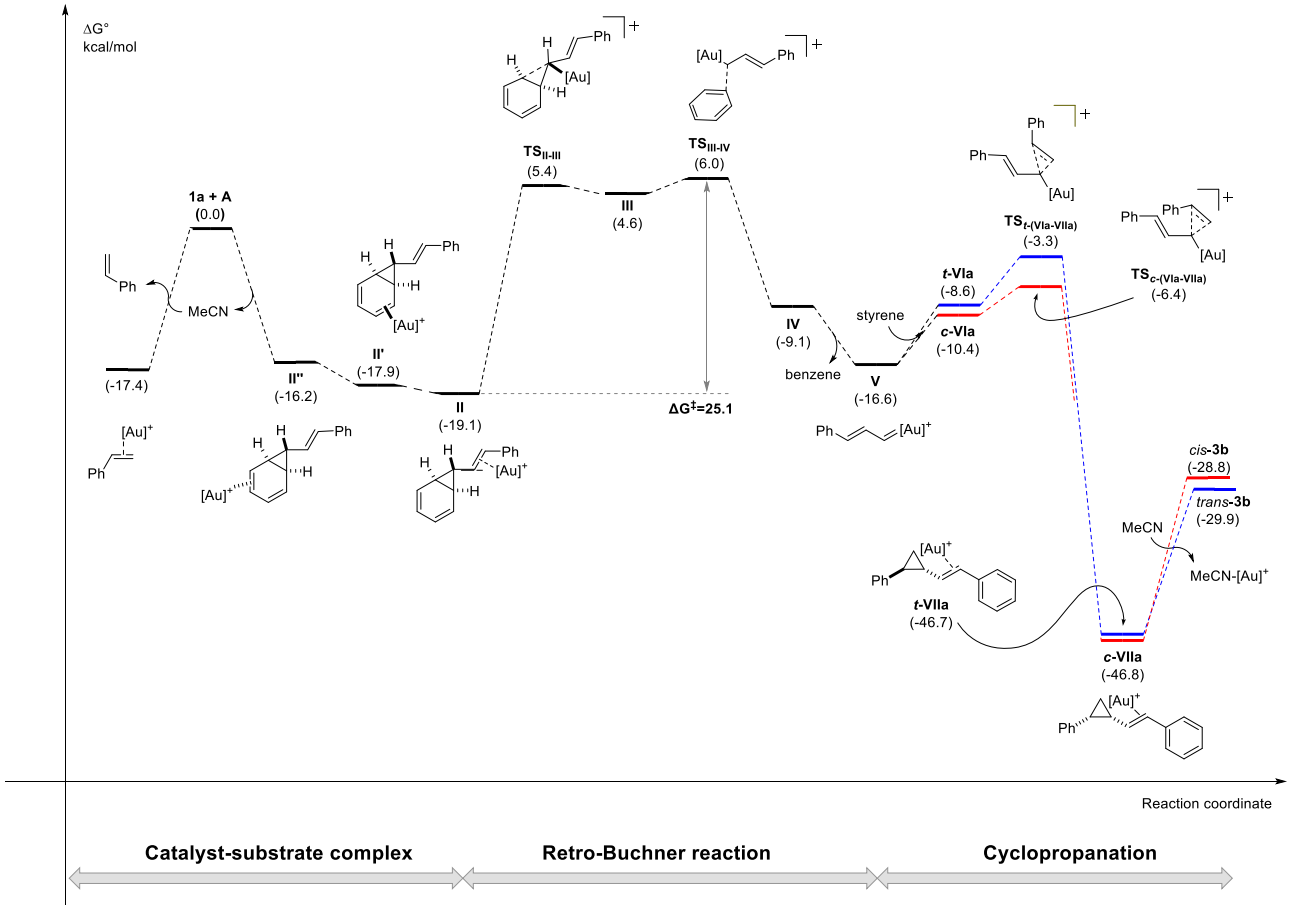
Computational details

Calculations were performed using SMD(CH_2Cl_2)-M06/6-311+G(2d,p), SDD(Au, ζ_f=1.05)//SMD(CH_2Cl_2)-M06/6-31G(d), SDD(Au) at the standard state (298.15 K, 1 atm). Full geometry optimizations were performed in solution, with the SMD method,[18] and using Gaussian 09[19] defaults for dichloromethane (DCM). In the article, all energies are given in kcal/mol. In the experimental section, energies are given in Hartree. The nature of the stationary points was characterized by a vibrational analysis performed within the harmonic approximation at 298 K and 1 atm. Transition states were identified by the presence of one imaginary frequency and minima by a full set of real frequencies.

Single point energies were calculated for all six cyclopropanation transition states using SMD(CH_2Cl_2)-PBE-D3(BJ)/6-311+G(2d,p), SDD(Au, ζ_f=1.05).

Optimized geometries were visualized using CYLview.[20]

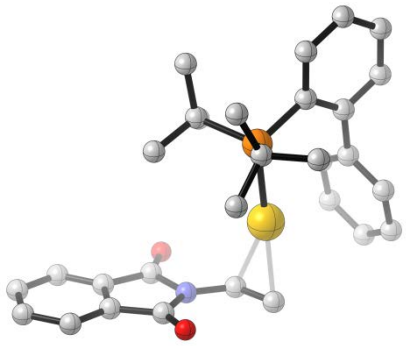
Calculated free energy profile for the formation of 3b



Computational details:
SMD(CH_2Cl_2)-M06/6-311+G(2d,p), SDD(Au, f=1.05)//SMD(CH_2Cl_2)-M06/6-31G(d), SDD(Au)
Gibbs free energies given in kcal/mol at the standard state (298.15 K, 1 atm)
[Au] = Au-JohnPhos

Cartesian coordinates (in Å) and energies (in h) for reactants, intermediates and transition states involved in the formation of 3b

Intermediate I

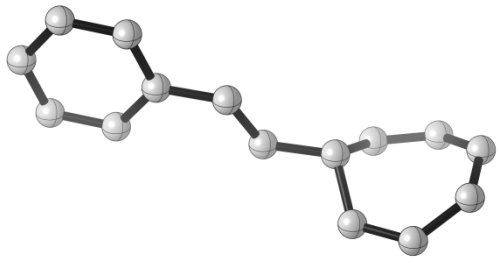


6	-1.844913000	2.101325000	-0.311194000
1	-1.590501000	2.658811000	0.592879000
79	0.111347000	0.657979000	-0.588759000
15	1.381722000	-1.266669000	-0.062609000
6	0.481240000	-2.138379000	1.352432000
6	1.521439000	-2.296867000	-1.651871000
6	3.088049000	-0.912745000	0.520760000
6	-0.895473000	-2.577910000	0.857873000
6	0.308286000	-1.089902000	2.452879000
6	1.222562000	-3.338180000	1.938043000
6	1.801516000	-3.783046000	-1.442669000
6	2.641010000	-1.666631000	-2.482447000
6	0.209129000	-2.157777000	-2.430538000
6	3.947930000	-1.995971000	0.768756000
6	3.596022000	0.396609000	0.664144000
1	-0.837185000	-3.394962000	0.126501000
1	-1.477247000	-2.945371000	1.716392000
1	-1.458560000	-1.746614000	0.405329000
1	-0.286055000	-0.226983000	2.113822000
1	-0.219263000	-1.550520000	3.301382000
1	1.273834000	-0.719419000	2.825600000
1	0.584706000	-3.787818000	2.713555000
1	1.435134000	-4.117356000	1.196449000
1	2.162657000	-3.045701000	2.421454000
1	1.895496000	-4.256617000	-2.431613000
1	2.738884000	-3.974693000	-0.907655000
1	0.983729000	-4.291364000	-0.915905000
1	3.632977000	-1.824380000	-2.039978000
1	2.640176000	-2.128812000	-3.480540000
1	2.493295000	-0.584348000	-2.621272000
1	0.290626000	-2.741336000	-3.359762000
1	-0.659119000	-2.536638000	-1.876495000
1	0.004874000	-1.114079000	-2.709934000
6	5.275120000	-1.810195000	1.130325000
1	3.577964000	-3.013774000	0.675824000
6	4.941872000	0.563009000	1.017931000
6	2.828019000	1.661969000	0.489675000
6	5.778349000	-0.519795000	1.247689000
1	5.910642000	-2.673700000	1.316196000
1	5.328053000	1.576908000	1.120454000
6	2.036115000	2.166638000	1.528379000
6	3.010719000	2.438564000	-0.659798000
1	6.818587000	-0.354502000	1.522323000
6	1.429844000	3.415778000	1.411933000
1	1.911389000	1.581835000	2.440292000
6	2.402186000	3.686293000	-0.776563000
1	3.649808000	2.063182000	-1.460420000
6	1.612163000	4.179030000	0.260037000
1	0.826383000	3.800170000	2.233419000
1	2.561711000	4.281303000	-1.674636000
1	1.149973000	5.161516000	0.175463000
6	-1.170209000	2.323397000	-1.484195000
1	-1.519313000	1.917334000	-2.430489000
1	-0.455312000	3.147252000	-1.502498000
7	-2.938120000	1.277980000	-0.125385000
6	-3.561728000	0.438326000	-1.085875000
6	-3.501569000	1.082917000	1.171968000
8	-3.087948000	1.618070000	2.171404000
8	-3.223004000	0.336787000	-2.241651000
6	-4.637394000	-0.259792000	-0.356097000
6	-4.601682000	0.123226000	0.984204000
6	-5.495488000	-0.386688000	1.908887000
1	-5.461131000	-0.084494000	2.953534000
6	-5.569032000	-1.167034000	-0.827319000
1	-5.589851000	-1.460537000	-1.874866000
6	-6.477842000	-1.684159000	0.098346000
1	-7.228938000	-2.398601000	-0.231877000
6	-6.441461000	-1.301411000	1.441386000
1	-7.164880000	-1.724320000	2.135356000

Zero-point correction= 0.570081
(Hartree/Particle)
Thermal correction to Energy= 0.604800
Thermal correction to Enthalpy= 0.605744
Thermal correction to Gibbs Free Energy= 0.504808
Sum of electronic and zero-point Energies= -1844.327363
Sum of electronic and thermal Energies= -1844.292644
Sum of electronic and thermal Enthalpies= -1844.291700
Sum of electronic and thermal Free Energies= -1844.392636

E(M06/6-311+G(2d,p))= -1845.31429483

Reactant 1a



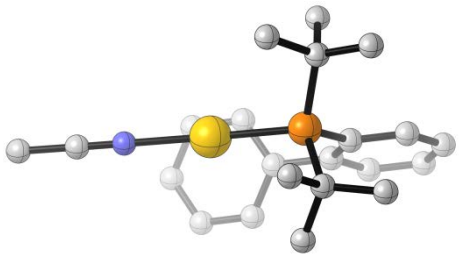
6	1.610298000	0.038795000	0.025044000
1	1.727478000	-0.836916000	-0.639474000
6	2.332806000	-0.242341000	1.316153000
1	1.809135000	-0.044105000	2.253837000
6	3.578132000	-0.762683000	1.329712000
1	4.003793000	-1.071964000	2.286617000
6	4.424308000	-0.909614000	0.173699000
1	5.220702000	-1.653265000	0.240942000
6	4.430036000	-0.083450000	-0.911913000
1	5.229891000	-0.221625000	-1.642021000
6	3.590540000	1.073869000	-1.082843000
1	4.023233000	1.913853000	-1.630365000
6	2.342370000	1.203619000	-0.586272000
1	1.823490000	2.162694000	-0.646043000
6	0.155745000	0.320207000	0.228404000
1	-0.070417000	1.187934000	0.857422000
6	-0.829854000	-0.415494000	-0.297660000
1	-0.553133000	-1.281859000	-0.907205000
6	-2.272257000	-0.202388000	-0.150097000
6	-3.152599000	-1.154065000	-0.682587000
6	-2.820704000	0.916366000	0.495613000

6	-4.530484000	-1.002241000	-0.570555000
1	-2.740489000	-2.026236000	-1.191876000
6	-4.195926000	1.069379000	0.607539000
1	-2.163610000	1.681049000	0.908911000
6	-5.058884000	0.110896000	0.076395000
1	-5.193975000	-1.756601000	-0.991272000
1	-4.600293000	1.946361000	1.111376000
1	-6.136984000	0.235546000	0.165363000

Zero-point correction= 0.241319
(Hartree/Particle)
Thermal correction to Energy= 0.253993
Thermal correction to Enthalpy= 0.254937
Thermal correction to Gibbs Free Energy= 0.200878
Sum of electronic and zero-point Energies= -579.253724
Sum of electronic and thermal Energies= -579.241051
Sum of electronic and thermal Enthalpies= -579.240106
Sum of electronic and thermal Free Energies= -579.294166

E(M06/6-311+G(2d,p))= -579.664368112

Catalyst A



79	-1.107991000	-0.641689000	-0.000382000
15	1.226928000	-0.691515000	-0.006240000
7	-3.212423000	-0.808817000	-0.039306000
6	2.038714000	0.953916000	0.117122000
6	-4.363974000	-0.907738000	-0.059490000
6	1.334122000	2.176608000	0.078952000
6	-5.798881000	-1.034451000	-0.080804000
1	-6.083355000	-2.054234000	0.201238000
1	-6.174514000	-0.821790000	-1.087742000
1	-6.243417000	-0.326268000	0.627035000
6	2.061478000	3.374910000	0.069135000
1	1.508661000	4.313264000	0.032253000
6	3.447460000	3.392031000	0.126003000
1	3.980578000	4.341012000	0.124386000
6	4.143229000	2.190753000	0.191812000
1	5.230004000	2.179577000	0.245593000
6	3.441778000	0.993193000	0.180125000
1	4.012106000	0.069031000	0.212224000
6	-0.146514000	2.336838000	0.074012000
6	-0.875797000	2.219560000	1.263785000
1	-0.361254000	1.917693000	2.177290000
6	-2.234728000	2.523971000	1.292944000
1	-2.784336000	2.446213000	2.230067000
6	-2.882591000	2.942815000	0.132419000
1	-3.942760000	3.190172000	0.157212000
6	-2.166862000	3.052526000	-1.057667000
1	-2.664700000	3.388604000	-1.966082000
6	-0.804804000	2.760699000	-1.084786000
1	-0.237883000	2.876991000	-2.009243000
6	1.754017000	-1.383282000	-1.684974000
6	1.070385000	-0.498734000	-2.731006000
1	1.369349000	-0.840266000	-3.733277000
1	1.369574000	0.555309000	-2.637581000
1	-0.026403000	-0.552972000	-2.667963000
6	3.257780000	-1.373001000	-1.950471000
1	3.435623000	-1.871470000	-2.915156000
1	3.830705000	-1.915925000	-1.189481000
1	3.659784000	-0.356143000	-2.034536000
6	1.234369000	-2.814877000	-1.808154000
1	1.368449000	-3.149831000	-2.847440000
1	0.163950000	-2.895355000	-1.568199000
1	1.792778000	-3.509458000	-1.166502000
6	1.766671000	-1.737839000	1.482402000
6	3.179057000	-2.311255000	1.398872000
1	3.372868000	-2.874895000	2.323837000
1	3.958175000	-1.543321000	1.327236000
1	3.292239000	-3.013171000	0.562411000
6	0.789081000	-2.907319000	1.637135000
1	1.080512000	-3.486731000	2.525999000
1	0.802812000	-3.591823000	0.779318000
1	-0.244337000	-2.563608000	1.785996000
6	1.641998000	-0.836396000	2.711069000
1	1.832246000	-1.439412000	3.611038000
1	0.633166000	-0.407697000	2.808608000
1	2.367789000	-0.013170000	2.699798000

Zero-point correction= 0.466168
(Hartree/Particle)
Thermal correction to Energy= 0.494403
Thermal correction to Enthalpy= 0.495347
Thermal correction to Gibbs Free Energy= 0.408409
Sum of electronic and zero-point Energies= -1386.985722
Sum of electronic and thermal Energies= -1386.957487
Sum of electronic and thermal Enthalpies= -1386.956543
Sum of electronic and thermal Free Energies= -1387.043481

E(M06/6-311+G(2d,p))= -1387.71502669

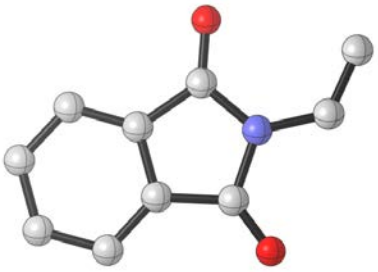
Reactant Acetonitrile

7	-1.435812000	-0.000095000	0.000013000
6	-0.274570000	0.000173000	0.000107000
6	1.173518000	0.000053000	-0.000006000
1	1.551565000	-0.601171000	-0.834293000
1	1.553175000	-0.422402000	0.936994000
1	1.552255000	1.022884000	-0.103398000

Zero-point correction= 0.045393
(Hartree/Particle)
Thermal correction to Energy= 0.048930
Thermal correction to Enthalpy= 0.049875
Thermal correction to Gibbs Free Energy= 0.021433
Sum of electronic and zero-point Energies= -132.616203
Sum of electronic and thermal Energies= -132.612666
Sum of electronic and thermal Enthalpies= -132.611721
Sum of electronic and thermal Free Energies= -132.640163

E(M06/6-311+G(2d,p))= -132.705649929

Reactant phthalimide

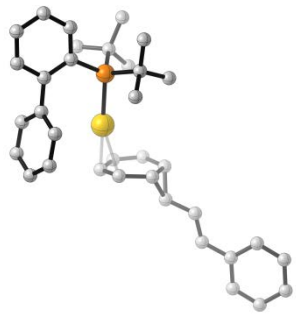


6	-3.723292000	-0.504295000	-0.005629000
1	-3.508602000	-1.567362000	-0.036504000
1	-4.763217000	-0.188396000	0.012081000
6	-2.773969000	0.429379000	0.012627000
1	-3.006620000	1.492953000	0.042446000
7	-1.388382000	0.212121000	-0.002197000
6	-0.477689000	1.294462000	-0.003420000
6	-0.711914000	-1.023759000	-0.001993000
6	0.871198000	0.692166000	-0.007414000
6	0.731279000	-0.692031000	-0.004057000
8	-0.796250000	2.461514000	-0.000333000
8	-1.232426000	-2.116782000	0.001327000
6	2.114548000	1.296847000	-0.003683000
1	2.213888000	2.380667000	-0.004224000
6	1.829134000	-1.531918000	0.002096000
1	1.710143000	-2.613779000	0.005718000
6	3.231468000	0.457556000	0.001769000
1	4.229216000	0.891998000	0.005642000
6	3.091055000	-0.932103000	0.005006000
1	3.982371000	-1.556607000	0.010458000

Zero-point correction= 0.148660
(Hartree/Particle)
Thermal correction to Energy= 0.158894
Thermal correction to Enthalpy= 0.159838
Thermal correction to Gibbs Free Energy= 0.112645
Sum of electronic and zero-point Energies= -589.953950
Sum of electronic and thermal Energies= -589.943716
Sum of electronic and thermal Enthalpies= -589.942771
Sum of electronic and thermal Free Energies= -589.989965

E(M06/6-311+G(2d,p))= -590.275558567

Intermediate II''

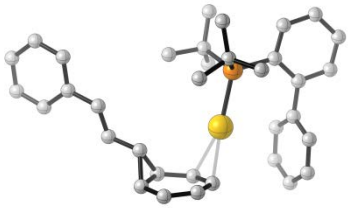


6	1.474512000	1.321287000	0.245915000
6	0.972932000	1.737663000	1.462880000
6	1.289169000	1.023216000	2.695113000
6	2.089271000	-0.061124000	2.676846000
1	1.276593000	1.903866000	-0.656101000
1	0.391174000	2.658729000	1.519318000
1	0.794675000	1.338577000	3.611749000
1	2.217705000	-0.661413000	3.576948000
79	-0.680094000	0.380987000	0.392538000
15	-2.402894000	-1.166089000	-0.069050000
6	-1.735597000	-2.314617000	-1.416141000
6	-2.809444000	-2.037080000	1.572391000
6	-3.975028000	-0.439336000	-0.685538000
6	-0.543308000	-3.088753000	-0.856239000
6	-1.252617000	-1.404374000	-2.547897000
6	-2.751964000	-3.296800000	-1.993121000
6	-3.496014000	-3.393921000	1.437038000
6	-3.702102000	-1.080449000	2.365163000
6	-1.507199000	-2.230945000	2.357624000
6	-5.063549000	-1.305783000	-0.882426000
6	-4.179642000	0.947387000	-0.858003000
1	-0.846261000	-3.850288000	-0.126501000
1	-0.044734000	-3.610830000	-1.686603000
1	0.199845000	-2.427403000	-0.385575000
1	-0.447801000	-0.727465000	-2.221510000
1	-0.856893000	-2.032926000	-3.359442000
1	-2.069195000	-0.798968000	-2.966252000
1	-2.234922000	-3.924373000	-2.734419000
1	-3.179688000	-3.967563000	-1.238309000
1	-3.570128000	-2.786101000	-2.515778000
1	-3.666628000	-3.793446000	2.447885000
1	-4.476527000	-3.335079000	0.950599000
1	-2.874984000	-4.123173000	0.901990000
1	-4.696497000	-0.959776000	1.917061000
1	-3.838865000	-1.488429000	3.377631000
1	-3.246732000	-0.083913000	2.472654000
1	-1.747564000	-2.726113000	3.310442000
1	-0.778596000	-2.862009000	1.832910000
1	-1.024607000	-1.271166000	2.592664000
6	-6.326147000	-0.835693000	-1.215127000
1	-4.930798000	-2.377702000	-0.764740000
6	-5.466986000	1.403640000	-1.174359000
6	-3.137131000	2.006777000	-0.764127000
6	-6.532266000	0.532115000	-1.349981000
1	-7.143647000	-1.539395000	-1.358612000
1	-5.618609000	2.475610000	-1.299192000
6	-2.209956000	2.190445000	-1.797105000
6	-3.168669000	2.929842000	0.287410000
1	-7.517764000	0.921288000	-1.599251000
6	-1.328217000	3.268472000	-1.773408000
1	-2.199362000	1.496156000	-2.638153000
6	-2.283389000	4.005312000	0.312939000
1	-3.907403000	2.807795000	1.080703000
6	-1.362215000	4.178204000	-0.718012000
1	-0.620987000	3.405855000	-2.590478000
1	-2.326706000	4.720348000	1.133303000
1	-0.682010000	5.028503000	-0.706573000
6	2.474840000	0.246014000	0.163761000
1	2.504262000	-0.327191000	-0.764016000
6	3.810413000	0.455760000	0.842050000
1	3.936236000	1.411659000	1.355994000
6	2.804153000	-0.488457000	1.468131000
1	3.056751000	-1.546269000	1.393396000
6	7.463307000	0.003188000	-0.323848000
6	8.592062000	0.834203000	-0.278623000
6	7.598162000	-1.261494000	-0.918041000
6	9.810583000	0.423928000	-0.807629000
1	8.501642000	1.818917000	0.182004000
6	8.814736000	-1.671789000	-1.446388000
1	6.745017000	-1.938536000	-0.958307000
6	9.927387000	-0.831777000	-1.396192000
1	10.672047000	1.088658000	-0.760792000
1	8.898897000	-2.658648000	-1.899820000
1	10.879979000	-1.159739000	-1.809071000
6	6.210779000	0.493935000	0.250659000
1	6.283014000	1.462468000	0.755163000
6	5.012686000	-0.108237000	0.220008000
1	4.879583000	-1.071709000	-0.282007000

Zero-point correction= 0.662826
(Hartree/Particle)
Thermal correction to Energy= 0.700129
Thermal correction to Enthalpy= 0.701073
Thermal correction to Gibbs Free Energy= 0.592965
Sum of electronic and zero-point Energies= -1833.630222
Sum of electronic and thermal Energies= -1833.592918
Sum of electronic and thermal Enthalpies= -1833.591974
Sum of electronic and thermal Free Energies= 1833.700082

E(M06/6-311+G(2d,p))= -1834.70465985

Intermediate II'

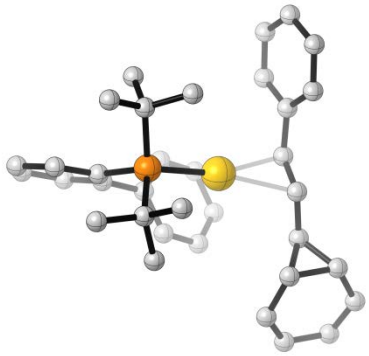


6	-0.479518000	-2.947177000	-0.591700000
6	-2.643360000	-1.870196000	0.406396000
6	0.303052000	-3.203022000	0.518618000
6	-1.941507000	-2.851502000	-0.497911000
6	-0.303801000	-3.517451000	1.802019000
6	-2.571854000	-3.314655000	0.839882000
6	-1.640163000	-3.675388000	1.907765000
1	-0.042420000	-3.060302000	-1.585135000
1	1.358158000	-3.449458000	0.375446000
1	-2.489086000	-3.098084000	-1.407200000
1	0.350733000	-3.773915000	2.632483000
1	-3.509891000	-3.867678000	0.786584000
1	-2.063551000	-4.108011000	2.813798000
1	-1.993956000	-1.185579000	0.961407000
6	-4.337516000	-0.073766000	0.243517000
1	-3.681261000	0.555457000	0.853867000
79	0.637023000	-0.922754000	0.085681000
15	1.133031000	1.386332000	0.286199000
6	-0.052149000	2.302394000	-0.869203000
6	0.938286000	1.834091000	2.124452000
6	2.839831000	1.871526000	-0.195154000
6	-1.476764000	2.032505000	-0.390348000
6	0.138943000	1.677170000	-2.251460000
6	0.175775000	3.807734000	-0.986219000
6	0.691166000	3.313192000	2.411590000
6	2.223558000	1.376262000	2.816541000
6	-0.230272000	1.031002000	2.704946000
6	3.202445000	3.220133000	-0.042088000
6	3.827069000	0.953121000	-0.615856000
1	-1.694098000	2.533051000	0.563374000
1	-2.188874000	2.417792000	-1.136423000
1	-1.670819000	0.955733000	-0.274292000
1	-0.098270000	0.602796000	-2.253679000
1	-0.541079000	2.172444000	-2.960415000
1	1.163336000	1.812253000	-2.626548000
1	-0.615350000	4.222331000	-1.628765000
1	0.122861000	4.329704000	-0.023081000
1	1.135129000	4.042877000	-1.463149000
1	0.637860000	3.445337000	3.502734000
1	1.493984000	3.966884000	2.050602000
1	-0.262666000	3.661901000	1.994954000
1	3.092716000	1.985350000	2.536494000
1	2.087316000	1.466159000	3.904376000
1	2.456003000	0.321934000	2.599702000
1	-0.328144000	1.282206000	3.771706000
1	-1.188749000	1.263847000	2.223112000
1	-0.059697000	-0.053347000	2.632265000
6	4.495579000	3.664795000	-0.279518000
1	2.459885000	3.946941000	0.275449000
6	5.130144000	1.420399000	-0.838373000
6	3.627866000	-0.502284000	-0.859351000
6	5.469357000	2.755656000	-0.675462000
1	4.737831000	4.717819000	-0.149726000
1	5.886584000	0.705473000	-1.160759000
6	2.961085000	-0.965184000	-2.000657000
6	4.240148000	-1.432932000	-0.012147000
1	6.490746000	3.083210000	-0.860776000
6	2.907131000	-2.328256000	-2.284583000
1	2.510144000	-0.246968000	-2.686472000
6	4.178327000	-2.796289000	-0.291506000
1	4.781614000	-1.077549000	0.865643000
6	3.513992000	-3.247220000	-1.430148000
1	2.401387000	-2.670881000	-3.186639000
1	4.665837000	-3.506560000	0.374626000
1	3.481664000	-4.311215000	-1.659816000
6	-3.925705000	-1.317310000	-0.044222000
1	-4.542669000	-1.985374000	-0.653207000
6	-5.580633000	0.565417000	-0.186824000
6	-6.596394000	-0.118067000	-0.873352000
6	-5.770946000	1.926178000	0.092662000
6	-7.753019000	0.540000000	-1.267767000
1	-6.482589000	-1.178753000	-1.096901000
6	-6.929131000	2.585983000	-0.303219000
1	-4.990530000	2.469116000	0.628762000
6	-7.926075000	1.895273000	-0.985953000
1	-8.530872000	-0.008654000	-1.797147000
1	-7.053679000	3.643784000	-0.075871000
1	-8.835506000	2.407735000	-1.295332000

Zero-point correction= 0.662806
(Hartree/Particle)
Thermal correction to Energy= 0.700150
Thermal correction to Enthalpy= 0.701094
Thermal correction to Gibbs Free Energy= 0.592739
Sum of electronic and zero-point Energies= -1833.632680
Sum of electronic and thermal Energies= -1833.595336
Sum of electronic and thermal Enthalpies= -1833.594392
Sum of electronic and thermal Free Energies= 1833.702747

E(M06/6-311+G(2d,p))= -1834.70716746

Intermediate II



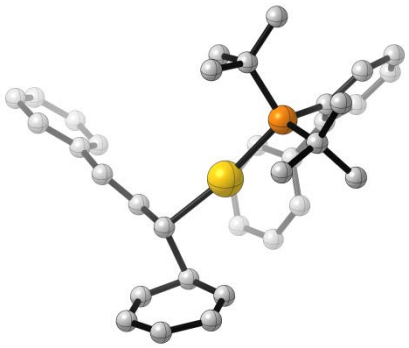
6	-0.601443000	0.783959000	-3.974596000
6	-1.951520000	-0.327689000	-2.096114000
6	-1.282674000	0.437940000	-5.087574000
6	-1.269299000	0.896897000	-2.675392000
6	-2.728755000	0.342297000	-5.083776000
6	-2.799512000	0.793444000	-2.669728000
6	-3.446129000	0.594612000	-3.969078000
1	0.463362000	1.014035000	-4.022100000
1	-0.758966000	0.333409000	-6.036897000
1	-0.809740000	1.550248000	-1.930279000
1	-3.238812000	0.170755000	-6.030738000
1	-3.338616000	1.381463000	-1.926467000
1	-4.531154000	0.679217000	-4.014027000
1	-1.888050000	-1.240038000	-2.693708000
6	-1.902189000	-1.735581000	-0.022826000
1	-1.865230000	-2.624909000	-0.662538000
79	0.321854000	-1.078440000	-0.000866000
15	2.581652000	-0.767201000	0.612795000
6	3.168746000	0.884966000	-0.089646000
6	2.623556000	-0.879196000	2.511926000
6	3.724853000	-2.067960000	-0.004103000
6	2.356485000	2.003984000	0.559822000
6	2.854143000	0.838075000	-1.586028000
6	4.659240000	1.173492000	0.080203000

6	3.847873000	-0.250843000	3.173139000
6	2.542986000	-2.367041000	2.860869000
6	1.374559000	-0.193954000	3.076047000
6	5.059657000	-2.020253000	0.431671000
6	3.309690000	-3.170083000	-0.784036000
1	2.633306000	2.159767000	1.610951000
1	2.560229000	2.943335000	0.024524000
1	1.273099000	1.817014000	0.506199000
1	1.778397000	0.705012000	-1.772863000
1	3.166372000	1.788391000	-2.044422000
1	3.397769000	0.030108000	-2.095979000
1	4.852921000	2.187755000	-0.299766000
1	4.987773000	1.146695000	1.126313000
1	5.282847000	0.486523000	-0.504986000
1	3.765936000	-0.401995000	4.259964000
1	4.794170000	-0.706609000	2.860043000
1	3.899196000	0.831958000	2.998807000
1	3.459996000	-2.914177000	2.608033000
1	2.383591000	-2.462817000	3.945117000
1	1.695616000	-2.862494000	2.360832000
1	1.395595000	-0.286301000	4.172246000
1	1.327768000	0.875425000	2.835485000
1	0.447990000	-0.669158000	2.721670000
6	5.964356000	-3.030861000	0.139183000
1	5.403398000	-1.176864000	1.024421000
6	4.234718000	-4.189019000	-1.052719000
6	1.963633000	-3.366927000	-1.391451000
6	5.544869000	-4.130629000	-0.599869000
1	6.989925000	-2.959268000	0.495977000
1	3.907656000	-5.039401000	-1.650498000
6	1.565472000	-2.632059000	-2.516370000
6	1.147274000	-4.412774000	-0.945245000
1	6.236062000	-4.939161000	-0.830437000
6	0.378394000	-2.938762000	-3.177277000
1	2.211794000	-1.837505000	-2.891821000
6	-0.043960000	-4.713322000	-1.602310000
1	1.460378000	-5.001276000	-0.081351000
6	-0.428541000	-3.980313000	-2.723011000
1	0.089057000	-2.365963000	-4.058370000
1	-0.664275000	-5.535772000	-1.248067000
1	-1.350780000	-4.224593000	-3.248692000
6	-1.935919000	-0.506183000	-0.646044000
1	-2.081056000	0.402127000	-0.050403000
6	-2.101290000	-1.997956000	1.414191000
6	-2.569104000	-1.027763000	2.311281000
6	-1.776276000	-3.270720000	1.905920000
6	-2.686480000	-1.320590000	3.664253000
1	-2.853160000	-0.039615000	1.950256000
6	-1.892343000	-3.560430000	3.260199000
1	-1.417975000	-4.030476000	1.208731000
6	-2.342658000	-2.583690000	4.145251000
1	-3.056806000	-0.559827000	4.349514000
1	-1.632265000	-4.552714000	3.625127000
1	-2.437284000	-2.808398000	5.206185000

Zero-point correction= 0.662232
(Hartree/Particle)
Thermal correction to Energy= 0.699592
Thermal correction to Enthalpy= 0.700537
Thermal correction to Gibbs Free Energy= 0.591961
Sum of electronic and zero-point Energies= -1833.637938
Sum of electronic and thermal Energies= -1833.600578
Sum of electronic and thermal Enthalpies= -1833.599634
Sum of electronic and thermal Free Energies= -1833.708210

E(M06/6-311+G(2d,p))= -1834.71086892

$TS_{II\text{-}III}$



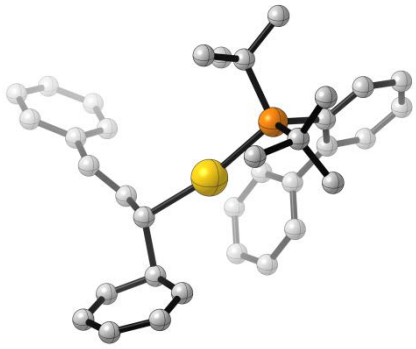
6	-0.896597000	3.551384000	1.187322000
6	-2.032609000	1.541778000	-0.049236000
6	-1.066756000	4.723453000	0.531888000
6	-1.965931000	2.551166000	1.234221000
6	-2.327633000	5.038854000	-0.074039000
6	-3.252783000	2.981663000	0.751301000
6	-3.399176000	4.194830000	0.041942000
1	0.049631000	3.316657000	1.677216000
1	-0.260053000	5.451718000	0.481744000
1	-1.953412000	1.889412000	2.105210000
1	-2.435460000	5.983364000	-0.604230000
1	-4.120856000	2.356514000	0.945872000
1	-4.368022000	4.456172000	-0.376293000
1	-2.123935000	2.050097000	-1.015701000
6	-3.454289000	-0.297910000	-0.925020000
1	-3.420864000	0.174370000	-1.912811000
79	-0.001472000	0.711080000	-0.185034000
15	2.127682000	-0.117024000	-0.802347000
6	1.815525000	-1.257276000	-2.284504000
6	3.229153000	1.383944000	-1.186904000
6	3.011926000	-1.164790000	0.427281000
6	1.206902000	-0.431953000	-3.417508000
6	0.788246000	-2.284209000	-1.799102000
6	3.034788000	-2.011881000	-2.808978000
6	4.399650000	1.118124000	-2.132093000
6	3.752576000	1.898428000	0.154973000
6	2.358069000	2.478481000	-1.811057000
6	4.300340000	-1.622103000	0.103489000
6	2.432326000	-1.598950000	1.638364000
1	1.934368000	0.256396000	-3.868963000
1	0.867967000	-1.116355000	-4.209885000
1	0.333138000	0.148724000	-3.085054000
1	-0.155030000	-1.814126000	-1.481091000
1	0.560356000	-2.975421000	-2.624262000
1	1.173648000	-2.883825000	-0.962001000
1	2.719624000	-2.602643000	-3.682311000
1	3.843800000	-1.348885000	-3.137728000
1	3.438384000	-2.716620000	-2.071281000
1	4.950446000	2.061081000	-2.269536000
1	5.117640000	0.385645000	-1.744668000
1	4.062977000	0.791455000	-3.124037000
1	4.449306000	1.197149000	0.631857000
1	4.291440000	2.842479000	-0.015992000
1	2.935232000	2.110820000	0.861967000
1	2.995157000	3.348902000	-2.028455000
1	1.893275000	2.165418000	-2.754001000
1	1.560423000	2.808754000	-1.130018000
6	5.002082000	-2.491136000	0.927181000
1	4.771366000	-1.301021000	-0.821481000
6	3.146349000	-2.496085000	2.445899000
6	1.114722000	-1.174623000	2.187170000
6	4.414663000	-2.941825000	2.103401000
1	6.000211000	-2.818245000	0.642175000
1	2.687023000	-2.832127000	3.375357000
6	0.055105000	-2.085843000	2.242034000
6	0.968360000	0.070559000	2.809723000
1	4.943975000	-3.632489000	2.757399000
6	-1.128217000	-1.758745000	2.900299000
1	0.172478000	-3.068322000	1.783178000

6	-0.211171000	0.393281000	3.477276000
1	1.802453000	0.773989000	2.798415000
6	-1.263823000	-0.519917000	3.522549000
1	-1.936772000	-2.487175000	2.949346000
1	-0.300358000	1.356090000	3.980503000
1	-2.180008000	-0.272121000	4.057472000
6	-2.846507000	0.335114000	0.101280000
1	-2.881730000	-0.091866000	1.109848000
6	-4.146739000	-1.579791000	-0.862523000
6	-4.113224000	-2.413336000	0.268452000
6	-4.895717000	-2.004463000	-1.971413000
6	-4.816253000	-3.609882000	0.291374000
1	-3.520203000	-2.123150000	1.136182000
6	-5.598140000	-3.203517000	-1.948280000
1	-4.925670000	-1.372641000	-2.860079000
6	-5.565761000	-4.011124000	-0.814485000
1	-4.777347000	-4.239992000	1.179138000
1	-6.175838000	-3.507126000	-2.820335000
1	-6.114458000	-4.951244000	-0.793458000

Zero-point correction= 0.659573
(Hartree/Particle)
Thermal correction to Energy= 0.697174
Thermal correction to Enthalpy= 0.698119
Thermal correction to Gibbs Free Energy= 0.589577
Sum of electronic and zero-point Energies= -1833.595693
Sum of electronic and thermal Energies= -1833.558091
Sum of electronic and thermal Enthalpies= -1833.557147
Sum of electronic and thermal Free Energies= -1833.665688

E(M06/6-311+G(2d,p))= -1834.66678314

Intermediate III

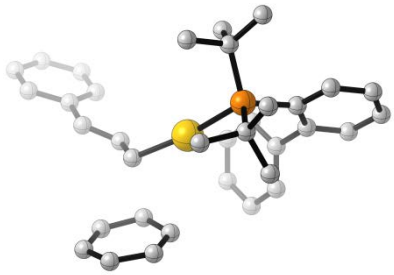


6	-1.328421000	3.564347000	0.649387000
6	-2.072015000	1.304170000	-0.258702000
6	-1.708418000	4.740027000	0.071400000
6	-2.282253000	2.489689000	0.885844000
6	-3.068061000	4.943557000	-0.259503000
6	-3.670930000	2.817988000	0.649036000
6	-4.045490000	3.995883000	0.031165000
1	-0.280200000	3.376913000	0.890646000
1	-0.981408000	5.520175000	-0.139207000
1	-2.093153000	1.929350000	1.813261000
1	-3.355158000	5.869889000	-0.755196000
1	-4.418148000	2.061385000	0.884797000
1	-5.085762000	4.185110000	-0.220538000
1	-2.364075000	1.731447000	-1.229637000
6	-3.535570000	-0.614692000	-0.854151000
1	-3.724001000	-0.148649000	-1.827150000
79	-0.020060000	0.681867000	-0.333194000
15	2.163173000	-0.150720000	-0.824497000
6	1.890707000	-1.539607000	-2.085566000
6	3.205321000	1.302021000	-1.472690000
6	3.116107000	-0.932283000	0.546006000
6	1.277214000	-0.933181000	-3.346002000
6	0.880026000	-2.492753000	-1.438531000
6	3.126499000	-2.349358000	-2.468848000
6	4.420677000	0.931287000	-2.318125000
6	3.650978000	2.085149000	-0.236236000
6	2.305283000	2.214032000	-2.313249000
6	4.407896000	-1.415115000	0.276735000
6	2.588672000	-1.124958000	1.839748000
1	2.002371000	-0.326707000	-3.905520000
1	0.950714000	-1.749015000	-4.008334000
1	0.396684000	-0.313145000	-3.121618000
1	-0.079164000	-1.998687000	-1.218887000
1	0.682101000	-3.322649000	-2.133658000
1	1.264442000	-2.928824000	-0.504720000
1	2.826006000	-3.091683000	-3.223682000
1	3.922742000	-1.738518000	-2.911610000
1	3.539823000	-2.902039000	-1.616446000
1	4.914486000	1.860935000	-2.639902000
1	5.170861000	0.349280000	-1.770118000
1	4.140711000	0.383470000	-3.227491000
1	4.346225000	1.517290000	0.395886000
1	4.165464000	3.001414000	-0.562110000
1	2.792922000	2.391668000	0.381953000
1	2.889081000	3.097653000	-2.612874000
1	1.949336000	1.728408000	-3.230221000
1	1.427489000	2.564480000	-1.750438000
6	5.161809000	-2.077678000	1.235485000
1	4.838417000	-1.281911000	-0.711687000
6	3.355182000	-1.815559000	2.789399000
6	1.275069000	-0.631570000	2.339977000
6	4.626663000	-2.288914000	2.500706000
1	6.160731000	-2.431593000	0.987759000
1	2.933499000	-1.963383000	3.783452000
6	0.220659000	-1.525072000	2.555475000
6	1.136437000	0.693755000	2.767446000
1	5.197745000	-2.814550000	3.263939000
6	-0.949036000	-1.102606000	3.183598000
1	0.329989000	-2.565471000	2.246012000
6	-0.030321000	1.114518000	3.401159000
1	1.965524000	1.389726000	2.630485000
6	-1.075289000	0.216521000	3.614149000
1	-1.755694000	-1.814009000	3.357275000
1	-0.115612000	2.144493000	3.747254000
1	-1.979888000	0.540306000	4.127739000
6	-2.808866000	0.074831000	0.051018000
1	-2.666542000	-0.334139000	1.058574000
6	-4.080288000	-1.955984000	-0.675591000
6	-3.599000000	-2.846609000	0.298696000
6	-5.118844000	-2.391798000	-1.513778000
6	-4.159722000	-4.108848000	0.446916000
1	-2.758081000	-2.551356000	0.928333000
6	-5.678705000	-3.654598000	-1.365102000
1	-5.492361000	-1.716201000	-2.284453000
6	-5.204791000	-4.518642000	-0.380458000
1	-3.768916000	-4.786712000	1.204893000
1	-6.488690000	-3.967764000	-2.022524000
1	-5.638453000	-5.510778000	-0.265322000

Zero-point correction= 0.660399
(Hartree/Particle)
Thermal correction to Energy= 0.698259
Thermal correction to Enthalpy= 0.699203
Thermal correction to Gibbs Free Energy= 0.589553
Sum of electronic and zero-point Energies= -1833.596387
Sum of electronic and thermal Energies= -1833.558526
Sum of electronic and thermal Enthalpies= -1833.557582
Sum of electronic and thermal Free Energies= -1833.667232

E(M06/6-311+G(2d,p))= -1834.66809433

$TS_{III\text{-}IV}$

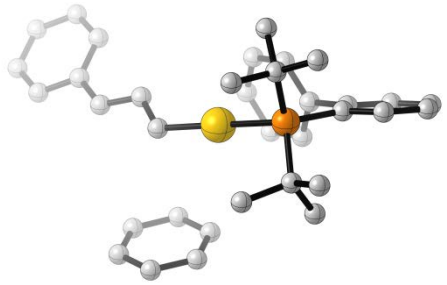


6	-0.658629000	3.073354000	1.159307000
6	-1.959279000	1.073249000	-0.261319000
6	-0.476160000	4.254668000	0.480158000
6	-1.937986000	2.437964000	1.181870000
6	-1.577075000	4.882091000	-0.129762000
6	-3.044758000	3.149753000	0.648723000
6	-2.857052000	4.345607000	-0.030551000
1	0.174000000	2.584805000	1.667350000
1	0.508185000	4.715735000	0.426464000
1	-2.109053000	1.689705000	1.958187000
1	-1.425698000	5.814083000	-0.672096000
1	-4.037139000	2.706617000	0.720261000
1	-3.702861000	4.857265000	-0.483707000
1	-2.232603000	1.701416000	-1.118931000
6	-4.103040000	-0.041640000	-0.664658000
1	-4.258118000	0.652510000	-1.497145000
79	0.024270000	0.384246000	-0.350139000
15	2.234446000	-0.360238000	-0.905434000
6	2.038547000	-1.708733000	-2.221200000
6	3.191121000	1.171262000	-1.514688000
6	3.271171000	-1.080810000	0.440616000
6	1.381378000	-1.088805000	-3.452714000
6	1.085380000	-2.740812000	-1.611883000
6	3.313356000	-2.435192000	-2.643617000
6	4.416836000	0.882390000	-2.377697000
6	3.610187000	1.944364000	-0.262577000
6	2.241052000	2.059448000	-2.324170000
6	4.587004000	-1.464918000	0.131425000
6	2.853616000	-1.155609000	1.787907000
1	2.068610000	-0.429516000	-3.999191000
1	1.085623000	-1.897226000	-4.138041000
1	0.475910000	-0.519016000	-3.197377000
1	0.104318000	-2.304909000	-1.371919000
1	0.927429000	-3.550862000	-2.339811000
1	1.499754000	-3.193125000	-0.699019000
1	3.052481000	-3.137989000	-3.449328000
1	4.086417000	-1.762616000	-3.034886000
1	3.742340000	-3.026670000	-1.825633000
1	4.861922000	1.842166000	-2.681377000
1	5.197725000	0.323770000	-1.847721000
1	4.154901000	0.342134000	-3.296923000
1	4.364452000	1.412143000	0.331565000
1	4.046677000	2.905791000	-0.572442000
1	2.751441000	2.170287000	0.389421000
1	2.778503000	2.979259000	-2.600238000
1	1.904133000	1.584560000	-3.253649000
1	1.350493000	2.349595000	-1.747799000
6	5.478048000	-1.895829000	1.104620000
1	4.933683000	-1.425290000	-0.896794000
6	3.773579000	-1.576384000	2.759457000
6	1.492987000	-0.846442000	2.303315000
6	5.070713000	-1.942586000	2.432643000
1	6.488637000	-2.185184000	0.822586000
1	3.441816000	-1.627245000	3.796261000
6	0.406901000	-1.688073000	2.035268000
6	1.315433000	0.219194000	3.192643000
1	5.756990000	-2.270031000	3.211623000
6	-0.823850000	-1.471209000	2.649049000
1	0.538401000	-2.536200000	1.362845000
6	0.079630000	0.445789000	3.794189000
1	2.163030000	0.866257000	3.423180000
6	-0.992346000	-0.403371000	3.528659000
1	-1.650810000	-2.151887000	2.448334000
1	-0.040023000	1.277811000	4.487038000
1	-1.953988000	-0.241826000	4.014853000
6	-3.001868000	0.140172000	0.103895000
1	-2.826542000	-0.495363000	0.976925000
6	-5.107619000	-1.084266000	-0.530355000
6	-5.018982000	-2.116788000	0.419134000
6	-6.222165000	-1.055063000	-1.383590000
6	-6.020617000	-3.070366000	0.519986000
1	-4.155557000	-2.173406000	1.080720000
6	-7.224538000	-2.011327000	-1.282107000
1	-6.295610000	-0.263355000	-2.129975000
6	-7.126860000	-3.022064000	-0.329376000
1	-5.937338000	-3.862747000	1.262119000
1	-8.082939000	-1.971557000	-1.950549000
1	-7.908328000	-3.775811000	-0.248327000

Zero-point correction= 0.660286
(Hartree/Particle)
Thermal correction to Energy= 0.697870
Thermal correction to Enthalpy= 0.698815
Thermal correction to Gibbs Free Energy= 0.588737
Sum of electronic and zero-point Energies= -1833.593628
Sum of electronic and thermal Energies= -1833.556044
Sum of electronic and thermal Enthalpies= -1833.555100
Sum of electronic and thermal Free Energies= -1833.665178

E(M06/6-311+G(2d,p))= -1834.66501576

Intermediate IV



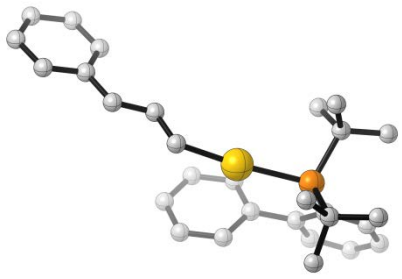
6	-1.044512000	2.500051000	2.278574000
6	-1.865176000	0.647254000	-0.692270000
6	-0.624661000	3.648701000	1.609093000
6	-2.393152000	2.147079000	2.277271000
6	-1.551439000	4.437699000	0.930023000
6	-3.321762000	2.944625000	1.610474000
6	-2.901001000	4.087338000	0.933278000
1	-0.322583000	1.881032000	2.812696000
1	0.427197000	3.934536000	1.619469000
1	-2.720169000	1.248455000	2.801555000
1	-1.223577000	5.335389000	0.407588000
1	-4.377697000	2.675538000	1.622917000
1	-3.626541000	4.712029000	0.413925000
1	-2.224990000	1.683851000	-0.762146000
6	-4.212215000	0.131911000	-0.769387000
1	-4.376261000	1.212989000	-0.828367000
79	0.141986000	0.291584000	-0.590101000
15	2.542428000	0.040473000	-0.733013000
6	2.918862000	-0.711060000	-2.429960000
6	3.291124000	1.770656000	-0.476885000
6	3.369381000	-1.039823000	0.513000000
6	2.427879000	0.257985000	-3.505472000
6	2.094628000	-1.999147000	-2.500133000
6	4.380876000	-1.060127000	-2.696481000
6	4.690468000	1.992534000	-1.045102000
6	3.303725000	2.008199000	1.035563000
6	2.352320000	2.800057000	-1.114910000

6	4.771772000	-1.126717000	0.496225000
6	2.673098000	-1.688604000	1.555225000
1	3.047714000	1.163053000	-3.562237000
1	2.486373000	-0.241032000	-4.484617000
1	1.382044000	0.559537000	-3.346657000
1	1.016825000	-1.805255000	-2.394329000
1	2.258127000	-2.476168000	-3.478545000
1	2.392936000	-2.721778000	-1.726639000
1	4.460918000	-1.439408000	-3.726534000
1	5.051674000	-0.196072000	-2.613215000
1	4.745513000	-1.852839000	-2.031679000
1	5.003999000	3.018659000	-0.798602000
1	5.444383000	1.319380000	-0.620714000
1	4.710539000	1.901730000	-2.138861000
1	4.077163000	1.420075000	1.546158000
1	3.511966000	3.071898000	1.226148000
1	2.334079000	1.771411000	1.500261000
1	2.759530000	3.805938000	-0.930146000
1	2.261710000	2.676108000	-2.201249000
1	1.341578000	2.760993000	-0.684309000
6	5.479796000	-1.807891000	1.476712000
1	5.332046000	-0.639928000	-0.297087000
6	3.405478000	-2.357477000	2.546066000
6	1.194297000	-1.755385000	1.707456000
6	4.791042000	-2.420353000	2.517124000
1	6.566227000	-1.850331000	1.428276000
1	2.857708000	-2.850546000	3.348944000
6	0.425765000	-2.600088000	0.897889000
6	0.571874000	-1.083875000	2.764522000
1	5.328261000	-2.949885000	3.301982000
6	-0.935050000	-2.766201000	1.140789000
1	0.909095000	-3.145857000	0.086506000
6	-0.792741000	-1.238733000	2.998227000
1	1.171120000	-0.443442000	3.413661000
6	-1.548722000	-2.084386000	2.190281000
1	-1.516742000	-3.440994000	0.512608000
1	-1.262411000	-0.710517000	3.827681000
1	-2.613979000	-2.216637000	2.379304000
6	-2.890973000	-0.288072000	-0.700900000
1	-2.659173000	-1.351968000	-0.636324000
6	-5.386353000	-0.675953000	-0.759735000
6	-5.344148000	-2.085297000	-0.669710000
6	-6.638035000	-0.028290000	-0.834890000
6	-6.518882000	-2.812491000	-0.660742000
1	-4.386870000	-2.599946000	-0.605646000
6	-7.810754000	-0.762531000	-0.825423000
1	-6.665860000	1.058521000	-0.902507000
6	-7.750093000	-2.153181000	-0.738605000
1	-6.487362000	-3.897486000	-0.591999000
1	-8.773298000	-0.259883000	-0.885864000
1	-8.670833000	-2.733788000	-0.731336000

Zero-point correction= 0.660111
(Hartree/Particle)
Thermal correction to Energy= 0.698786
Thermal correction to Enthalpy= 0.699730
Thermal correction to Gibbs Free Energy= 0.587937
Sum of electronic and zero-point Energies= -1833.615261
Sum of electronic and thermal Energies= -1833.576586
Sum of electronic and thermal Enthalpies= -1833.575642
Sum of electronic and thermal Free Energies= -1833.687435

E(M06/6-311+G(2d,p))= -1834.68832615

Intermediate V



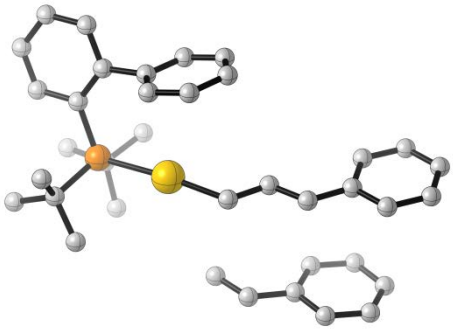
79	-1.343559000	0.389961000	0.642414000
15	-3.296393000	1.724974000	0.151321000
6	-2.929957000	2.618611000	-1.479030000
6	-4.800671000	0.567206000	0.070414000
6	0.293519000	-0.815880000	0.820857000
1	0.170717000	-1.878091000	1.076860000
6	1.618703000	-0.440543000	0.658714000
1	1.867427000	0.588689000	0.393654000
6	2.635471000	-1.368256000	0.856838000
1	2.324117000	-2.384300000	1.117761000
6	4.041227000	-1.155921000	0.772243000
6	4.894407000	-2.252951000	1.023823000
6	4.607672000	0.100115000	0.456370000
6	6.268400000	-2.101995000	0.963551000
1	4.451744000	-3.218621000	1.265467000
6	5.980219000	0.242965000	0.396871000
1	3.966407000	0.956555000	0.258775000
6	6.808960000	-0.854487000	0.651456000
1	6.922252000	-2.948346000	1.160191000
1	6.418276000	1.208475000	0.154320000
1	7.889506000	-0.732470000	0.604208000
6	-3.697780000	3.076618000	1.340372000
6	-4.850464000	3.849649000	1.119917000
6	-2.854212000	3.427863000	2.416258000
6	-5.167279000	4.942887000	1.914249000
1	-5.519678000	3.604320000	0.299494000
6	-3.177963000	4.549413000	3.193504000
6	-4.317494000	5.303238000	2.953357000
1	-6.071537000	5.513593000	1.711066000
1	-2.516841000	4.815739000	4.017907000
1	-4.544253000	6.164496000	3.579331000
6	-1.629600000	2.699649000	2.846756000
6	-0.372546000	3.293730000	2.693097000
6	-1.725136000	1.495364000	3.554100000
6	0.763932000	2.699284000	3.236323000
1	-0.292772000	4.244167000	2.164098000
6	-0.589186000	0.906225000	4.106855000
1	-2.705423000	1.040880000	3.704121000
6	0.657018000	1.509445000	3.952595000
1	1.733707000	3.180687000	3.117040000
1	-0.683457000	-0.020320000	4.671701000
1	1.542471000	1.056083000	4.395850000
6	-5.996034000	1.080945000	-0.727395000
1	-6.777030000	0.305425000	-0.715332000
1	-6.445655000	1.987997000	-0.306306000
1	-5.741303000	1.269237000	-1.778302000
6	-5.217231000	0.299110000	1.517682000
1	-5.603902000	1.196851000	2.017262000
1	-6.015879000	-0.457577000	1.521343000
1	-4.384582000	-0.098815000	2.117292000
6	-4.353669000	-0.759384000	-0.551955000
1	-5.204208000	-1.457532000	-0.532831000
1	-4.040769000	-0.652491000	-1.597877000
1	-3.527125000	-1.222229000	0.005579000
6	-2.744384000	1.569738000	-2.573854000
1	-3.691670000	1.084919000	-2.845963000
1	-2.356961000	2.064024000	-3.477463000
1	-2.023718000	0.790800000	-2.284634000
6	-1.605312000	3.351354000	-1.247724000

1	-0.789624000	2.660357000	-0.986301000
1	-1.321220000	3.878546000	-2.171215000
1	-1.687955000	4.103862000	-0.450011000
6	-3.967670000	3.642693000	-1.932165000
1	-3.645447000	4.048665000	-2.903070000
1	-4.965929000	3.211478000	-2.073645000
1	-4.047425000	4.488326000	-1.238150000

Zero-point correction= 0.559400
(Hartree/Particle)
Thermal correction to Energy= 0.591765
Thermal correction to Enthalpy= 0.592709
Thermal correction to Gibbs Free Energy= 0.494791
Sum of electronic and zero-point Energies= -1601.648822
Sum of electronic and thermal Energies= -1601.616457
Sum of electronic and thermal Enthalpies= -1601.615513
Sum of electronic and thermal Free Energies= -1601.713432

E(M06/6-311+G(2d,p))= -1602.55313656

Intermediate *c*-VIa

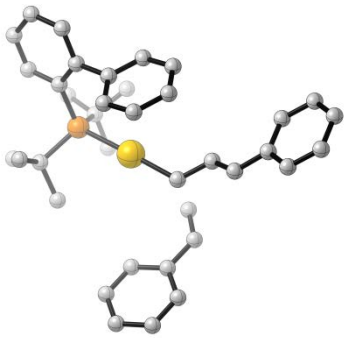


79	0.615878000	-0.297551000	-0.459985000
15	2.901623000	-0.767970000	0.167115000
6	2.824108000	-1.477126000	1.923721000
6	3.633924000	-1.967295000	-1.113151000
6	-1.360452000	-0.091657000	-0.953506000
1	-1.712709000	-0.443128000	-1.933444000
6	-1.750739000	-2.913447000	-0.087522000
1	-1.619506000	-2.574351000	0.940866000
1	-0.864867000	-3.305184000	-0.584994000
6	-4.210513000	-2.440950000	-0.161831000
6	-5.350418000	-2.472304000	-0.981394000
6	-4.346154000	-1.947310000	1.147522000
6	-6.581822000	-2.031549000	-0.513102000
1	-5.257499000	-2.857772000	-1.997577000
6	-5.577219000	-1.512181000	1.617452000
1	-3.478192000	-1.910829000	1.805691000
6	-6.698924000	-1.547486000	0.788637000
1	-7.454328000	-2.065487000	-1.163936000
1	-5.664757000	-1.133748000	2.635075000
1	-7.662591000	-1.200301000	1.158424000
6	-2.942093000	-2.915358000	-0.705647000
1	-2.994449000	-3.291525000	-1.730930000
6	-2.347678000	0.533771000	-0.199383000
1	-2.111918000	0.915128000	0.796726000
6	-3.622651000	0.705977000	-0.718089000
1	-3.802812000	0.300605000	-1.719181000
6	-4.729307000	1.386632000	-0.120667000
6	-5.927959000	1.478586000	-0.856135000
6	-4.679509000	1.932079000	1.180286000
6	-7.041526000	2.102963000	-0.316026000
1	-5.963605000	1.052002000	-1.858353000
6	-5.795089000	2.547712000	1.716677000
1	-3.765059000	1.865181000	1.767318000
6	-6.974489000	2.634766000	0.970078000
1	-7.961701000	2.173303000	-0.891830000
1	-5.756506000	2.965139000	2.720581000
1	-7.847781000	3.122182000	1.399700000
6	4.056995000	0.664212000	0.298893000
6	5.397629000	0.418337000	0.642481000
6	3.643497000	2.005213000	0.148835000
6	6.306155000	1.446493000	0.851514000
1	5.748808000	-0.602601000	0.764217000
6	4.569156000	3.031577000	0.386672000
6	5.885472000	2.765976000	0.734717000
1	7.335895000	1.211154000	1.113976000
1	4.236351000	4.063309000	0.275175000
1	6.580934000	3.585589000	0.906683000
6	2.293165000	2.467650000	-0.274898000
6	1.449632000	3.100784000	0.643846000
6	1.918473000	2.431095000	-1.622861000
6	0.256725000	3.685335000	0.224829000
1	1.748369000	3.158297000	1.691344000
6	0.727842000	3.020847000	-2.042607000
1	2.584308000	1.963145000	-2.349291000
6	-0.102699000	3.654252000	-1.120604000
1	-0.383092000	4.186075000	0.950443000
1	0.457912000	2.999380000	-3.097597000
1	-1.024971000	4.129634000	-1.451551000
6	4.819389000	-2.804210000	-0.640661000
1	5.122419000	-3.468913000	-1.464014000
1	5.699522000	-2.205620000	-0.377983000
1	4.559326000	-3.442489000	0.213822000
6	4.041855000	-1.116396000	-2.316951000
1	4.873847000	-0.437445000	-2.089240000
1	4.366251000	-1.783762000	-3.129280000
1	3.200867000	-0.517704000	-2.698535000
6	2.528998000	-2.929395000	-1.560789000
1	2.931063000	-3.577409000	-2.354325000
1	2.184078000	-3.582286000	-0.749293000
1	1.657696000	-2.399300000	-1.971196000
6	2.008910000	-2.768093000	1.886553000
1	2.546264000	-3.582465000	1.382435000
1	1.812480000	-3.093899000	2.919144000
1	1.037412000	-2.629482000	1.390213000
6	2.071860000	-0.426972000	2.746418000
1	1.063669000	-0.234858000	2.348811000
1	1.966680000	-0.789165000	3.780509000
1	2.613836000	0.529148000	2.784727000
6	4.161595000	-1.749471000	2.607716000
1	3.954998000	-2.191193000	3.594450000
1	4.792011000	-2.459470000	2.058749000
1	4.735777000	-0.831161000	2.779386000

Zero-point correction= 0.693875
(Hartree/Particle)
Thermal correction to Energy= 0.734397
Thermal correction to Enthalpy= 0.735342
Thermal correction to Gibbs Free Energy= 0.619721
Sum of electronic and zero-point Energies= -1910.923046
Sum of electronic and thermal Energies= -1910.882523
Sum of electronic and thermal Enthalpies= -1910.881579
Sum of electronic and thermal Free Energies= -1910.997200

E(M06/6-311+G(2d,p))= - -1912.05193883

Intermediate *t*-VIa



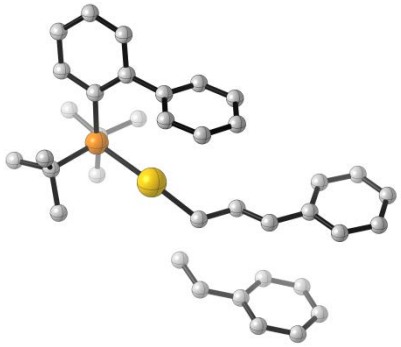
79	-0.014779000	0.124418000	-0.191625000
15	-2.368324000	-0.310259000	0.126883000
6	-2.743517000	0.233543000	1.904096000

6	-3.335663000	0.664296000	-1.185568000
6	1.939946000	0.663283000	-0.407002000
1	2.195259000	1.528165000	-1.036624000
6	1.416378000	2.770581000	2.259774000
1	2.241968000	2.252829000	2.745876000
1	0.443374000	2.699933000	2.748723000
6	1.601283000	3.454250000	1.124223000
6	3.055276000	0.017006000	0.113527000
1	2.930520000	-0.848748000	0.765985000
6	4.326514000	0.410699000	-0.274956000
1	4.390790000	1.302169000	-0.907519000
6	5.564142000	-0.234866000	0.022339000
6	6.750686000	0.323689000	-0.497281000
6	5.639972000	-1.411761000	0.799677000
6	7.975264000	-0.271465000	-0.248055000
1	6.688638000	1.230269000	-1.098315000
6	6.865670000	-2.000619000	1.045388000
1	4.732305000	-1.857148000	1.202938000
6	8.031401000	-1.432776000	0.522144000
1	8.887728000	0.161754000	-0.651318000
1	6.923553000	-2.907623000	1.642959000
1	8.992821000	-1.905142000	0.716269000
6	-2.934855000	-2.064694000	0.040521000
6	-4.296189000	-2.341315000	0.254230000
6	-2.055578000	-3.154833000	-0.145193000
6	-4.786819000	-3.638939000	0.307866000
1	-4.999951000	-1.526826000	0.403370000
6	-2.564774000	-4.458811000	-0.058062000
6	-3.910651000	-4.708162000	0.165177000
1	-5.849240000	-3.808760000	0.472229000
1	-1.874751000	-5.291320000	-0.193356000
1	-4.273516000	-5.733102000	0.217512000
6	-0.605588000	-3.066341000	-0.468466000
6	0.343702000	-3.542765000	0.442061000
6	-0.175945000	-2.645735000	-1.732393000
6	1.692955000	-3.591324000	0.100162000
1	0.012908000	-3.892578000	1.420927000
6	1.172804000	-2.701314000	-2.077193000
1	-0.912640000	-2.295505000	-2.456729000
6	2.110560000	-3.174099000	-1.161626000
1	2.417539000	-3.972656000	0.819089000
1	1.488735000	-2.381227000	-3.069393000
1	3.165410000	-3.217971000	-1.431485000
6	-4.788493000	0.974212000	-0.837557000
1	-5.238122000	1.521644000	-1.680063000
1	-5.397158000	0.076026000	-0.680671000
1	-4.872859000	1.616640000	0.048700000
6	-3.274735000	-0.161742000	-2.470715000
1	-3.826789000	-1.107421000	-2.391561000
1	-3.723904000	0.421036000	-3.288762000
1	-2.237830000	-0.389325000	-2.760007000
6	-2.607864000	1.988863000	-1.436105000
1	-3.144122000	2.541347000	-2.223220000
1	-2.573120000	2.631814000	-0.547367000
1	-1.575843000	1.832322000	-1.781263000
6	-2.467962000	1.733520000	2.015587000
1	-3.241982000	2.336295000	1.519992000
1	-2.464243000	2.015267000	3.080511000
1	-1.490322000	2.010283000	1.593713000
6	-1.740380000	-0.527183000	2.776640000
1	-0.699290000	-0.269810000	2.528969000
1	-1.914991000	-0.268200000	3.832067000
1	-1.855716000	-1.617008000	2.680797000
6	-4.148692000	-0.057178000	2.425789000
1	-4.240431000	0.388432000	3.428121000
1	-4.940625000	0.375784000	1.802776000
1	-4.336811000	-1.131936000	2.534601000
6	0.574308000	4.185022000	0.374573000
6	-0.634195000	4.598476000	0.954696000
6	0.798134000	4.476083000	-0.977959000
6	-1.594403000	5.257685000	0.196799000
1	-0.814680000	4.418778000	2.014779000
6	-0.165950000	5.129032000	-1.739316000
1	1.744861000	4.181053000	-1.433572000
6	-1.367423000	5.520133000	-1.154263000
1	-2.524576000	5.577274000	0.665311000
1	0.026672000	5.342230000	-2.789758000
1	-2.121167000	6.039139000	-1.744256000
1	2.598115000	3.459987000	0.672810000

Zero-point correction= 0.694799
(Hartree/Particle)
Thermal correction to Energy= 0.735242
Thermal correction to Enthalpy= 0.736186
Thermal correction to Gibbs Free Energy= 0.620165
Sum of electronic and zero-point Energies= -1910.919075
Sum of electronic and thermal Energies= -1910.878632
Sum of electronic and thermal Enthalpies= -1910.877688
Sum of electronic and thermal Free Energies= -1910.993709

E(M06/6-311+G(2d,p))= -1912.04940280

Transition state $TS_{c\text{-(VIa-VIIa)}}$



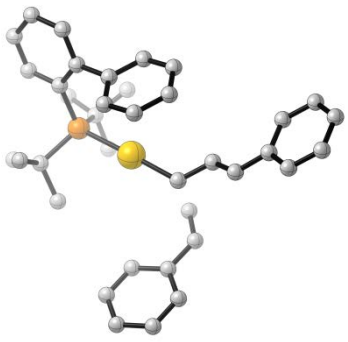
79	-1.424985000	0.268381000	0.185890000
15	-3.333162000	1.712268000	0.054745000
6	-3.073270000	2.758612000	-1.504108000
6	-4.894368000	0.621724000	-0.007617000
6	0.221859000	-0.999442000	0.149643000
1	0.135154000	-2.005971000	0.578352000
6	-0.119506000	-1.600221000	-2.011054000
1	0.339816000	-0.701126000	-2.421489000
1	-1.207191000	-1.623286000	-2.023501000
6	1.996713000	-2.954249000	-1.884917000
6	2.531382000	-4.170790000	-1.418921000
6	2.885357000	-1.963075000	-2.344579000
6	3.900180000	-4.388222000	-1.406986000
1	1.848948000	-4.941817000	-1.060254000
6	4.254681000	-2.187694000	-2.343054000
1	2.497749000	-1.016916000	-2.720658000
6	4.765505000	-3.394491000	-1.867393000
1	4.298039000	-5.332011000	-1.038497000
1	4.931173000	-1.413156000	-2.700855000
1	5.841144000	-3.563022000	-1.857834000
6	0.568877000	-2.763792000	-1.820423000
1	-0.005596000	-3.641470000	-1.513131000
6	1.545359000	-0.491603000	0.148300000
1	1.718669000	0.508119000	-0.259814000
6	2.585333000	-1.205750000	0.676944000
1	2.363896000	-2.218037000	1.030704000
6	3.954723000	-0.775547000	0.841029000
6	4.900630000	-1.714076000	1.288238000
6	4.388654000	0.525220000	0.523942000
6	6.241161000	-1.370985000	1.405111000
1	4.568784000	-2.722828000	1.535351000
6	5.725940000	0.865022000	0.645375000
1	3.672011000	1.271916000	0.184867000
6	6.655325000	-0.081064000	1.084304000
1	6.963218000	-2.107994000	1.751451000
1	6.051591000	1.874186000	0.399519000
1	7.704973000	0.192596000	1.176923000
6	-3.573382000	2.947124000	1.403474000
6	-4.739086000	3.730052000	1.380712000
6	-2.613294000	3.206441000	2.405902000
6	-4.963221000	4.748531000	2.296632000
1	-5.495684000	3.546442000	0.622546000
6	-2.844930000	4.256736000	3.306478000

6	-4.000964000	5.022039000	3.261810000
1	-5.883160000	5.328068000	2.248902000
1	-2.094575000	4.452251000	4.072184000
1	-4.151272000	5.822100000	3.984484000
6	-1.352481000	2.446943000	2.632376000
6	-0.116372000	3.063235000	2.411282000
6	-1.375648000	1.167023000	3.199719000
6	1.070382000	2.411721000	2.739093000
1	-0.089144000	4.069899000	1.992482000
6	-0.189379000	0.523388000	3.544956000
1	-2.335311000	0.685551000	3.393035000
6	1.036603000	1.144555000	3.316245000
1	2.023907000	2.909925000	2.568315000
1	-0.225919000	-0.465009000	4.001685000
1	1.963554000	0.643089000	3.591633000
6	-6.105673000	1.210311000	-0.727532000
1	-6.926246000	0.478789000	-0.670289000
1	-6.476948000	2.138508000	-0.278310000
1	-5.908260000	1.391210000	-1.791952000
6	-5.257020000	0.298245000	1.442914000
1	-5.623789000	1.175431000	1.990719000
1	-6.054990000	-0.459164000	1.447689000
1	-4.402841000	-0.120198000	1.996802000
6	-4.527200000	-0.691237000	-0.709616000
1	-5.414504000	-1.342303000	-0.718519000
1	-4.217994000	-0.544101000	-1.753057000
1	-3.722922000	-1.227483000	-0.186235000
6	-2.993860000	1.819565000	-2.707048000
1	-3.960829000	1.352299000	-2.935807000
1	-2.692468000	2.400062000	-3.592167000
1	-2.246958000	1.024374000	-2.560502000
6	-1.717780000	3.444797000	-1.315665000
1	-0.901217000	2.717802000	-1.187504000
1	-1.496314000	4.049371000	-2.208204000
1	-1.715200000	4.121644000	-0.449122000
6	-4.124063000	3.833596000	-1.763808000
1	-3.866990000	4.349494000	-2.701361000
1	-5.134645000	3.424986000	-1.879774000
1	-4.142097000	4.591450000	-0.970796000

Zero-point correction= 0.694297
(Hartree/Particle)
Thermal correction to Energy= 0.733708
Thermal correction to Enthalpy= 0.734652
Thermal correction to Gibbs Free Energy= 0.621923
Sum of electronic and zero-point Energies= -1910.919092
Sum of electronic and thermal Energies= -1910.879680
Sum of electronic and thermal Enthalpies= -1910.878736
Sum of electronic and thermal Free Energies= -1910.991465

E(M06/6-311+G(2d,p))= -1912.04773405
E(PBE/6-311+G(2d,p))= -1911.144414
E(PBE-D3(BJ)/6-311+G(2d,p))= -1911.28439877

Transition state $TS_{t\text{-(VIa-VIIa)}}$



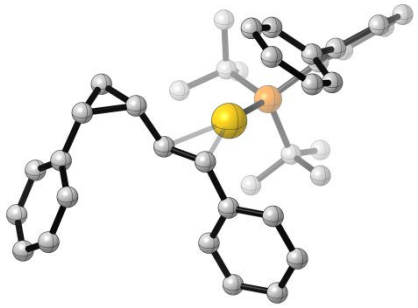
79	-0.194591000	0.294931000	0.168721000
15	-2.582289000	0.046300000	0.301386000
6	-2.970497000	-0.065158000	2.153918000
6	-3.395688000	1.533274000	-0.558929000
6	1.857242000	0.598924000	0.135266000
1	2.246620000	1.257104000	-0.652564000
6	1.743296000	2.114540000	1.867457000
1	2.137480000	1.405154000	2.591840000
1	0.683667000	2.348184000	1.957305000
6	2.580093000	2.857193000	1.094422000
6	2.818109000	-0.336619000	0.615906000
1	2.522395000	-1.028267000	1.408460000
6	4.034050000	-0.454408000	0.010552000
1	4.279451000	0.288277000	-0.755810000
6	5.036318000	-1.475690000	0.222941000
6	6.217660000	-1.416069000	-0.536230000
6	4.881142000	-2.523264000	1.150224000
6	7.217378000	-2.364579000	-0.372307000
1	6.339665000	-0.610960000	-1.261209000
6	5.882647000	-3.466754000	1.313824000
1	3.971756000	-2.598358000	1.744531000
6	7.052063000	-3.390634000	0.554822000
1	8.126815000	-2.306651000	-0.967252000
1	5.754463000	-4.270232000	2.036810000
1	7.833177000	-4.137464000	0.686467000
6	-3.327703000	-1.482406000	-0.409794000
6	-4.725710000	-1.618687000	-0.378270000
6	-2.561456000	-2.566814000	-0.889535000
6	-5.362090000	-2.786009000	-0.776765000
1	-5.341983000	-0.796366000	-0.024003000
6	-3.219661000	-3.748990000	-1.258126000
6	-4.600747000	-3.867659000	-1.203942000
1	-6.447909000	-2.849943000	-0.740721000
1	-2.617142000	-4.584199000	-1.614548000
1	-5.079828000	-4.797589000	-1.505215000
6	-1.086203000	-2.577351000	-1.085897000
6	-0.277919000	-3.403178000	-0.298185000
6	-0.505952000	-1.886223000	-2.156266000
6	1.082327000	-3.531290000	-0.569535000
1	-0.728429000	-3.963244000	0.522396000
6	0.852255000	-2.022946000	-2.434090000
1	-1.134640000	-1.262160000	-2.793353000
6	1.648774000	-2.848093000	-1.643191000
1	1.696343000	-4.185648000	0.048046000
1	1.285976000	-1.493831000	-3.281873000
1	2.707460000	-2.967146000	-1.870171000
6	-4.785565000	1.923211000	-0.061863000
1	-5.131275000	2.784637000	-0.653469000
1	-5.534788000	1.132139000	-0.184246000
1	-4.775640000	2.236299000	0.989874000
6	-3.449790000	1.197835000	-2.049794000
1	-4.179558000	0.409909000	-2.275537000
1	-3.745144000	2.098975000	-2.607731000
1	-2.468709000	0.879571000	-2.433505000
6	-2.472481000	2.741919000	-0.375052000
1	-2.925772000	3.609459000	-0.879105000
1	-2.331055000	3.008838000	0.681293000
1	-1.483091000	2.569866000	-0.823139000
6	-2.485785000	1.217377000	2.828968000
1	-3.093120000	2.090169000	2.553141000
1	-2.564368000	1.095552000	3.919896000
1	-1.432293000	1.435935000	2.595874000
6	-2.145875000	-1.247759000	2.669712000
1	-1.069192000	-1.111594000	2.485855000
1	-2.296528000	-1.342743000	3.755674000
1	-2.456470000	-2.195830000	2.207323000
6	-4.432976000	-0.303726000	2.520812000
1	-4.512912000	-0.318113000	3.618268000
1	-5.104031000	0.482424000	2.154498000
1	-4.798964000	-1.271943000	2.158000000
6	2.192289000	3.915704000	0.178757000
6	0.852755000	4.294603000	-0.011888000
6	3.188455000	4.560422000	-0.571107000
6	0.524825000	5.282004000	-0.929073000
1	0.062370000	3.810123000	0.561343000
6	2.859160000	5.556688000	-1.481105000
1	4.229696000	4.269744000	-0.426960000
6	1.526263000	5.917541000	-1.664629000
1	-0.518588000	5.560452000	-1.070758000
1	3.643345000	6.051997000	-2.050740000
1	1.265650000	6.695260000	-2.380321000

1	3.646090000	2.616606000	1.113553000

Zero-point correction= 0.695008
(Hartree/Particle)
Thermal correction to Energy= 0.734448
Thermal correction to Enthalpy= 0.735392
Thermal correction to Gibbs Free Energy= 0.622012
Sum of electronic and zero-point Energies= -1910.913301
Sum of electronic and thermal Energies= -1910.873862
Sum of electronic and thermal Enthalpies= -1910.872917
Sum of electronic and thermal Free Energies= -1910.986297

E(M06/6-311+G(2d,p))= -1912.04286925
E(PBE/6-311+G(2d,p))= -1911.142374
E(PBE-D3(BJ)/6-311+G(2d,p))= -1911.27929964

Intermediate *c*-VIIa

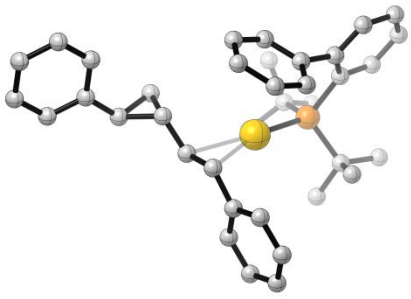


79	0.013347000	-0.019980000	-0.179152000
15	2.006250000	-1.035932000	0.606882000
6	2.075696000	-0.573841000	2.444145000
6	1.926624000	-2.900107000	0.267402000
6	-2.569790000	-0.409608000	-1.999919000
1	-2.166041000	0.178516000	-2.824886000
6	-2.696265000	-1.899259000	-2.194912000
1	-2.540874000	-2.517367000	-1.309008000
1	-2.311454000	-2.323947000	-3.119860000
6	-4.948616000	-1.100324000	-1.156701000
6	-5.621277000	0.076465000	-0.806783000
6	-5.245088000	-2.274229000	-0.462401000
6	-6.561174000	0.080069000	0.217431000
1	-5.393698000	0.999400000	-1.342877000
6	-6.190172000	-2.274408000	0.562193000
1	-4.732626000	-3.198620000	-0.729919000
6	-6.847752000	-1.097631000	0.906790000
1	-7.071600000	1.005326000	0.481224000
1	-6.411063000	-3.199892000	1.092222000
1	-7.583267000	-1.095972000	1.709684000
6	-3.928573000	-1.067126000	-2.244823000
1	-4.322713000	-0.857349000	-3.240934000
6	-2.309945000	0.123359000	-0.657592000
1	-2.699904000	-0.467957000	0.176655000
6	-1.828391000	1.390382000	-0.411959000
1	-1.554299000	2.007204000	-1.275829000
6	-1.834980000	2.085535000	0.886736000
6	-1.206603000	3.334439000	0.976433000
6	-2.428012000	1.543763000	2.036610000
6	-1.149457000	4.016918000	2.186319000
1	-0.754426000	3.763320000	0.080701000
6	-2.363928000	2.223928000	3.245527000
1	-2.952367000	0.588934000	1.984600000
6	-1.720789000	3.459255000	3.326892000
1	-0.656468000	4.986239000	2.238489000
1	-2.829538000	1.793024000	4.130449000
1	-1.676336000	3.990146000	4.276225000
6	3.558364000	-0.373816000	-0.122958000
6	4.781330000	-0.890265000	0.335431000
6	3.582278000	0.704145000	-1.035290000
6	5.998475000	-0.345951000	-0.051340000
1	4.792205000	-1.735069000	1.019259000
6	4.819748000	1.260061000	-1.388332000
6	6.016348000	0.751927000	-0.903385000
1	6.926475000	-0.773633000	0.323003000
1	4.828851000	2.099896000	-2.082843000
1	6.959678000	1.204945000	-1.202953000
6	2.401412000	1.296100000	-1.719862000
6	2.047466000	2.629790000	-1.489020000
6	1.728279000	0.581463000	-2.720523000
6	1.042670000	3.236324000	-2.239823000
1	2.577315000	3.196180000	-0.721677000
6	0.730136000	1.191306000	-3.476351000
1	2.019089000	-0.449553000	-2.926976000
6	0.385482000	2.520870000	-3.238559000
1	0.785644000	4.278425000	-2.053536000
1	0.231387000	0.628178000	-4.264332000
1	-0.387214000	3.001645000	-3.836956000
6	2.793032000	-3.757177000	1.185836000
1	2.676449000	-4.808982000	0.884142000
1	3.861081000	-3.521124000	1.116260000
1	2.482661000	-3.682761000	2.235472000
6	2.352925000	-3.099174000	-1.187145000
1	3.405834000	-2.838528000	-1.356498000
1	2.223700000	-4.159678000	-1.449078000
1	1.734950000	-2.510384000	-1.881883000
6	0.472530000	-3.355047000	0.413424000
1	0.412789000	-4.424842000	0.163322000
1	0.093517000	-3.233885000	1.435901000
1	-0.195399000	-2.808910000	-0.268406000
6	0.849647000	-1.173521000	3.132594000
1	0.921971000	-2.265387000	3.227291000
1	0.776268000	-0.757144000	4.148288000
1	-0.084689000	-0.930341000	2.604216000
6	1.989731000	0.954539000	2.487902000
1	1.061862000	1.335622000	2.035009000
1	2.008402000	1.282365000	3.538199000
1	2.840139000	1.429209000	1.977489000
6	3.333384000	-1.002164000	3.196996000
1	3.212208000	-0.705923000	4.249716000
1	3.500885000	-2.085527000	3.181176000
1	4.233969000	-0.500363000	2.823313000

Zero-point correction= 0.697400
(Hartree/Particle)
Thermal correction to Energy= 0.736660
Thermal correction to Enthalpy= 0.737604
Thermal correction to Gibbs Free Energy= 0.624113
Sum of electronic and zero-point Energies= -1910.984919
Sum of electronic and thermal Energies= -1910.945659
Sum of electronic and thermal Enthalpies= -1910.944715
Sum of electronic and thermal Free Energies= -1911.058206

E(M06/6-311+G(2d,p))= -1912.11420726

Intermediate *t*-VIIa



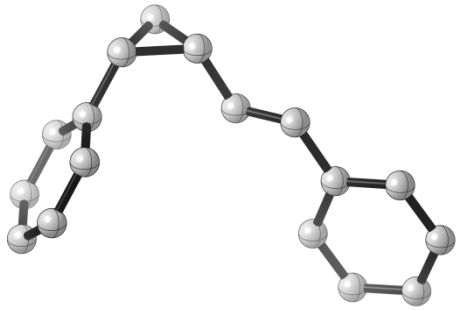
79	0.196112000	0.412894000	0.130812000
15	2.329885000	-0.320564000	0.826650000
6	3.460089000	1.188791000	0.669701000
6	2.155127000	-1.002005000	2.588399000
6	-2.922834000	-0.107373000	0.435331000
1	-3.052920000	-0.595926000	-0.533012000
6	-2.948420000	-0.992257000	1.646228000

1	-2.310834000	-0.714880000	2.486577000
1	-3.047362000	-2.065308000	1.478087000
6	-4.134904000	-0.125911000	1.363423000
6	-2.085083000	1.095898000	0.418846000
1	-2.001715000	1.635619000	1.368995000
6	-1.577941000	1.649102000	-0.736066000
1	-1.805729000	1.132321000	-1.675003000
6	-0.914895000	2.956194000	-0.882691000
6	-0.455553000	3.324126000	-2.154257000
6	-0.684705000	3.824432000	0.195004000
6	0.226580000	4.520785000	-2.345787000
1	-0.636072000	2.655304000	-2.997066000
6	-0.001333000	5.017306000	0.002146000
1	-1.039149000	3.561675000	1.191793000
6	0.461054000	5.368389000	-1.266717000
1	0.576938000	4.791122000	-3.340434000
1	0.169782000	5.682430000	0.847071000
1	0.996042000	6.305192000	-1.411939000
6	3.080053000	-1.633618000	-0.216547000
6	4.359244000	-2.109319000	0.118144000
6	2.444924000	-2.158281000	-1.361836000
6	5.012271000	-3.058907000	-0.655406000
1	4.869925000	-1.725360000	0.997670000
6	3.127518000	-3.104054000	-2.138838000
6	4.395997000	-3.552636000	-1.799294000
1	6.002334000	-3.405253000	-0.365157000
1	2.632440000	-3.499432000	-3.025590000
1	4.897837000	-4.290305000	-2.422812000
6	1.064420000	-1.840291000	-1.826879000
6	0.846658000	-0.943809000	-2.878796000
6	-0.017070000	-2.574615000	-1.325317000
6	-0.429545000	-0.785000000	-3.416793000
1	1.689155000	-0.383013000	-3.286463000
6	-1.289831000	-2.418289000	-1.867402000
1	0.153381000	-3.293826000	-0.523405000
6	-1.498478000	-1.526116000	-2.917531000
1	-0.583438000	-0.094272000	-4.245057000
1	-2.117697000	-3.011369000	-1.479881000
1	-2.491936000	-1.413315000	-3.349881000
6	3.457489000	-1.084731000	3.378306000
1	3.229903000	-1.497110000	4.372974000
1	4.197189000	-1.752030000	2.921101000
1	3.914219000	-0.098376000	3.534193000
6	1.540056000	-2.395066000	2.449494000
1	2.216417000	-3.105860000	1.956511000
1	1.319575000	-2.784365000	3.454530000
1	0.591886000	-2.372217000	1.890264000
6	1.176053000	-0.117794000	3.366149000
1	1.034695000	-0.553770000	4.366453000
1	1.542633000	0.907446000	3.501099000
1	0.190721000	-0.068820000	2.880051000
6	2.980327000	2.260874000	1.646311000
1	3.201826000	1.993354000	2.688161000
1	3.511717000	3.199056000	1.426148000
1	1.902416000	2.461553000	1.553765000
6	3.287626000	1.694804000	-0.765654000
1	2.255871000	2.012922000	-0.979662000
1	3.943774000	2.565945000	-0.911118000
1	3.574827000	0.936976000	-1.508755000
6	4.944994000	0.924110000	0.906993000
1	5.474219000	1.887381000	0.858421000
1	5.152446000	0.487236000	1.890848000
1	5.379314000	0.277264000	0.135577000
6	-5.429719000	-0.671518000	0.888873000
6	-5.514668000	-1.801342000	0.067322000
6	-6.614938000	-0.032901000	1.266850000
6	-6.748882000	-2.273552000	-0.365368000
1	-4.607810000	-2.323239000	-0.241888000
6	-7.850685000	-0.506068000	0.836944000
1	-6.561668000	0.847116000	1.909052000
6	-7.923047000	-1.628244000	0.016849000
1	-6.794163000	-3.153481000	-1.005693000
1	-8.761051000	0.006767000	1.144228000
1	-8.888596000	-1.999223000	-0.323001000
1	-4.230202000	0.757237000	1.997502000

Zero-point correction= 0.698576
(Hartree/Particle)
Thermal correction to Energy= 0.737422
Thermal correction to Enthalpy= 0.738367
Thermal correction to Gibbs Free Energy= 0.627312
Sum of electronic and zero-point Energies= -1910.986467
Sum of electronic and thermal Energies= -1910.947620
Sum of electronic and thermal Enthalpies= -1910.946676
Sum of electronic and thermal Free Energies= -1911.057730

E(M06/6-311+G(2d,p))= -1912.11734643

Product *cis*-3b

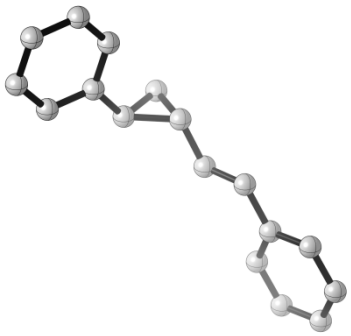


6	3.791657000	-0.705256000	-0.600196000
6	4.869836000	0.149438000	-0.396606000
6	4.697481000	1.336104000	0.309935000
6	3.434637000	1.658919000	0.807018000
6	2.358948000	0.805913000	0.602722000
6	2.517207000	-0.398666000	-0.101083000
1	3.930331000	-1.635188000	-1.153613000
1	5.849653000	-0.114295000	-0.793013000
1	5.539194000	2.008142000	0.469600000
1	3.286783000	2.588635000	1.355225000
1	1.378284000	1.085167000	0.987010000
6	1.416309000	-1.333599000	-0.336947000
1	1.656732000	-2.181619000	-0.986330000
6	0.175552000	-1.252579000	0.167555000
1	-0.092444000	-0.425674000	0.832533000
6	-0.890940000	-2.221189000	-0.105336000
6	-2.332844000	-1.743673000	-0.253175000
6	-1.924781000	-2.505758000	0.958557000
1	-0.608031000	-3.055761000	-0.748648000
1	-2.892245000	-2.309422000	-1.001014000
1	-2.270953000	-3.530866000	1.075208000
1	-1.817733000	-1.955051000	1.893637000
6	-2.666384000	-0.291405000	-0.207626000
6	-3.235655000	0.304552000	0.919315000
6	-2.411537000	0.507112000	-1.329174000
6	-3.545088000	1.663347000	0.927369000
1	-3.445626000	-0.304128000	1.799053000
6	-2.720096000	1.862355000	-1.325197000
1	-1.957963000	0.051915000	-2.211057000
6	-3.288527000	2.446282000	-0.193929000
1	-3.989691000	2.110204000	1.815891000
1	-2.512083000	2.468069000	-2.206358000
1	-3.528854000	3.508487000	-0.187324000

Zero-point correction= 0.276661
(Hartree/Particle)
Thermal correction to Energy= 0.290854
Thermal correction to Enthalpy= 0.291798
Thermal correction to Gibbs Free Energy= 0.233887
Sum of electronic and zero-point Energies= -656.609280
Sum of electronic and thermal Energies= -656.595087
Sum of electronic and thermal Enthalpies= -656.594143
Sum of electronic and thermal Free Energies= -656.652054

E(M06/6-311+G(2d,p))= -657.072960834

Product *trans*-3b

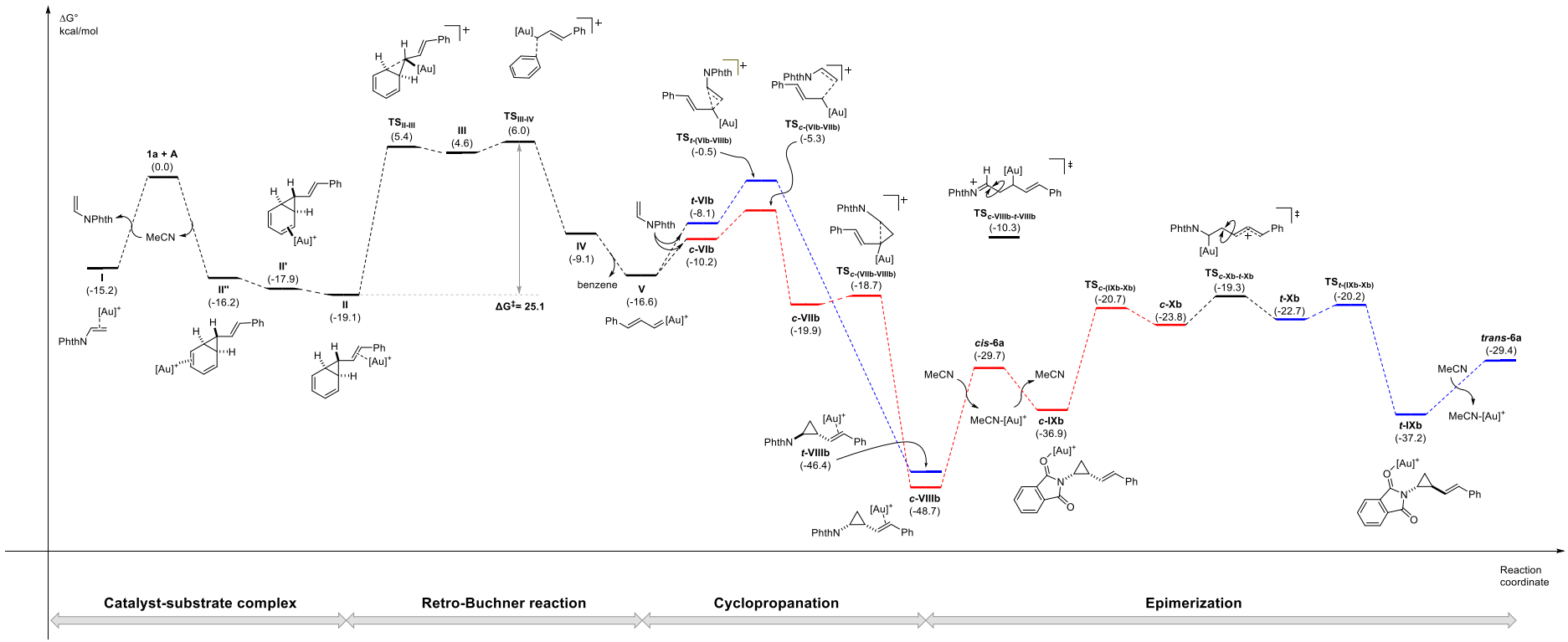


6	3.926107000	-1.327892000	-0.562125000
6	5.251931000	-1.381301000	-0.145128000
6	5.786561000	-0.348653000	0.619586000
6	4.981265000	0.738591000	0.959134000
6	3.658516000	0.791622000	0.541717000
6	3.100943000	-0.245598000	-0.222915000
1	3.509788000	-2.140061000	-1.159819000
1	5.869700000	-2.235580000	-0.419537000
1	6.824196000	-0.387564000	0.947369000
1	5.391119000	1.555366000	1.552141000
1	3.051923000	1.656870000	0.808111000
6	1.709925000	-0.241885000	-0.678123000
1	1.431790000	-1.073385000	-1.333404000
6	0.767331000	0.660738000	-0.366155000
1	1.004859000	1.499586000	0.296761000
6	-0.618038000	0.617701000	-0.843419000
6	-1.728742000	1.061061000	0.106808000
6	-1.366171000	1.897992000	-1.078943000
1	-0.873243000	-0.222011000	-1.493825000
1	-2.066329000	1.929702000	-1.913196000
1	-0.835830000	2.831968000	-0.895047000
6	-3.001350000	0.306123000	0.185114000
6	-3.596400000	0.097595000	1.433785000
6	-3.636620000	-0.216249000	-0.947895000
6	-4.788816000	-0.609822000	1.551427000
1	-3.112124000	0.501240000	2.323902000
6	-4.827141000	-0.925909000	-0.831653000
1	-3.198032000	-0.069872000	-1.935976000
6	-5.410017000	-1.126326000	0.417990000
1	-5.233066000	-0.756782000	2.535252000
1	-5.304426000	-1.325506000	-1.725669000
1	-6.343164000	-1.680549000	0.507096000
1	-1.372865000	1.429853000	1.070614000

Zero-point correction= 0.277221
(Hartree/Particle)
Thermal correction to Energy= 0.291318
Thermal correction to Enthalpy= 0.292262
Thermal correction to Gibbs Free Energy= 0.234655
Sum of electronic and zero-point Energies= -656.611124
Sum of electronic and thermal Energies= -656.597027
Sum of electronic and thermal Enthalpies= -656.596083
Sum of electronic and thermal Free Energies= -656.653691

E(M06/6-311+G(2d,p))= -657.075488356

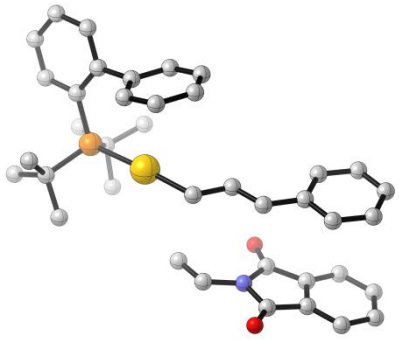
Calculated free energy profile for the formation and isomerization of 6a



Computational details:
SMD(CH_2Cl_2)-M06/6-311+G(2d,p), SDD(Au, f=1.05)//SMD(CH_2Cl_2)-M06/6-31G(d), SDD(Au)
Gibbs free energies given in kcal/mol at the standard state (298.15 K, 1 atm)
[Au] = Au-JohnPhos

Cartesian coordinates (in Å) and energies (in h) for reactants, intermediates and transition states involved in the formation and isomerization of 6a

Intermediate *c*-VIb

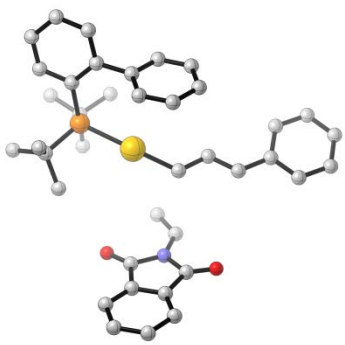


79	-1.338241000	0.381218000	0.620439000
15	-3.256436000	1.748772000	0.109277000
6	-2.824856000	2.669403000	-1.490466000
6	-4.778815000	0.621125000	-0.035682000
6	0.307100000	-0.810816000	0.863622000
1	0.211358000	-1.845957000	1.220454000
6	-0.287554000	-1.858645000	-1.798270000
1	0.023624000	-0.915482000	-2.237049000
1	-1.348752000	-2.023529000	-1.624212000
6	0.565864000	-2.849335000	-1.513819000
1	0.230935000	-3.794099000	-1.086873000
6	1.626594000	-0.405807000	0.665479000
1	1.830992000	0.607152000	0.312101000
6	2.676428000	-1.272739000	0.909446000
1	2.412933000	-2.281691000	1.246870000
6	4.075045000	-1.001003000	0.771638000
6	4.990451000	-2.032010000	1.066423000
6	4.564190000	0.245482000	0.324616000
6	6.353391000	-1.821272000	0.935260000
1	4.608822000	-2.996709000	1.402805000
6	5.925551000	0.447962000	0.191885000
1	3.872629000	1.049926000	0.081504000
6	6.819589000	-0.582244000	0.497310000
1	7.054739000	-2.620563000	1.164682000
1	6.301104000	1.408923000	-0.153068000
1	7.890168000	-0.414755000	0.392318000
6	-3.669939000	3.075332000	1.320956000
6	-4.787535000	3.890058000	1.072657000
6	-2.874017000	3.360122000	2.451251000
6	-5.112146000	4.963967000	1.889790000
1	-5.420995000	3.691955000	0.212115000
6	-3.202716000	4.463455000	3.251415000
6	-4.305145000	5.261631000	2.981720000
1	-5.988639000	5.568431000	1.663835000
1	-2.576162000	4.680455000	4.116411000
1	-4.536980000	6.107840000	3.626079000
6	-1.701188000	2.569972000	2.919313000
6	-0.406524000	3.082382000	2.784567000
6	-1.888199000	1.385978000	3.641776000
6	0.679247000	2.421601000	3.354416000
1	-0.256553000	4.019191000	2.246392000
6	-0.802938000	0.729545000	4.218315000
1	-2.898003000	0.995530000	3.774871000
6	0.482689000	1.247674000	4.078195000
1	1.680297000	2.837844000	3.248649000
1	-0.967324000	-0.182020000	4.791419000
1	1.328937000	0.742281000	4.541486000
6	-5.948006000	1.172609000	-0.846878000
1	-6.742135000	0.410756000	-0.868836000
1	-6.390623000	2.077230000	-0.412762000
1	-5.669610000	1.380145000	-1.888205000
6	-5.233194000	0.330251000	1.396013000
1	-5.617045000	1.223488000	1.905890000
1	-6.043255000	-0.413621000	1.365406000
1	-4.420979000	-0.094376000	2.005001000
6	-4.338890000	-0.701311000	-0.672522000
1	-5.200024000	-1.386614000	-0.683514000
1	-4.002706000	-0.580791000	-1.709920000
1	-3.532589000	-1.185124000	-0.102062000
6	-2.655354000	1.643200000	-2.608726000
1	-3.614397000	1.205427000	-2.917284000
1	-2.225423000	2.145227000	-3.488641000
1	-1.973292000	0.828099000	-2.326170000
6	-1.479360000	3.348058000	-1.218837000
1	-0.688209000	2.621243000	-0.978983000
1	-1.170141000	3.900432000	-2.119235000
1	-1.545045000	4.072511000	-0.394007000
6	-3.816066000	3.739809000	-1.939542000
1	-3.464965000	4.151711000	-2.897817000
1	-4.826291000	3.346375000	-2.103307000
1	-3.876738000	4.574428000	-1.230411000
7	1.947670000	-2.834960000	-1.704872000
6	2.737856000	-3.971477000	-1.380753000
6	2.729327000	-1.837048000	-2.334122000
6	4.096486000	-3.675576000	-1.869690000
6	4.095884000	-2.398086000	-2.423355000
8	2.318914000	-4.949640000	-0.807078000
8	2.327345000	-0.758981000	-2.708673000
6	5.242095000	-4.449716000	-1.825893000
1	5.231214000	-5.448277000	-1.393270000
6	5.244606000	-1.835700000	-2.948261000
1	5.237443000	-0.832645000	-3.370939000
6	6.405380000	-3.895450000	-2.364670000
1	7.327881000	-4.472495000	-2.357514000
6	6.407191000	-2.610085000	-2.912590000
1	7.332514000	-2.207249000	-3.319839000

Zero-point correction= 0.709580
(Hartree/Particle)
Thermal correction to Energy= 0.753568
Thermal correction to Enthalpy= 0.754512
Thermal correction to Gibbs Free Energy= 0.631286
Sum of electronic and zero-point Energies= -2191.617480
Sum of electronic and thermal Energies= -2191.573492
Sum of electronic and thermal Enthalpies= -2191.572547
Sum of electronic and thermal Free Energies= -2191.695774

E(M06/6-311+G(2d,p))= -2192.84239272

Intermediate *t*-VIb



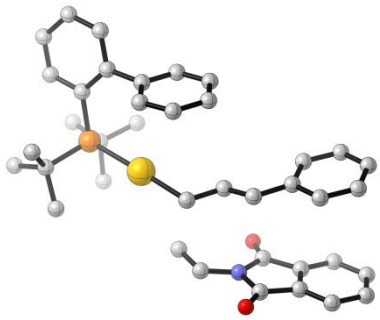
79	0.518130000	0.028345000	0.119289000
15	2.765316000	-0.805382000	0.415590000
6	3.227112000	-0.448706000	2.220380000
6	2.795636000	-2.657522000	-0.020105000
6	-1.387825000	0.760622000	0.006225000

1	-2.207944000	0.176197000	-0.435995000
6	-1.950847000	-0.937702000	2.619141000
1	-1.794083000	-0.101584000	3.297173000
1	-1.197450000	-1.717751000	2.579904000
6	-3.070516000	-0.973626000	1.893172000
6	-1.758436000	2.052704000	0.370128000
1	-1.020195000	2.720459000	0.817490000
6	-3.033676000	2.516287000	0.094925000
1	-3.742701000	1.785714000	-0.307915000
6	-3.533993000	3.842943000	0.268018000
6	-4.896126000	4.083741000	-0.008482000
6	-2.722328000	4.910844000	0.710298000
6	-5.435722000	5.346747000	0.165198000
1	-5.518196000	3.258484000	-0.353637000
6	-3.266555000	6.170207000	0.877190000
1	-1.665587000	4.746763000	0.914005000
6	-4.621188000	6.387990000	0.608965000
1	-6.488297000	5.525660000	-0.042476000
1	-2.641042000	6.992634000	1.217148000
1	-5.043223000	7.382322000	0.743941000
6	4.093578000	0.027933000	-0.556675000
6	5.385527000	-0.522271000	-0.516441000
6	3.905241000	1.235288000	-1.264478000
6	6.468368000	0.086822000	-1.134650000
1	5.558707000	-1.448675000	0.024450000
6	5.016265000	1.850750000	-1.859662000
6	6.284280000	1.291168000	-1.803588000
1	7.451805000	-0.376558000	-1.081801000
1	4.861343000	2.787174000	-2.395288000
1	7.122912000	1.792075000	-2.283855000
6	2.613152000	1.947300000	-1.470196000
6	2.381592000	3.170532000	-0.832631000
6	1.685637000	1.495806000	-2.417088000
6	1.245116000	3.921165000	-1.124329000
1	3.113742000	3.544324000	-0.115753000
6	0.554574000	2.252410000	-2.717717000
1	1.871201000	0.558326000	-2.943240000
6	0.329777000	3.464958000	-2.070260000
1	1.084439000	4.874606000	-0.622328000
1	-0.149084000	1.894112000	-3.468217000
1	-0.554087000	4.056862000	-2.307017000
6	3.857427000	-3.504181000	0.678367000
1	3.745410000	-4.543707000	0.334280000
1	4.886236000	-3.204850000	0.446503000
1	3.733709000	-3.510650000	1.768670000
6	2.963913000	-2.757524000	-1.536329000
1	3.966239000	-2.464259000	-1.872583000
1	2.802356000	-3.802508000	-1.840920000
1	2.226156000	-2.141246000	-2.072029000
6	1.422205000	-3.230324000	0.342003000
1	1.407268000	-4.302630000	0.094201000
1	1.187721000	-3.135669000	1.409618000
1	0.615476000	-2.743696000	-0.223396000
6	2.271739000	-1.212771000	3.135163000
1	2.414677000	-2.300249000	3.080362000
1	2.459452000	-0.909751000	4.176508000
1	1.219160000	-0.986759000	2.909741000
6	3.004191000	1.053243000	2.414245000
1	1.959560000	1.342350000	2.222586000
1	3.243320000	1.317791000	3.455483000
1	3.654908000	1.653039000	1.762335000
6	4.669376000	-0.773530000	2.596779000
1	4.807942000	-0.547558000	3.664884000
1	4.925498000	-1.828692000	2.449193000
1	5.390132000	-0.160829000	2.040831000
1	-3.823828000	-0.188458000	1.950642000
7	-3.431018000	-1.964764000	0.972558000
6	-2.764431000	-3.179706000	0.709842000
6	-4.561036000	-1.809733000	0.134718000
6	-3.549793000	-3.846024000	-0.353158000
6	-4.628811000	-3.033102000	-0.688215000
8	-1.758864000	-3.567355000	1.261606000
8	-5.279638000	-0.835434000	0.127626000
6	-5.545426000	-3.403913000	-1.654858000
1	-6.388509000	-2.764219000	-1.908891000
6	-3.336216000	-5.061292000	-0.976213000
1	-2.488247000	-5.689472000	-0.709900000
6	-4.255533000	-5.445503000	-1.956252000
1	-4.123503000	-6.394295000	-2.472384000
6	-5.341407000	-4.632715000	-2.287970000
1	-6.039274000	-4.963544000	-3.054506000

Zero-point correction= 0.709078
(Hartree/Particle)
Thermal correction to Energy= 0.753602
Thermal correction to Enthalpy= 0.754546
Thermal correction to Gibbs Free Energy= 0.628362
Sum of electronic and zero-point Energies= -2191.612043
Sum of electronic and thermal Energies= -2191.567519
Sum of electronic and thermal Enthalpies= -2191.566575
Sum of electronic and thermal Free Energies= -2191.692759

E(M06/6-311+G(2d,p))= -2192.83609959

Transition state $TS_{c\text{-(VIb-VIIb)}}$



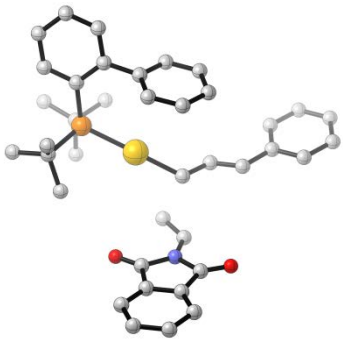
79	-1.468853000	0.241093000	0.193020000
15	-3.339689000	1.725265000	0.038982000
6	-3.039787000	2.786735000	-1.501846000
6	-4.921252000	0.667878000	-0.057416000
6	0.154489000	-1.050464000	0.209116000
1	0.052760000	-2.047957000	0.656403000
6	-0.181871000	-1.698090000	-1.964967000
1	0.212416000	-0.795444000	-2.422359000
1	-1.260390000	-1.833092000	-1.950813000
6	0.593926000	-2.788633000	-1.723434000
1	0.161388000	-3.720308000	-1.358785000
6	1.486886000	-0.562948000	0.190283000
1	1.668148000	0.429082000	-0.230607000
6	2.522619000	-1.285453000	0.710445000
1	2.291482000	-2.282974000	1.101445000
6	3.904470000	-0.872876000	0.816884000
6	4.845980000	-1.799384000	1.296379000
6	4.350116000	0.395497000	0.400038000
6	6.193347000	-1.472220000	1.359128000
1	4.502683000	-2.783876000	1.616683000
6	5.695562000	0.719692000	0.467350000
1	3.635636000	1.128514000	0.027498000
6	6.619740000	-0.212335000	0.944144000
1	6.912874000	-2.199059000	1.731787000
1	6.031990000	1.703538000	0.145394000
1	7.675774000	0.047702000	0.993129000
6	-3.563108000	2.939654000	1.409612000
6	-4.712305000	3.747035000	1.395563000
6	-2.606774000	3.154740000	2.426374000
6	-4.924408000	4.747366000	2.334021000
1	-5.467073000	3.594866000	0.628525000
6	-2.826617000	4.186644000	3.350905000
6	-3.966099000	4.976761000	3.314400000
1	-5.831967000	5.346543000	2.292630000
1	-2.079604000	4.348950000	4.127588000
1	-4.106959000	5.761899000	4.055161000
6	-1.362166000	2.366375000	2.648915000
6	-0.112926000	2.956236000	2.429152000
6	-1.413644000	1.088275000	3.218720000
6	1.059444000	2.280973000	2.761058000
1	-0.063885000	3.961051000	2.007938000

6	-0.241642000	0.420950000	3.568391000
1	-2.384055000	0.627133000	3.409265000
6	0.997448000	1.016785000	3.342277000
1	2.024278000	2.756560000	2.588011000
1	-0.300189000	-0.565542000	4.027127000
1	1.913596000	0.496910000	3.619938000
6	-6.107922000	1.289895000	-0.790094000
1	-6.949358000	0.581836000	-0.743902000
1	-6.457916000	2.228712000	-0.345706000
1	-5.892048000	1.466296000	-1.851681000
6	-5.312017000	0.334945000	1.383620000
1	-5.682909000	1.209885000	1.932196000
1	-6.114448000	-0.417600000	1.367764000
1	-4.469936000	-0.092660000	1.949116000
6	-4.567896000	-0.643693000	-0.769280000
1	-5.473073000	-1.267237000	-0.823302000
1	-4.211837000	-0.488554000	-1.796527000
1	-3.800781000	-1.212020000	-0.224477000
6	-2.959865000	1.861637000	-2.715841000
1	-3.930250000	1.410429000	-2.962044000
1	-2.640613000	2.449542000	-3.589708000
1	-2.224944000	1.054626000	-2.572173000
6	-1.675742000	3.447199000	-1.287531000
1	-0.873443000	2.705502000	-1.155356000
1	-1.431248000	4.055460000	-2.171501000
1	-1.674820000	4.116835000	-0.415566000
6	-4.069339000	3.882743000	-1.758850000
1	-3.789129000	4.411351000	-2.682605000
1	-5.084148000	3.492363000	-1.898189000
1	-4.087898000	4.626647000	-0.952529000
7	1.962135000	-2.841406000	-1.799626000
6	2.686042000	-3.981538000	-1.324278000
6	2.847525000	-1.881899000	-2.373767000
6	4.100273000	-3.709158000	-1.622262000
6	4.196959000	-2.464071000	-2.240133000
8	2.167481000	-4.929301000	-0.787202000
8	2.512008000	-0.829944000	-2.863002000
6	5.220140000	-4.477086000	-1.354737000
1	5.133691000	-5.448103000	-0.871089000
6	5.418624000	-1.933732000	-2.613264000
1	5.487485000	-0.955384000	-3.085179000
6	6.457362000	-3.952838000	-1.734193000
1	7.363496000	-4.523944000	-1.542866000
6	6.554763000	-2.702706000	-2.350710000
1	7.535096000	-2.322370000	-2.630323000

Zero-point correction= 0.710651
(Hartree/Particle)
Thermal correction to Energy= 0.753167
Thermal correction to Enthalpy= 0.754111
Thermal correction to Gibbs Free Energy= 0.636258
Sum of electronic and zero-point Energies= -2191.614076
Sum of electronic and thermal Energies= -2191.571560
Sum of electronic and thermal Enthalpies= -2191.570615
Sum of electronic and thermal Free Energies= -2191.688469

E(M06/6-311+G(2d,p))= -2192.83951082
E(PBE/6-311+G(2d,p))= -2191.797188
E(PBE-D3(BJ)/6-311+G(2d,p))= -2191.9486528

Transition state TS$_{f\text{-(VIb-VIIIb)}}$



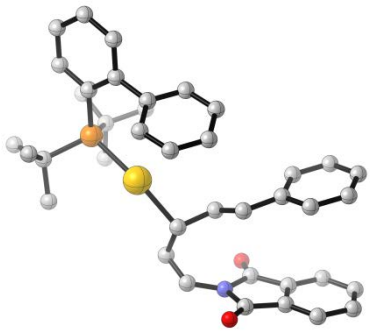
79	-0.519411000	-0.058943000	-0.333565000
15	-2.744913000	-0.950192000	-0.419930000
6	-3.407043000	-0.492479000	-2.134552000
6	-2.650490000	-2.826695000	-0.115928000
6	1.398119000	0.731883000	-0.397541000
1	2.142048000	0.345951000	0.311518000
6	1.934820000	-0.516286000	-2.229390000
1	1.744850000	0.298834000	-2.923272000
1	1.255313000	-1.362333000	-2.240084000
6	3.141522000	-0.577534000	-1.611429000
6	1.646374000	2.077773000	-0.804317000
1	0.925991000	2.559141000	-1.470763000
6	2.667994000	2.794806000	-0.258558000
1	3.388243000	2.250190000	0.361953000
6	2.898501000	4.219254000	-0.368560000
6	4.042803000	4.762372000	0.239379000
6	2.018304000	5.082162000	-1.046435000
6	4.308798000	6.122340000	0.163692000
1	4.723967000	4.097591000	0.770819000
6	2.285100000	6.439783000	-1.118415000
1	1.117885000	4.683135000	-1.511418000
6	3.429939000	6.963537000	-0.514669000
1	5.200579000	6.529025000	0.636805000
1	1.596934000	7.099885000	-1.643326000
1	3.633140000	8.031568000	-0.571190000
6	-3.980851000	-0.247048000	0.753531000
6	-5.268016000	-0.808763000	0.775036000
6	-3.733572000	0.884788000	1.562051000
6	-6.294842000	-0.275194000	1.541998000
1	-5.484726000	-1.684586000	0.169330000
6	-4.790896000	1.427657000	2.306792000
6	-6.057845000	0.863011000	2.303607000
1	-7.276644000	-0.744739000	1.534090000
1	-4.591410000	2.308123000	2.917065000
1	-6.852355000	1.307047000	2.900683000
6	-2.423119000	1.570488000	1.735498000
6	-2.247209000	2.875051000	1.262300000
6	-1.400083000	0.982107000	2.488576000
6	-1.068754000	3.570791000	1.521159000
1	-3.049874000	3.348444000	0.695439000
6	-0.226499000	1.682750000	2.758864000
1	-1.539822000	-0.024507000	2.885417000
6	-0.057454000	2.977688000	2.273506000
1	-0.951404000	4.588984000	1.152484000
1	0.554443000	1.215603000	3.358071000
1	0.858708000	3.527085000	2.487286000
6	-3.750581000	-3.675174000	-0.748620000
1	-3.565375000	-4.727689000	-0.484982000
1	-4.756734000	-3.430206000	-0.388509000
1	-3.746889000	-3.612675000	-1.844575000
6	-2.644226000	-3.028599000	1.399296000
1	-3.615860000	-2.807604000	1.858767000
1	-2.404463000	-4.080541000	1.615705000
1	-1.879730000	-2.409034000	1.891986000
6	-1.304208000	-3.310526000	-0.664166000
1	-1.218778000	-4.394290000	-0.492282000
1	-1.199224000	-3.138756000	-1.743676000
1	-0.458024000	-2.823485000	-0.160597000
6	-2.512479000	-1.138372000	-3.192737000

1	-2.620048000	-2.231034000	-3.222482000
1	-2.801409000	-0.753378000	-4.182522000
1	-1.449090000	-0.897133000	-3.041468000
6	-3.278039000	1.030047000	-2.233053000
1	-2.234044000	1.364733000	-2.134144000
1	-3.647512000	1.356392000	-3.216906000
1	-3.878175000	1.542111000	-1.467299000
6	-4.862313000	-0.867321000	-2.400695000
1	-5.106476000	-0.591107000	-3.437628000
1	-5.056838000	-1.940222000	-2.292651000
1	-5.555078000	-0.319674000	-1.749609000
1	3.847723000	0.251167000	-1.663616000
7	3.593253000	-1.607437000	-0.813292000
6	3.025454000	-2.899525000	-0.646663000
6	4.762872000	-1.454627000	-0.011396000
6	3.928092000	-3.607878000	0.281863000
6	4.965040000	-2.753472000	0.651236000
8	2.012579000	-3.291449000	-1.176907000
8	5.395562000	-0.429302000	0.066476000
6	5.966722000	-3.156880000	1.515836000
1	6.773233000	-2.482978000	1.797787000
6	3.850404000	-4.902853000	0.760789000
1	3.037746000	-5.564597000	0.467776000
6	4.859151000	-5.321003000	1.631916000
1	4.837121000	-6.333698000	2.028966000
6	5.898910000	-4.464511000	2.001477000
1	6.668897000	-4.824627000	2.680485000

Zero-point correction= 0.710746
(Hartree/Particle)
Thermal correction to Energy= 0.753561
Thermal correction to Enthalpy= 0.754505
Thermal correction to Gibbs Free Energy= 0.634523
Sum of electronic and zero-point Energies= -2191.605785
Sum of electronic and thermal Energies= -2191.562970
Sum of electronic and thermal Enthalpies= -2191.562026
Sum of electronic and thermal Free Energies= -2191.682008

E(M06/6-311+G(2d,p))= -2192.83026447
E(PBE/6-311+G(2d,p))= -2191.794519
E(PBE-D3(BJ)/6-311+G(2d,p))= -2191.9391044

Intermediate *c*-VIIb



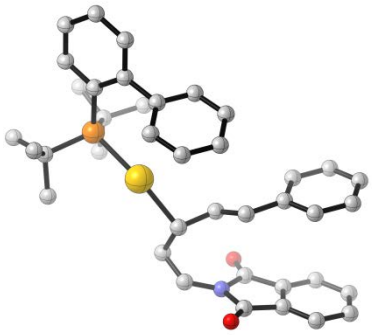
79	-1.480385000	0.108071000	-0.004541000
15	-3.236173000	1.706023000	0.017173000
6	-2.859409000	2.856330000	-1.439602000
6	-4.878571000	0.761260000	-0.151906000
6	0.053313000	-1.403970000	-0.435694000
1	-0.114925000	-2.114265000	0.388252000
6	-0.336787000	-1.932508000	-1.865065000
1	0.016323000	-1.255752000	-2.644096000
1	-1.392563000	-2.182823000	-1.971757000
6	0.492883000	-3.065651000	-1.547714000
1	0.056841000	-3.907914000	-1.010918000
6	1.330090000	-0.696261000	-0.376686000
1	1.487331000	0.072905000	-1.139918000
6	2.328836000	-1.003594000	0.478197000
1	2.164316000	-1.830014000	1.179781000
6	3.651539000	-0.392767000	0.526429000
6	4.655138000	-1.020651000	1.279707000
6	3.985548000	0.764918000	-0.196429000
6	5.954341000	-0.526183000	1.294711000
1	4.404100000	-1.916816000	1.849901000
6	5.280706000	1.263752000	-0.171853000
1	3.218531000	1.285732000	-0.769881000
6	6.272589000	0.617469000	0.566934000
1	6.720898000	-1.034204000	1.878241000
1	5.521768000	2.164567000	-0.734611000
1	7.287860000	1.010373000	0.579626000
6	-3.373592000	2.823430000	1.474748000
6	-4.466560000	3.704110000	1.530339000
6	-2.390150000	2.909815000	2.484663000
6	-4.594822000	4.657737000	2.530356000
1	-5.240029000	3.651131000	0.768422000
6	-2.522114000	3.900005000	3.469270000
6	-3.604692000	4.766843000	3.499877000
1	-5.460698000	5.317051000	2.541357000
1	-1.755813000	3.965587000	4.241329000
1	-3.679942000	5.517256000	4.284918000
6	-1.214447000	2.013124000	2.644278000
6	0.080129000	2.536241000	2.556713000
6	-1.376402000	0.679035000	3.039193000
6	1.187825000	1.748037000	2.857238000
1	0.214213000	3.580443000	2.271392000
6	-0.268458000	-0.107702000	3.347606000
1	-2.382143000	0.269521000	3.143903000
6	1.015704000	0.425707000	3.259788000
1	2.188120000	2.174001000	2.790057000
1	-0.412622000	-1.137940000	3.672181000
1	1.882163000	-0.183683000	3.514381000
6	-6.023875000	1.530368000	-0.808394000
1	-6.914227000	0.883206000	-0.810219000
1	-6.302040000	2.447487000	-0.276306000
1	-5.807431000	1.784691000	-1.854163000
6	-5.283734000	0.329781000	1.257911000
1	-5.583976000	1.178183000	1.885489000
1	-6.140060000	-0.357063000	1.186791000
1	-4.473385000	-0.208313000	1.772192000
6	-4.620830000	-0.500429000	-0.983293000
1	-5.567240000	-1.053028000	-1.084775000
1	-4.258583000	-0.277444000	-1.995529000
1	-3.892314000	-1.166522000	-0.498301000
6	-2.858454000	2.034175000	-2.727311000
1	-3.866050000	1.701174000	-3.009726000
1	-2.479185000	2.662586000	-3.547178000
1	-2.206249000	1.150033000	-2.656151000
6	-1.448842000	3.393599000	-1.182233000
1	-0.701497000	2.586878000	-1.127640000
1	-1.167313000	4.062988000	-2.008881000
1	-1.394956000	3.975105000	-0.250660000
6	-3.804006000	4.045556000	-1.598372000
1	-3.482623000	4.624014000	-2.477745000
1	-4.845795000	3.748616000	-1.767614000
1	-3.769085000	4.722830000	-0.735800000
7	1.829686000	-3.152151000	-1.683086000
6	2.595030000	-4.065021000	-0.861792000
6	2.708172000	-2.300493000	-2.438986000
6	4.002086000	-3.775362000	-1.156756000
6	4.068930000	-2.725547000	-2.072542000
8	2.088201000	-4.848055000	-0.100948000
8	2.345580000	-1.449806000	-3.212659000
6	5.143503000	-4.345350000	-0.619947000
1	5.080773000	-5.160502000	0.098164000
6	5.280685000	-2.203293000	-2.487597000
1	5.325306000	-1.377881000	-3.195139000
6	6.370834000	-3.825361000	-1.035460000
1	7.292858000	-4.242553000	-0.636110000
6	6.437763000	-2.771770000	-1.950369000
1	7.410634000	-2.386395000	-2.248094000

Zero-point correction= 0.711652
(Hartree/Particle)
Thermal correction to Energy= 0.754683
Thermal correction to Enthalpy= 0.755627
Thermal correction to Gibbs Free Energy= 0.634997
Sum of electronic and zero-point Energies= -2191.636077

Sum of electronic and thermal Energies=	-2191.593046
Sum of electronic and thermal Enthalpies=	-2191.592102
Sum of electronic and thermal Free Energies=	-2191.712732

E(M06/6-311+G(2d,p))= -2192.86157272

Transition state $TS_{c\text{-(VIIIb-VIIIb)}}$

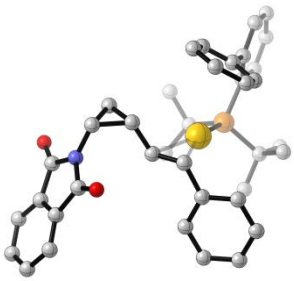


79	-1.478987000	0.107505000	-0.002181000
15	-3.233137000	1.704435000	0.015953000
6	-2.853038000	2.855597000	-1.439119000
6	-4.874567000	0.759161000	-0.157694000
6	0.056844000	-1.409922000	-0.436627000
1	-0.124026000	-2.110232000	0.392575000
6	-0.343549000	-1.925747000	-1.865899000
1	0.013066000	-1.249679000	-2.643665000
1	-1.399750000	-2.174099000	-1.971802000
6	0.486824000	-3.052626000	-1.533958000
1	0.049825000	-3.893925000	-0.997117000
6	1.330733000	-0.696178000	-0.374396000
1	1.487076000	0.072521000	-1.138195000
6	2.328781000	-1.001245000	0.481489000
1	2.165201000	-1.827402000	1.183544000
6	3.651669000	-0.390384000	0.527600000
6	4.657337000	-1.020537000	1.276062000
6	3.983888000	0.768297000	-0.194309000
6	5.957030000	-0.527140000	1.287285000
1	4.407702000	-1.917508000	1.845530000
6	5.279687000	1.265672000	-0.174030000
1	3.215218000	1.290742000	-0.764022000
6	6.273675000	0.617279000	0.560064000
1	6.725276000	-1.036739000	1.867196000
1	5.519532000	2.167132000	-0.736267000
1	7.289404000	1.009134000	0.569543000
6	-3.373015000	2.819639000	1.474692000
6	-4.466153000	3.700195000	1.528988000
6	-2.391451000	2.905032000	2.486534000
6	-4.596261000	4.652964000	2.529601000
1	-5.238170000	3.647912000	0.765580000
6	-2.525217000	3.894460000	3.471647000
6	-3.607874000	4.761273000	3.500988000
1	-5.462190000	5.312175000	2.539625000
1	-1.760363000	3.959372000	4.245152000
1	-3.684536000	5.511057000	4.286486000
6	-1.216173000	2.008092000	2.647686000
6	0.078674000	2.530962000	2.562486000
6	-1.379159000	0.673888000	3.041844000
6	1.185642000	1.742270000	2.864396000
1	0.213525000	3.575268000	2.277981000
6	-0.271908000	-0.113340000	3.351592000
1	-2.385221000	0.264738000	3.145023000
6	1.012550000	0.419786000	3.265986000
1	2.186144000	2.167946000	2.799063000
1	-0.416888000	-1.143658000	3.675639000
1	1.878534000	-0.189915000	3.521469000
6	-6.018514000	1.529496000	-0.815182000
1	-6.909009000	0.882603000	-0.819261000
1	-6.297257000	2.445983000	-0.282310000
1	-5.800340000	1.785140000	-1.860268000
6	-5.282605000	0.325658000	1.250662000
1	-5.584718000	1.173088000	1.878599000
1	-6.138442000	-0.361476000	1.176623000
1	-4.473200000	-0.212735000	1.766088000
6	-4.615132000	-0.501363000	-0.990366000
1	-5.561473000	-1.053523000	-1.094693000
1	-4.250578000	-0.277231000	-2.001528000
1	-3.888012000	-1.168385000	-0.504510000
6	-2.850655000	2.034635000	-2.727576000
1	-3.858068000	1.702768000	-3.011987000
1	-2.469485000	2.663534000	-3.546129000
1	-2.199341000	1.149862000	-2.656258000
6	-1.442664000	3.392028000	-1.178997000
1	-0.695727000	2.584939000	-1.124213000
1	-1.159673000	4.062184000	-2.004511000
1	-1.389852000	3.972526000	-0.246735000
6	-3.797056000	4.045283000	-1.597999000
1	-3.474255000	4.624341000	-2.476439000
1	-4.838726000	3.748893000	-1.768884000
1	-3.762969000	4.721788000	-0.734825000
7	1.825081000	-3.146105000	-1.678146000
6	2.590031000	-4.050751000	-0.850926000
6	2.700995000	-2.300416000	-2.440328000
6	3.997555000	-3.766285000	-1.151563000
6	4.063237000	-2.723663000	-2.075351000
8	2.084761000	-4.826701000	-0.081215000
8	2.337434000	-1.452192000	-3.216792000
6	5.139511000	-4.334198000	-0.614008000
1	5.077527000	-5.143927000	0.110344000
6	5.274388000	-2.205494000	-2.496966000
1	5.318368000	-1.385103000	-3.210426000
6	6.366495000	-3.819129000	-1.036911000
1	7.289070000	-4.234995000	-0.637410000
6	6.432316000	-2.771986000	-1.959198000
1	7.404876000	-2.390214000	-2.262562000

Zero-point correction=	0.711563
(Hartree/Particle)	
Thermal correction to Energy=	0.753774
Thermal correction to Enthalpy=	0.754718
Thermal correction to Gibbs Free Energy=	0.636870
Sum of electronic and zero-point Energies=	-2191.636165
Sum of electronic and thermal Energies=	-2191.593955
Sum of electronic and thermal Enthalpies=	-2191.593010
Sum of electronic and thermal Free Energies=	-2191.710858

E(M06/6-311+G(2d,p))= -2192.86157473

Intermediate *c*-VIIIb



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15	2.453780000	0.083762000	1.238311000
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6	1.842895000	-0.930294000	2.726199000
6	-1.729153000	-1.365143000	-1.645685000
1	-1.291933000	-1.442930000	-2.642051000
6	-1.705003000	-2.600876000	-0.787349000
1	-1.624728000	-2.451317000	0.288479000
1	-1.197082000	-3.483593000	-1.171029000
6	-1.618224000	-0.042270000	-1.015614000
1	-2.134428000	0.084579000	-0.057673000
6	-1.074685000	1.058520000	-1.636121000
1	-0.653197000	0.922276000	-2.638323000
6	-1.170585000	2.449975000	-1.160908000
6	-0.314978000	3.409809000	-1.718152000
6	-2.071878000	2.845626000	-0.162702000

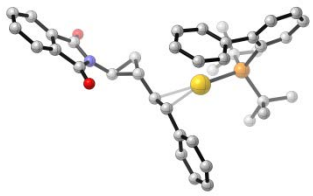
6	-0.337810000	4.725949000	-1.272080000
1	0.380108000	3.106683000	-2.503067000
6	-2.094113000	4.162187000	0.280438000
1	-2.775539000	2.126088000	0.256467000
6	-1.223920000	5.104500000	-0.266091000
1	0.336754000	5.458423000	-1.712142000
1	-2.803322000	4.459048000	1.051214000
1	-1.247082000	6.135512000	0.082106000
6	3.928041000	-0.783395000	0.563869000
6	4.998630000	-1.046706000	1.435328000
6	4.001646000	-1.278066000	-0.756801000
6	6.105063000	-1.785025000	1.039786000
1	4.972882000	-0.678545000	2.457530000
6	5.121771000	-2.032796000	-1.132739000
6	6.163986000	-2.289266000	-0.254057000
1	6.912259000	-1.968102000	1.746183000
1	5.167418000	-2.413822000	-2.152633000
1	7.019638000	-2.877757000	-0.580210000
6	2.996726000	-1.073595000	-1.838010000
6	2.924615000	0.138004000	-2.536327000
6	2.228791000	-2.156479000	-2.282589000
6	2.102245000	0.261204000	-3.654621000
1	3.542266000	0.978722000	-2.218319000
6	1.403767000	-2.030648000	-3.397677000
1	2.298151000	-3.109840000	-1.756587000
6	1.341107000	-0.822447000	-4.088769000
1	2.072697000	1.203100000	-4.201223000
1	0.817174000	-2.885369000	-3.733139000
1	0.708725000	-0.729019000	-4.970467000
6	2.619355000	-0.729397000	4.025792000
1	2.192222000	-1.402509000	4.784364000
1	3.682909000	-0.979438000	3.942462000
1	2.526844000	0.294462000	4.411009000
6	1.905549000	-2.398841000	2.302809000
1	2.935340000	-2.770645000	2.226894000
1	1.383894000	-3.005308000	3.057656000
1	1.406595000	-2.572843000	1.336220000
6	0.378260000	-0.566587000	2.990568000
1	0.023768000	-1.157107000	3.848609000
1	0.239255000	0.493337000	3.237773000
1	-0.265025000	-0.804579000	2.131271000
6	1.828781000	2.548676000	2.377993000
1	1.640591000	2.136002000	3.377736000
1	2.086451000	3.610827000	2.502859000
1	0.894589000	2.500038000	1.797168000
6	3.261590000	2.555669000	0.341996000
1	2.363785000	2.610620000	-0.291535000
1	3.582260000	3.586210000	0.556094000
1	4.066414000	2.071167000	-0.229103000
6	4.243860000	1.932717000	2.530250000
1	4.432567000	2.993404000	2.753361000
1	4.147025000	1.408514000	3.488499000
1	5.128543000	1.549838000	2.006632000
7	-4.030897000	-1.673955000	-0.610903000
6	-4.500318000	-2.261026000	0.579776000
6	-4.816190000	-0.570757000	-0.991107000
6	-5.636408000	-1.415616000	1.017808000
6	-5.828765000	-0.407297000	0.076999000
8	-4.044186000	-3.250708000	1.106053000
8	-4.649804000	0.086066000	-1.995138000
6	-6.435799000	-1.522005000	2.140706000
1	-6.280401000	-2.314639000	2.870461000
6	-6.826000000	0.539518000	0.222555000
1	-6.969469000	1.324029000	-0.518168000
6	-7.446498000	-0.570013000	2.297825000
1	-8.097322000	-0.616051000	3.168774000
6	-7.638302000	0.442577000	1.355421000
1	-8.434384000	1.168855000	1.506995000
6	-2.984048000	-2.195955000	-1.428799000
1	-3.325111000	-2.761093000	-2.295998000

Zero-point correction= 0.711309
(Hartree/Particle)
Thermal correction to Energy= 0.754600
Thermal correction to Enthalpy= 0.755545
Thermal correction to Gibbs Free Energy= 0.633331

Sum of electronic and zero-point Energies= -2191.681139
Sum of electronic and thermal Energies= -2191.637847
Sum of electronic and thermal Enthalpies= -2191.636903
Sum of electronic and thermal Free Energies= -2191.759117

E(M06/6-311+G(2d,p))= -2192.90576079

Intermediate *t*-VIIIb



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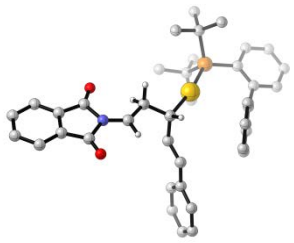
6	-2.645328000	-1.914494000	-2.207941000
6	2.229498000	0.225662000	-0.635677000
1	2.421068000	-0.081608000	0.392297000
6	2.394283000	-0.831738000	-1.690656000
1	1.761734000	-0.779767000	-2.576503000
1	2.639509000	-1.836571000	-1.350567000
6	3.438087000	0.222781000	-1.542025000
1	3.488275000	1.000225000	-2.305662000
6	1.249112000	1.310057000	-0.790709000
1	1.098078000	1.682432000	-1.809209000
6	0.714717000	1.980744000	0.285917000
1	1.017988000	1.637977000	1.283189000
6	-0.093238000	3.209946000	0.268536000
6	-0.589207000	3.681598000	1.491252000
6	-0.418055000	3.903629000	-0.906178000
6	-1.396305000	4.812427000	1.542327000
1	-0.336179000	3.143643000	2.406291000
6	-1.227319000	5.030427000	-0.853189000
1	-0.039643000	3.560606000	-1.869114000
6	-1.720952000	5.487840000	0.369193000
1	-1.771822000	5.167680000	2.500363000
1	-1.470217000	5.562222000	-1.771733000
1	-2.353087000	6.373365000	0.403955000
6	-3.529072000	-1.774172000	0.685925000
6	-4.752603000	-2.448033000	0.535435000
6	-2.882968000	-1.826273000	1.941338000
6	-5.349883000	-3.128671000	1.587767000
1	-5.269145000	-2.433153000	-0.420506000
6	-3.516465000	-2.494669000	2.998187000
6	-4.735050000	-3.137345000	2.833968000
1	-6.298100000	-3.639633000	1.432096000
1	-3.015673000	-2.522266000	3.965653000
1	-5.196750000	-3.651890000	3.674728000
6	-1.540667000	-1.268709000	2.262670000
6	-1.414604000	-0.217997000	3.178234000
6	-0.379696000	-1.893909000	1.787815000
6	-0.156900000	0.203943000	3.604353000
1	-2.313727000	0.258376000	3.571408000
6	0.875602000	-1.483753000	2.229314000
1	-0.468617000	-2.730036000	1.092895000
6	0.991052000	-0.431311000	3.135953000
1	-0.075804000	1.019424000	4.322047000
1	1.766732000	-1.998098000	1.869972000
1	1.973540000	-0.112730000	3.482224000
6	-3.918256000	-2.421923000	-2.879208000
1	-3.629467000	-3.062961000	-3.725693000
1	-4.539942000	-3.034386000	-2.215319000
1	-4.529425000	-1.605971000	-3.285298000
6	-1.829448000	-3.095415000	-1.678839000
1	-2.382761000	-3.692158000	-0.941551000
1	-1.577676000	-3.754764000	-2.522645000
1	-0.881986000	-2.766942000	-1.223738000

6	-1.805802000	-1.180375000	-3.256293000
1	-1.582297000	-1.882300000	-4.073500000
1	-2.329419000	-0.321998000	-3.694629000
1	-0.847913000	-0.826935000	-2.846097000
6	-3.840216000	1.415806000	-2.206084000
1	-4.032214000	0.873692000	-3.141326000
1	-4.459754000	2.324990000	-2.222782000
1	-2.787017000	1.734534000	-2.194300000
6	-4.115259000	1.489019000	0.269929000
1	-3.124166000	1.958290000	0.368663000
1	-4.862715000	2.291845000	0.184411000
1	-4.329918000	0.934971000	1.195312000
6	-5.658370000	0.119343000	-1.099439000
1	-6.286564000	0.993454000	-1.326880000
1	-5.804302000	-0.607296000	-1.907281000
1	-6.034310000	-0.314288000	-0.165041000
7	4.685526000	-0.122687000	-0.945021000
6	5.226738000	0.529923000	0.175534000
6	5.563339000	-1.092154000	-1.462299000
6	6.541642000	-0.110241000	0.413654000
6	6.742930000	-1.080526000	-0.564717000
8	4.690107000	1.423722000	0.792604000
8	5.355414000	-1.769918000	-2.443153000
6	7.480326000	0.131996000	1.399418000
1	7.316103000	0.894232000	2.159086000
6	7.891476000	-1.849372000	-0.596658000
1	8.040569000	-2.606229000	-1.364548000
6	8.644329000	-0.640532000	1.376690000
1	9.408591000	-0.482954000	2.135298000
6	8.846291000	-1.614180000	0.396307000
1	9.764128000	-2.198732000	0.406918000

Zero-point correction= 0.713708
(Hartree/Particle)
Thermal correction to Energy= 0.756419
Thermal correction to Enthalpy= 0.757364
Thermal correction to Gibbs Free Energy= 0.636897
Sum of electronic and zero-point Energies= -2191.678331
Sum of electronic and thermal Energies= -2191.635619
Sum of electronic and thermal Enthalpies= -2191.634675
Sum of electronic and thermal Free Energies= -2191.755142

E(M06/6-311+G(2d,p))= -2192.90573305

Transition state TS$_{c\text{-VIIIb-}t\text{-VIIIb}}$



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6	-4.647822000	-0.324460000	-2.751973000
6	-0.118032000	-1.493509000	-0.059416000
1	-0.087858000	-2.581372000	0.114312000
6	0.716415000	-1.147802000	-1.293307000
1	0.653368000	-0.087053000	-1.579727000
1	0.367509000	-1.693085000	-2.192604000
6	2.125926000	-1.532521000	-1.124086000
1	2.383458000	-2.294075000	-0.375506000
6	0.346457000	-0.768232000	1.139469000
1	0.466513000	0.316341000	1.015185000
6	0.587211000	-1.317901000	2.347398000
1	0.510121000	-2.407061000	2.438419000
6	0.911549000	-0.609344000	3.582104000
6	1.340379000	-1.342219000	4.700641000
6	0.786038000	0.783879000	3.722893000
6	1.651842000	-0.713539000	5.900802000
1	1.430210000	-2.426721000	4.616166000
6	1.103768000	1.412519000	4.919530000
1	0.417391000	1.381131000	2.888274000
6	1.539884000	0.669736000	6.016497000
1	1.980869000	-1.308455000	6.752096000
1	0.997263000	2.493653000	5.002825000
1	1.779283000	1.165868000	6.955778000
6	-5.747958000	-0.167588000	0.065515000
6	-6.989498000	0.302042000	-0.393715000
6	-5.699096000	-0.786482000	1.334322000
6	-8.150419000	0.185177000	0.358291000
1	-7.056815000	0.786383000	-1.363943000
6	-6.877420000	-0.873479000	2.091163000
6	-8.091927000	-0.400296000	1.617769000
1	-9.092251000	0.560595000	-0.037644000
1	-6.825238000	-1.346075000	3.071895000
1	-8.988474000	-0.491639000	2.228405000
6	-4.493469000	-1.376404000	1.974574000
6	-3.984327000	-0.801347000	3.144077000
6	-3.933939000	-2.572923000	1.513070000
6	-2.934416000	-1.401069000	3.833408000
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6	-2.889674000	-3.179637000	2.208464000
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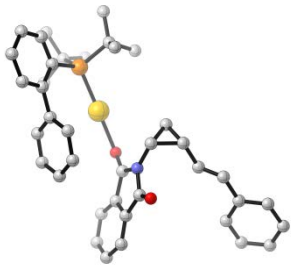
6	-2.387826000	-2.595277000	3.368774000
1	-2.549687000	-0.942014000	4.743410000
1	-2.472645000	-4.117048000	1.840655000
1	-1.578375000	-3.076087000	3.916842000
6	-5.475187000	0.670500000	-3.565240000
1	-5.626054000	0.249458000	-4.571185000
1	-6.470545000	0.862696000	-3.149932000
1	-4.960304000	1.631489000	-3.691085000
6	-5.367988000	-1.672681000	-2.694192000
1	-6.381584000	-1.593552000	-2.280796000
1	-5.454687000	-2.075338000	-3.714670000
1	-4.810285000	-2.409841000	-2.097114000
6	-3.317961000	-0.528557000	-3.488100000
1	-3.533040000	-0.811119000	-4.529919000
1	-2.702918000	0.380865000	-3.511370000
1	-2.720237000	-1.332456000	-3.035914000
6	-2.825252000	2.461593000	-1.676380000
1	-3.116728000	2.437714000	-2.734972000
1	-2.545275000	3.498781000	-1.436849000
1	-1.929041000	1.835011000	-1.549599000
6	-3.507937000	2.219080000	0.704323000
1	-2.575587000	1.675815000	0.924091000
1	-3.326714000	3.289736000	0.884731000
1	-4.274250000	1.887711000	1.419751000
6	-5.182211000	2.909474000	-0.987333000
1	-4.888147000	3.960462000	-0.843415000
1	-5.584432000	2.818048000	-2.003458000
1	-5.989004000	2.697853000	-0.274162000
7	3.155744000	-1.070758000	-1.771759000
6	4.538679000	-1.537401000	-1.480185000
6	3.190150000	-0.049048000	-2.838215000
6	5.385359000	-0.765214000	-2.377483000
6	4.606223000	0.095488000	-3.160519000
8	4.763487000	-2.373761000	-0.656407000
8	2.210230000	0.478234000	-3.279670000
6	6.765238000	-0.810295000	-2.502363000
1	7.362659000	-1.480350000	-1.888398000
6	5.181105000	0.939714000	-4.097342000
1	4.569676000	1.604279000	-4.703557000
6	7.346488000	0.038578000	-3.442226000
1	8.426175000	0.034365000	-3.571856000
6	6.568164000	0.898032000	-4.225936000
1	7.057527000	1.545846000	-4.949557000

Zero-point correction= 0.708373
(Hartree/Particle)
Thermal correction to Energy= 0.751434
Thermal correction to Enthalpy= 0.752378
Thermal correction to Gibbs Free Energy= 0.630302
Sum of electronic and zero-point Energies= -2191.618431
Sum of electronic and thermal Energies= -2191.575370

Sum of electronic and thermal Enthalpies= -2191.574426
Sum of electronic and thermal Free Energies= -2191.696502

E(M06/6-311+G(2d,p))= -2192.84162580

Intermediate *c*-IXb

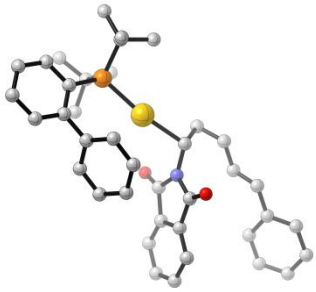


79	1.303614000	-0.991434000	0.576692000
15	3.102250000	-2.441391000	0.449534000
6	3.187043000	-3.420024000	2.061998000
6	4.635587000	-1.377964000	0.091394000
6	0.639499000	1.890068000	-1.419011000
1	0.996249000	1.328780000	-2.282991000
6	1.629248000	2.317916000	-0.387863000
1	1.301588000	2.375075000	0.649543000
1	2.660012000	1.998154000	-0.528273000
6	2.953061000	-3.657059000	-0.922339000
6	4.061066000	-4.482678000	-1.178979000
6	1.832776000	-3.750481000	-1.778275000
6	4.092209000	-5.358156000	-2.255120000
1	4.929940000	-4.444108000	-0.527600000
6	1.889561000	-4.633854000	-2.865508000
6	3.001368000	-5.425925000	-3.113239000
1	4.970841000	-5.977617000	-2.423345000
1	1.022981000	-4.695360000	-3.523472000
1	3.009769000	-6.098887000	-3.968717000
6	0.541813000	-3.016573000	-1.639770000
6	-0.433572000	-3.452408000	-0.734276000
6	0.221636000	-1.988591000	-2.534060000
6	-1.699313000	-2.871203000	-0.723417000
1	-0.204222000	-4.270419000	-0.050459000
6	-1.041962000	-1.400975000	-2.516799000
1	0.969942000	-1.658959000	-3.256567000
6	-2.008656000	-1.848267000	-1.617945000
1	-2.452509000	-3.232864000	-0.024502000
1	-1.275786000	-0.601116000	-3.219996000
1	-3.007973000	-1.413082000	-1.624747000
6	5.978879000	-2.047762000	0.369735000
1	6.774952000	-1.319201000	0.155020000
1	6.170277000	-2.920948000	-0.263599000
1	6.082352000	-2.340743000	1.422482000
6	4.540319000	-0.979716000	-1.383120000
1	4.700244000	-1.829142000	-2.059298000
1	5.316925000	-0.230522000	-1.596527000
1	3.566064000	-0.525937000	-1.624813000
6	4.564043000	-0.106497000	0.943322000
1	5.378455000	0.563569000	0.630654000
1	4.697778000	-0.306269000	2.013072000
1	3.614350000	0.430350000	0.814881000
6	3.497740000	-2.455748000	3.204393000
1	4.531639000	-2.089431000	3.165275000
1	3.375242000	-2.990739000	4.157629000
1	2.818076000	-1.591055000	3.218303000
6	1.795350000	-4.019508000	2.270099000
1	1.017885000	-3.244884000	2.340279000
1	1.794036000	-4.588739000	3.211548000
1	1.524724000	-4.715154000	1.463283000
6	4.204833000	-4.558315000	2.065066000
1	4.193156000	-5.018397000	3.064324000
1	5.231186000	-4.222747000	1.873331000
1	3.949313000	-5.345004000	1.344689000
6	1.070757000	3.346655000	-1.332363000
1	1.714818000	3.673451000	-2.148807000
6	0.134060000	4.355681000	-0.817554000
1	-0.511173000	4.039873000	0.009502000
6	0.046838000	5.608212000	-1.285386000
1	0.733091000	5.920199000	-2.078374000
6	-0.882085000	6.635870000	-0.812155000
6	-0.624369000	7.980449000	-1.111098000
6	-2.036090000	6.329738000	-0.074774000
6	-1.472687000	8.989239000	-0.667962000
1	0.261922000	8.230405000	-1.695616000
6	-2.883327000	7.336643000	0.368674000
1	-2.283878000	5.288184000	0.133660000
6	-2.604219000	8.671635000	0.078171000
1	-1.249307000	10.027859000	-0.907984000
1	-3.775407000	7.078388000	0.937952000
1	-3.272662000	9.458417000	0.424235000
7	-0.703694000	1.576258000	-1.031103000
6	-1.820465000	2.040504000	-1.791610000
6	-1.125370000	0.908197000	0.090218000
6	-3.018406000	1.664046000	-1.014107000
8	-1.722837000	2.597070000	-2.855529000
6	-2.594588000	0.994865000	0.132009000
8	-0.419486000	0.326459000	0.923261000
6	-4.359415000	1.829749000	-1.301989000
6	-3.491324000	0.461452000	1.039215000
1	-4.683934000	2.342832000	-2.205175000
6	-5.276229000	1.304959000	-0.385647000
1	-3.154539000	-0.073231000	1.925480000
6	-4.850549000	0.634395000	0.762439000
1	-6.342413000	1.415616000	-0.572550000
1	-5.591539000	0.234676000	1.451620000

Zero-point correction= 0.712946
(Hartree/Particle)
Thermal correction to Energy= 0.755736
Thermal correction to Enthalpy= 0.756680
Thermal correction to Gibbs Free Energy= 0.636403
Sum of electronic and zero-point Energies= -2191.666222
Sum of electronic and thermal Energies= -2191.623432
Sum of electronic and thermal Enthalpies= -2191.622488
Sum of electronic and thermal Free Energies= -2191.742766

E(M06/6-311+G(2d,p))= -2192.89004110

Transition state $TS_{c\text{-}(IXb\text{-}Xb)}$



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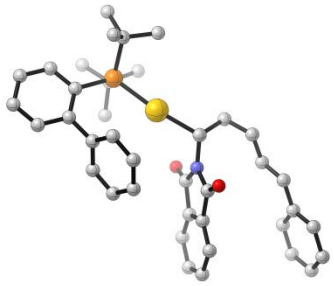
6	-5.110053000	1.849632000	0.650317000
6	-1.083020000	-1.698724000	0.488694000
1	-1.386707000	-1.881425000	1.524637000
6	-1.887214000	-2.369737000	-0.687113000
1	-1.427855000	-2.153558000	-1.653000000
1	-2.950259000	-2.133337000	-0.655732000
6	-2.821006000	3.813812000	0.993815000
6	-3.655111000	4.940622000	0.906930000
6	-1.581015000	3.946856000	1.656254000
6	-3.284028000	6.172466000	1.428501000
1	-4.619622000	4.863948000	0.411529000
6	-1.209679000	5.206333000	2.147042000
6	-2.043557000	6.310020000	2.040112000
1	-3.961487000	7.020269000	1.347195000
1	-0.245262000	5.302428000	2.645343000
1	-1.726679000	7.271296000	2.440584000
6	-0.615804000	2.846661000	1.922438000

6	0.636928000	2.842255000	1.301788000
6	-0.896732000	1.871813000	2.887870000
6	1.585010000	1.875502000	1.628255000
1	0.869362000	3.609862000	0.563025000
6	0.056717000	0.914595000	3.225758000
1	-1.862030000	1.886145000	3.396015000
6	1.299946000	0.915072000	2.595600000
1	2.558816000	1.888980000	1.140080000
1	-0.167944000	0.169904000	3.988647000
1	2.052220000	0.177899000	2.874336000
6	-6.222029000	2.632019000	-0.046374000
1	-7.183916000	2.312007000	0.381802000
1	-6.154620000	3.716606000	0.095895000
1	-6.261122000	2.422427000	-1.123169000
6	-5.179125000	2.071084000	2.161658000
1	-5.141605000	3.133120000	2.434995000
1	-6.129926000	1.663245000	2.536074000
1	-4.365889000	1.550087000	2.689799000
6	-5.343892000	0.360036000	0.375320000
1	-6.377912000	0.109827000	0.656974000
1	-5.217294000	0.097292000	-0.683331000
1	-4.671523000	-0.273889000	0.971102000
6	-3.633033000	1.505111000	-2.544660000
1	-4.714173000	1.332286000	-2.458561000
1	-3.413675000	1.696318000	-3.605856000
1	-3.104561000	0.582659000	-2.256389000
6	-1.674014000	2.930654000	-1.965490000
1	-1.073180000	2.042866000	-1.718211000
1	-1.519524000	3.151724000	-3.032345000
1	-1.287231000	3.784986000	-1.391965000
6	-3.920701000	3.956608000	-2.174937000
1	-3.723041000	4.106397000	-3.247000000
1	-5.006215000	3.873231000	-2.051043000
1	-3.576541000	4.858827000	-1.654059000
6	-1.440341000	-3.524628000	0.027214000
1	-2.067302000	-3.922304000	0.825285000
6	-0.228962000	-4.219068000	-0.297689000
1	0.298900000	-3.915057000	-1.205186000
6	0.259536000	-5.208145000	0.485374000
1	-0.328533000	-5.502953000	1.359688000
6	1.511260000	-5.918522000	0.297903000
6	1.739656000	-7.096269000	1.026324000
6	2.522459000	-5.446426000	-0.556843000
6	2.929126000	-7.798622000	0.884859000
1	0.965584000	-7.458503000	1.703284000
6	3.714685000	-6.142264000	-0.686945000
1	2.381577000	-4.511218000	-1.099039000
6	3.918686000	-7.323552000	0.027177000
1	3.089809000	-8.715476000	1.449152000
1	4.494852000	-5.756051000	-1.341135000
1	4.856499000	-7.866440000	-0.077922000
7	0.330470000	-1.593736000	0.371868000
6	1.208068000	-2.122366000	1.343713000
6	1.026733000	-1.098974000	-0.738996000
6	2.565169000	-1.999272000	0.767926000
8	0.862648000	-2.559966000	2.418314000
6	2.457540000	-1.383812000	-0.477746000
8	0.519281000	-0.575670000	-1.710071000
6	3.782044000	-2.421728000	1.268536000
6	3.566746000	-1.161721000	-1.272213000
1	3.854129000	-2.908864000	2.239319000
6	4.909064000	-2.210739000	0.467551000
1	3.476401000	-0.681244000	-2.244735000
6	4.803056000	-1.591068000	-0.778505000
1	5.885359000	-2.538561000	0.818976000
1	5.700113000	-1.440036000	-1.375642000

Zero-point correction= 0.711463
(Hartree/Particle)
Thermal correction to Energy= 0.753762
Thermal correction to Enthalpy= 0.754706
Thermal correction to Gibbs Free Energy= 0.636382
Sum of electronic and zero-point Energies= -2191.641256
Sum of electronic and thermal Energies= -2191.598956
Sum of electronic and thermal Enthalpies= -2191.598012
Sum of electronic and thermal Free Energies= -2191.716337

E(M06/6-311+G(2d,p))= -2192.86421689

Intermediate *c*-Xb



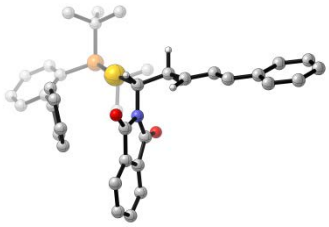
79	2.145862000	-0.290267000	-0.522192000
15	3.354372000	-2.313405000	-0.110116000
6	3.123572000	-2.668549000	1.736486000
6	5.168921000	-2.011706000	-0.595225000
6	1.255307000	1.655730000	-0.722140000
1	1.448293000	1.987231000	-1.750771000
6	1.982607000	2.628333000	0.299357000
1	1.716130000	2.356957000	1.326889000
1	3.060555000	2.528904000	0.145112000
6	2.793652000	-3.859668000	-0.945955000
6	3.564110000	-5.024789000	-0.793700000
6	1.569046000	-3.957637000	-1.643176000
6	3.148994000	-6.254629000	-1.286014000
1	4.511230000	-4.982275000	-0.262119000
6	1.152028000	-5.213682000	-2.107036000
6	1.924124000	-6.353143000	-1.935550000
1	3.777834000	-7.132301000	-1.149306000
1	0.200363000	-5.278803000	-2.634179000
1	1.573030000	-7.310904000	-2.315638000
6	0.660183000	-2.826455000	-1.972414000
6	-0.612766000	-2.761648000	-1.397395000
6	1.007342000	-1.888183000	-2.951544000
6	-1.515039000	-1.773215000	-1.782070000
1	-0.898176000	-3.500530000	-0.647770000
6	0.101354000	-0.905757000	-3.344341000
1	1.988213000	-1.947958000	-3.425289000
6	-1.161195000	-0.844809000	-2.758435000
1	-2.505258000	-1.740563000	-1.328953000
1	0.383043000	-0.189178000	-4.115228000
1	-1.872200000	-0.081452000	-3.074283000
6	6.211823000	-2.841329000	0.150642000
1	7.206352000	-2.572952000	-0.237340000
1	6.096460000	-3.922155000	0.009926000
1	6.215175000	-2.628245000	1.227041000
6	5.272462000	-2.271562000	-2.098208000
1	5.187114000	-3.336650000	-2.347693000
1	6.253701000	-1.922567000	-2.453583000
1	4.503081000	-1.722938000	-2.662554000
6	5.481879000	-0.531225000	-0.346127000
1	6.533672000	-0.345006000	-0.611777000
1	5.347899000	-0.238063000	0.703566000
1	4.855880000	0.126016000	-0.966314000
6	3.679181000	-1.487015000	2.531173000
1	4.775152000	-1.430733000	2.485084000
1	3.400502000	-1.608212000	3.588940000
1	3.265254000	-0.526977000	2.184834000
6	1.609481000	-2.746079000	1.951629000
1	1.100138000	-1.816413000	1.655991000
1	1.411885000	-2.917628000	3.020808000
1	1.158768000	-3.580926000	1.395599000
6	3.745929000	-3.965850000	2.245733000
1	3.542545000	-4.044339000	3.324604000
1	4.833701000	-4.004569000	2.114123000
1	3.303562000	-4.849724000	1.768896000
6	1.447935000	3.904091000	-0.137203000
1	1.910700000	4.383858000	-1.003944000
6	0.251580000	4.421121000	0.341183000
1	-0.198604000	3.966953000	1.226728000
6	-0.399329000	5.426082000	-0.345874000

1	0.101031000	5.828504000	-1.231738000
6	-1.693742000	5.956964000	-0.061174000
6	-2.244754000	6.891119000	-0.962183000
6	-2.455248000	5.546874000	1.055811000
6	-3.520244000	7.391731000	-0.762528000
1	-1.654082000	7.204384000	-1.822282000
6	-3.727101000	6.050920000	1.249643000
1	-2.039711000	4.838450000	1.770415000
6	-4.261049000	6.969808000	0.341039000
1	-3.941463000	8.108989000	-1.463357000
1	-4.312789000	5.735206000	2.110335000
1	-5.264245000	7.362046000	0.498097000
7	-0.177123000	1.654576000	-0.568935000
6	-1.054758000	2.239092000	-1.499461000
6	-0.869000000	1.160850000	0.543153000
6	-2.413226000	2.109251000	-0.923203000
8	-0.721127000	2.741482000	-2.551891000
6	-2.303511000	1.455847000	0.301323000
8	-0.362992000	0.627341000	1.510007000
6	-3.632362000	2.539355000	-1.412202000
6	-3.413641000	1.190957000	1.081320000
1	-3.705024000	3.060614000	-2.365384000
6	-4.762106000	2.276041000	-0.630972000
1	-3.321625000	0.677820000	2.036985000
6	-4.654425000	1.612406000	0.592284000
1	-5.741807000	2.597849000	-0.978847000
1	-5.553512000	1.420119000	1.174621000

Zero-point correction= 0.712434
(Hartree/Particle)
Thermal correction to Energy= 0.755212
Thermal correction to Enthalpy= 0.756156
Thermal correction to Gibbs Free Energy= 0.636677
Sum of electronic and zero-point Energies= -2191.645258
Sum of electronic and thermal Energies= -2191.602480
Sum of electronic and thermal Enthalpies= -2191.601536
Sum of electronic and thermal Free Energies= -2191.721015

E(M06/6-311+G(2d,p))= -2192.86947838

Transition state $TS_{c\text{-}Xb\text{-}t\text{-}Xb}$

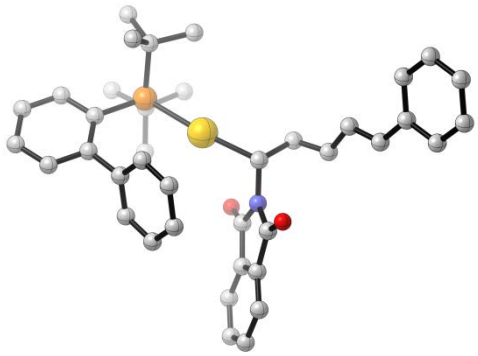


79	1.685168000	-0.349324000	-0.684118000
15	3.167607000	-2.141103000	-0.041546000
6	2.760271000	-2.511247000	1.773291000
6	4.961789000	-1.552991000	-0.297416000
6	0.458462000	1.343753000	-1.058861000
1	0.615006000	1.669856000	-2.096474000
6	0.751137000	2.523430000	-0.139313000
1	0.622825000	2.261774000	0.925286000
1	1.819935000	2.799437000	-0.217136000
6	3.008348000	-3.789216000	-0.860770000
6	3.941981000	-4.788020000	-0.540113000
6	1.925003000	-4.135089000	-1.697796000
6	3.817527000	-6.092720000	-0.997349000
1	4.788817000	-4.546155000	0.096828000
6	1.795670000	-5.466153000	-2.122226000
6	2.722990000	-6.439456000	-1.780933000
1	4.567534000	-6.834639000	-0.729600000
1	0.949548000	-5.724187000	-2.758875000
1	2.597460000	-7.460418000	-2.137412000
6	0.901797000	-3.197031000	-2.232659000
6	-0.445918000	-3.352699000	-1.890752000
6	1.248968000	-2.239820000	-3.193063000
6	-1.425532000	-2.568007000	-2.494546000
1	-0.725786000	-4.106753000	-1.153931000
6	0.268749000	-1.461788000	-3.803642000
1	2.295557000	-2.125398000	-3.479005000
6	-1.070768000	-1.627050000	-3.458426000
1	-2.473032000	-2.706803000	-2.225522000
1	0.552944000	-0.726391000	-4.555741000
1	-1.836547000	-1.023520000	-3.944601000
6	6.023853000	-2.158677000	0.618966000
1	7.000401000	-1.735000000	0.338192000
1	6.115931000	-3.247455000	0.532150000
1	5.853228000	-1.906182000	1.673560000
6	5.313399000	-1.839559000	-1.758640000
1	5.412421000	-2.912642000	-1.966956000
1	6.277130000	-1.362177000	-1.991864000
1	4.564351000	-1.424232000	-2.450147000
6	4.993661000	-0.033805000	-0.094772000
1	6.018478000	0.322655000	-0.280862000
1	4.721222000	0.260728000	0.927122000
1	4.321301000	0.487713000	-0.790403000
6	2.966060000	-1.228804000	2.579399000
1	4.027655000	-0.959933000	2.669703000
1	2.576426000	-1.380764000	3.597642000
1	2.426930000	-0.374958000	2.139947000
6	1.274659000	-2.879854000	1.786582000
1	0.643536000	-2.072174000	1.389064000
1	0.964849000	-3.073116000	2.825053000
1	1.074221000	-3.791761000	1.205559000
6	3.538480000	-3.650845000	2.425417000
1	3.205008000	-3.739695000	3.470756000
1	4.621364000	-3.481877000	2.441494000
1	3.343355000	-4.615721000	1.941405000
6	-0.037384000	3.740499000	-0.422391000
1	-0.654821000	3.746911000	-1.328556000
6	-0.037320000	4.864928000	0.363185000
1	0.563363000	4.883382000	1.273264000
6	-0.822141000	5.952173000	-0.018174000
1	-1.392672000	5.834713000	-0.943555000
6	-0.979220000	7.191262000	0.649658000
6	-1.868809000	8.134710000	0.083793000
6	-0.292085000	7.517268000	1.844288000
6	-2.067895000	9.360975000	0.688802000
1	-2.396961000	7.875430000	-0.832972000
6	-0.493664000	8.745789000	2.439069000
1	0.398272000	6.806609000	2.293018000
6	-1.379057000	9.664520000	1.864054000
1	-2.754876000	10.083496000	0.255048000
1	0.035751000	9.001615000	3.353834000
1	-1.531409000	10.630704000	2.342024000
7	-0.968547000	1.013357000	-0.997043000
6	-1.841861000	1.154658000	-2.080708000
6	-1.582565000	0.345235000	0.064384000
6	-3.121095000	0.524041000	-1.671095000
8	-1.572146000	1.694439000	-3.135901000
6	-2.967791000	0.042882000	-0.375118000
8	-1.057306000	0.073950000	1.126862000
6	-4.297877000	0.354073000	-2.375199000
6	-3.987497000	-0.627844000	0.273250000
1	-4.405331000	0.728123000	-3.392352000
6	-5.336412000	-0.325340000	-1.730011000
1	-3.860112000	-1.007054000	1.285775000
6	-5.183703000	-0.808156000	-0.429484000
1	-6.279542000	-0.484109000	-2.249739000
1	-6.009741000	-1.334968000	0.044611000

Zero-point correction= 0.710923
(Hartree/Particle)
Thermal correction to Energy= 0.753629
Thermal correction to Enthalpy= 0.754574
Thermal correction to Gibbs Free Energy= 0.634515
Sum of electronic and zero-point Energies= -2191.638179
Sum of electronic and thermal Energies= -2191.595473
Sum of electronic and thermal Enthalpies= -2191.594529
Sum of electronic and thermal Free Energies= -2191.714587

E(M06/6-311+G(2d,p))= -2192.86008044

Intermediate *t*-Xb



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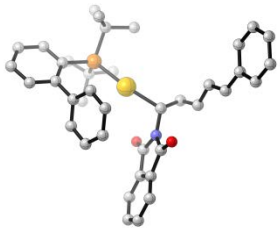
6	4.691305000	-1.102454000	0.310619000
6	-0.166115000	1.234662000	0.123990000
1	0.063742000	1.910944000	-0.709470000
6	-0.058338000	1.999638000	1.495361000
1	-0.547831000	1.402914000	2.271934000
1	0.992710000	2.166125000	1.756097000
6	3.110746000	-3.281954000	-1.069945000
6	4.125246000	-4.250076000	-0.980928000
6	2.151829000	-3.410892000	-2.099604000
6	4.191800000	-5.331370000	-1.848734000
1	4.882025000	-4.171156000	-0.204108000
6	2.220473000	-4.525071000	-2.949607000
6	3.220002000	-5.479412000	-2.831206000
1	4.994227000	-6.059577000	-1.745992000
1	1.472531000	-4.621024000	-3.736299000
1	3.245742000	-6.328393000	-3.512120000
6	1.065761000	-2.444821000	-2.414829000
6	-0.271428000	-2.851596000	-2.344518000
6	1.359452000	-1.177842000	-2.933867000
6	-1.293716000	-2.014029000	-2.785016000
1	-0.505250000	-3.842533000	-1.953261000
6	0.338008000	-0.341890000	-3.379502000
1	2.400473000	-0.860842000	-3.013908000
6	-0.989250000	-0.760568000	-3.310975000
1	-2.329830000	-2.349667000	-2.735306000
1	0.580697000	0.638788000	-3.787880000
1	-1.785935000	-0.109382000	-3.670332000
6	5.812681000	-1.845390000	1.031498000
1	6.724709000	-1.231220000	0.979421000
1	6.056215000	-2.814034000	0.579404000
1	5.587468000	-2.000420000	2.094424000
6	5.094700000	-0.830272000	-1.138775000
1	5.351321000	-1.749163000	-1.681901000
1	5.980922000	-0.177769000	-1.146722000
1	4.298191000	-0.312700000	-1.694783000
6	4.485797000	0.243171000	1.014775000
1	5.453417000	0.765191000	1.069239000
1	4.111218000	0.129805000	2.040608000
1	3.783752000	0.887540000	0.466188000
6	2.594225000	-1.984694000	3.000479000
1	3.602292000	-1.629835000	3.255622000
1	2.192644000	-2.499271000	3.886658000
1	1.953527000	-1.111474000	2.802888000
6	1.188519000	-3.505284000	1.613164000
1	0.453215000	-2.703327000	1.451375000
1	0.885596000	-4.064423000	2.511684000
1	1.139494000	-4.199433000	0.761433000
6	3.517542000	-4.141685000	2.160220000
1	3.171898000	-4.579111000	3.109268000
1	4.567815000	-3.857590000	2.295757000
1	3.462910000	-4.932850000	1.402752000
6	-0.752924000	3.226955000	1.150997000
1	-1.838180000	3.171938000	1.028839000
6	-0.130914000	4.422840000	0.821910000
1	0.948552000	4.511155000	0.953468000
6	-0.889133000	5.477368000	0.354455000
1	-1.961069000	5.294441000	0.233485000
6	-0.442432000	6.789574000	0.008896000
6	-1.399691000	7.713548000	-0.459351000
6	0.907233000	7.191741000	0.110758000
6	-1.023289000	8.996874000	-0.817144000
1	-2.440668000	7.401025000	-0.534873000
6	1.276060000	8.475225000	-0.245764000
1	1.660185000	6.493319000	0.471149000
6	0.313966000	9.377215000	-0.709656000
1	-1.765459000	9.704182000	-1.180634000
1	2.316283000	8.783560000	-0.166830000
1	0.612017000	10.386218000	-0.989048000
7	-1.495165000	0.733162000	-0.118749000
6	-2.343240000	1.230250000	-1.122168000
6	-2.040144000	-0.404859000	0.490758000
6	-3.516683000	0.326289000	-1.154676000
8	-2.115789000	2.210008000	-1.800712000
6	-3.339837000	-0.649125000	-0.177269000
8	-1.511750000	-1.045012000	1.377233000
6	-4.617710000	0.327347000	-1.989730000
6	-4.263138000	-1.660186000	0.012142000
1	-4.741813000	1.088748000	-2.758046000
6	-5.556380000	-0.693385000	-1.809971000
1	-4.118128000	-2.421054000	0.777055000
6	-5.382353000	-1.668404000	-0.826024000
1	-6.437266000	-0.730780000	-2.447908000
1	-6.131779000	-2.449401000	-0.712217000

Zero-point correction= 0.712649
(Hartree/Particle)
Thermal correction to Energy= 0.755680
Thermal correction to Enthalpy= 0.756624
Thermal correction to Gibbs Free Energy= 0.635206
Sum of electronic and zero-point Energies= -2191.643047
Sum of electronic and thermal Energies= -2191.600016
Sum of electronic and thermal Enthalpies= -2191.599072
Sum of electronic and thermal Free Energies= -2191.720490

E(M06/6-311+G(2d,p))= -2192.86619429

Transition state TS$_{t\text{-IXb-}c\text{-IXb}}$



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6	4.513150000	-0.782895000	0.406810000
6	-0.469996000	1.221031000	0.411849000
1	-0.131789000	1.802355000	-0.452788000
6	-0.192730000	1.754553000	1.865636000
1	-0.780845000	1.184595000	2.583824000
1	0.866689000	1.800100000	2.126214000
6	3.137692000	-2.910184000	-1.265199000
6	4.267490000	-3.742994000	-1.325593000
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6	4.440138000	-4.677838000	-2.336822000
1	5.034097000	-3.668780000	-0.558084000
6	2.345056000	-3.991954000	-3.281338000
6	3.462270000	-4.813727000	-3.315175000
1	5.331821000	-5.301717000	-2.349902000
1	1.586281000	-4.079241000	-4.058686000
1	3.572498000	-5.550941000	-4.108489000
6	0.948705000	-2.179501000	-2.439042000

6	-0.322266000	-2.745136000	-2.291605000
6	1.052145000	-0.858123000	-2.891921000
6	-1.466390000	-2.009497000	-2.594383000
1	-0.408406000	-3.779589000	-1.957042000
6	-0.091034000	-0.123959000	-3.198648000
1	2.039572000	-0.417114000	-3.036282000
6	-1.351787000	-0.699909000	-3.055138000
1	-2.449713000	-2.467731000	-2.487722000
1	0.004465000	0.897953000	-3.564840000
1	-2.242459000	-0.132196000	-3.322368000
6	5.690075000	-1.490194000	1.076283000
1	6.542897000	-0.794805000	1.096506000
1	6.023810000	-2.387095000	0.541528000
1	5.469637000	-1.763795000	2.116372000
6	4.914006000	-0.315312000	-0.992108000
1	5.295458000	-1.133766000	-1.615116000
1	5.712535000	0.436024000	-0.899514000
1	4.075599000	0.160017000	-1.523087000
6	4.169482000	0.455240000	1.243919000
1	5.085601000	1.049568000	1.379201000
1	3.787987000	0.203666000	2.242355000
1	3.425318000	1.092561000	0.744019000
6	2.529320000	-2.199831000	2.938215000
1	3.499868000	-1.776210000	3.230246000
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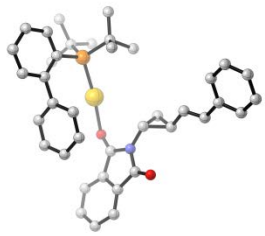
1	1.796173000	-1.381319000	2.865556000
6	1.254895000	-3.651551000	1.357790000
1	0.446601000	-2.907704000	1.311461000
1	1.017759000	-4.358008000	2.167466000
1	1.261668000	-4.218365000	0.415365000
6	3.643575000	-4.128658000	1.811795000
1	3.360527000	-4.726011000	2.691595000
1	4.661075000	-3.757663000	1.980652000
1	3.656225000	-4.808420000	0.950614000
6	-0.760581000	2.930577000	1.286956000
1	-1.846376000	3.008873000	1.226610000
6	0.012470000	4.035876000	0.814299000
1	1.093448000	3.998208000	0.970816000
6	-0.584112000	5.098661000	0.223258000
1	-1.667693000	5.048601000	0.079267000
6	0.053771000	6.314249000	-0.243977000
6	-0.733485000	7.281129000	-0.889010000
6	1.427105000	6.563515000	-0.078413000
6	-0.167916000	8.457517000	-1.362976000
1	-1.799871000	7.093554000	-1.017074000
6	1.989460000	7.739037000	-0.550628000
1	2.054373000	5.832434000	0.430002000
6	1.194782000	8.688883000	-1.194865000
1	-0.791013000	9.196764000	-1.862980000
1	3.053965000	7.922252000	-0.414854000
1	1.640339000	9.611195000	-1.563776000
7	-1.769828000	0.681917000	0.198835000
6	-2.678978000	1.198785000	-0.745421000
6	-2.247352000	-0.507298000	0.776252000
6	-3.830618000	0.269465000	-0.748121000
8	-2.495863000	2.204739000	-1.395010000
6	-3.579853000	-0.741303000	0.177192000
8	-1.641645000	-1.180929000	1.582883000
6	-4.980993000	0.283421000	-1.513986000
6	-4.474550000	-1.775295000	0.381325000
1	-5.162732000	1.071430000	-2.242675000
6	-5.891739000	-0.758890000	-1.317053000
1	-4.272285000	-2.562874000	1.104861000
6	-5.643949000	-1.767799000	-0.384442000
1	-6.809591000	-0.785890000	-1.900842000
1	-6.375137000	-2.563337000	-0.255499000

Zero-point correction= 0.712012
(Hartree/Particle)
Thermal correction to Energy= 0.754433
Thermal correction to Enthalpy= 0.755377
Thermal correction to Gibbs Free Energy= 0.636580
Sum of electronic and zero-point Energies= -2191.640669
Sum of electronic and thermal Energies= -2191.598249
Sum of electronic and thermal Enthalpies= -2191.597305
Sum of electronic and thermal Free Energies= -2191.716101

E(M06/6-311+G(2d,p))= -2192.86366014

Intermediate *t*-IXb



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6	3.732783000	-0.280344000	0.490218000
6	-0.927588000	1.568240000	0.397662000
1	-0.073895000	1.315878000	-0.238800000
6	-0.679180000	1.838764000	1.849089000
1	-1.458910000	1.531603000	2.544726000
1	0.339336000	1.732642000	2.220617000
6	3.096098000	-2.678813000	-1.234607000
6	4.424179000	-3.085763000	-1.449091000
6	2.131508000	-2.984753000	-2.219883000
6	4.798672000	-3.805623000	-2.574986000
1	5.192575000	-2.845911000	-0.718744000
6	2.526118000	-3.734920000	-3.336860000
6	3.837714000	-4.148657000	-3.518409000
1	5.837741000	-4.101165000	-2.706269000
1	1.774747000	-3.971992000	-4.089542000
1	4.108623000	-4.725118000	-4.401075000
6	0.709734000	-2.540726000	-2.238925000
6	-0.324716000	-3.474895000	-2.112847000
6	0.389014000	-1.216093000	-2.563480000
6	-1.650290000	-3.093737000	-2.307006000
1	-0.080421000	-4.511957000	-1.878852000
6	-0.936320000	-0.837557000	-2.767640000
1	1.192187000	-0.488664000	-2.690375000
6	-1.958201000	-1.777514000	-2.645505000
1	-2.444232000	-3.833479000	-2.211303000
1	-1.168282000	0.191868000	-3.042282000
1	-2.992970000	-1.490283000	-2.832498000
6	5.193622000	-0.492635000	0.878256000
1	5.687817000	0.490093000	0.896692000
1	5.746356000	-1.115392000	0.165112000
1	5.293938000	-0.927690000	1.880578000
6	3.647156000	0.403401000	-0.875072000
1	4.142174000	-0.170611000	-1.668877000
1	4.146660000	1.381382000	-0.807072000
1	2.604959000	0.587573000	-1.177980000
6	3.086791000	0.643093000	1.524027000
1	3.655926000	1.584394000	1.556968000
1	3.086697000	0.220651000	2.536379000
1	2.050340000	0.882412000	1.250861000
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1	2.910781000	-3.288212000	3.845128000
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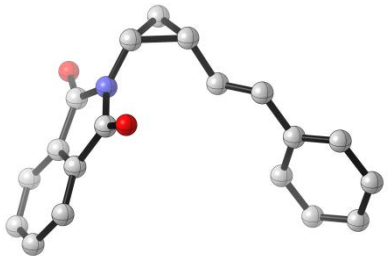
1	2.224791000	-5.053435000	2.272395000
1	2.148417000	-4.758108000	0.524444000
6	4.472944000	-3.784655000	1.659239000
1	4.573851000	-4.445429000	2.532890000
1	5.282503000	-3.047441000	1.711504000
1	4.617768000	-4.405438000	0.767439000
6	-0.992133000	2.982785000	0.926672000
1	-1.990716000	3.411078000	1.011571000
6	0.069245000	3.907355000	0.502900000
1	1.069395000	3.470096000	0.411461000
6	-0.136827000	5.200818000	0.221166000

1	-1.152116000	5.594553000	0.328826000
6	0.860750000	6.169741000	-0.234867000
6	0.459379000	7.492973000	-0.465400000
6	2.205069000	5.837767000	-0.465517000
6	1.362339000	8.452254000	-0.911016000
1	-0.582298000	7.765796000	-0.291344000
6	3.106881000	6.794642000	-0.910454000
1	2.550942000	4.817192000	-0.299680000
6	2.691307000	8.106937000	-1.136686000
1	1.025214000	9.473364000	-1.083880000
1	4.145088000	6.515551000	-1.086035000
1	3.401384000	8.853137000	-1.489552000
7	-2.149788000	0.919855000	0.032663000
6	-3.174388000	1.501869000	-0.770584000
6	-2.465323000	-0.377241000	0.358605000
6	-4.239692000	0.479279000	-0.850874000
8	-3.116647000	2.597730000	-1.268355000
6	-3.818984000	-0.647499000	-0.147095000
8	-1.729012000	-1.177380000	0.949410000
6	-5.445506000	0.503882000	-1.523856000
6	-4.583596000	-1.797941000	-0.086454000
1	-5.761116000	1.382326000	-2.083394000
6	-6.231916000	-0.651224000	-1.463075000
1	-4.241316000	-2.680390000	0.451374000
6	-5.810371000	-1.778816000	-0.755897000
1	-7.188758000	-0.674908000	-1.980346000
1	-6.446247000	-2.661331000	-0.734007000

Zero-point correction= 0.712733 (Hartree/Particle)
Thermal correction to Energy= 0.755641
Thermal correction to Enthalpy= 0.756585
Thermal correction to Gibbs Free Energy= 0.636653
Sum of electronic and zero-point Energies= -2191.666788
Sum of electronic and thermal Energies= -2191.623880
Sum of electronic and thermal Enthalpies= -2191.622936
Sum of electronic and thermal Free Energies= -2191.742868

E(M06/6-311+G(2d,p))= -2192.89079352

Product *cis*-6a

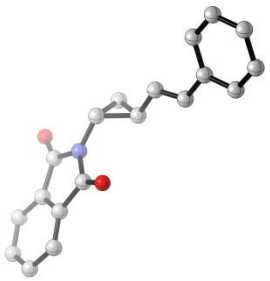


6	-0.999130000	-2.535189000	-0.450601000
1	-1.416973000	-3.145954000	-1.250866000
6	-0.455969000	-3.229138000	0.747606000
1	-0.545204000	-2.716232000	1.703289000
1	-0.562317000	-4.310389000	0.797049000
6	0.503969000	-2.638893000	-0.252372000
1	0.997972000	-3.334475000	-0.931478000
6	1.294718000	-1.459411000	0.120758000
1	0.805620000	-0.744397000	0.789251000
6	2.549582000	-1.245050000	-0.300336000
1	3.000783000	-1.985943000	-0.967691000
6	3.406362000	-0.105843000	0.030223000
6	4.688585000	-0.038741000	-0.533346000
6	3.007779000	0.935225000	0.883894000
6	5.541565000	1.024970000	-0.260267000
1	5.013979000	-0.839512000	-1.198800000
6	3.858587000	1.997186000	1.157554000
1	2.018820000	0.912681000	1.340993000
6	5.130426000	2.049971000	0.586761000
1	6.532032000	1.053114000	-0.712605000
1	3.527102000	2.793277000	1.823241000
1	5.794582000	2.885003000	0.804188000
7	-1.637425000	-1.266305000	-0.289919000
6	-1.475186000	-0.217127000	-1.211597000
6	-2.591123000	-0.950645000	0.692340000
6	-2.337667000	0.885974000	-0.725579000
8	-0.771930000	-0.258676000	-2.195919000
6	-3.001105000	0.448247000	0.415900000
8	-2.984116000	-1.690514000	1.566744000
6	-2.532246000	2.156723000	-1.235133000
6	-3.887302000	1.261693000	1.097320000
1	-2.009441000	2.490427000	-2.129675000
6	-3.423283000	2.989002000	-0.552499000
1	-4.403966000	0.909103000	1.988273000
6	-4.088920000	2.549409000	0.593697000
1	-3.603253000	3.997846000	-0.919041000
1	-4.777239000	3.222932000	1.100774000

Zero-point correction= 0.292509 (Hartree/Particle)
Thermal correction to Energy= 0.310261
Thermal correction to Enthalpy= 0.311206
Thermal correction to Gibbs Free Energy= 0.243913
Sum of electronic and zero-point Energies= -937.302816
Sum of electronic and thermal Energies= -937.285064
Sum of electronic and thermal Enthalpies= -937.284120
Sum of electronic and thermal Free Energies= -937.351413

E(M06/6-311+G(2d,p))= -937.863691691

Product *trans*-6a



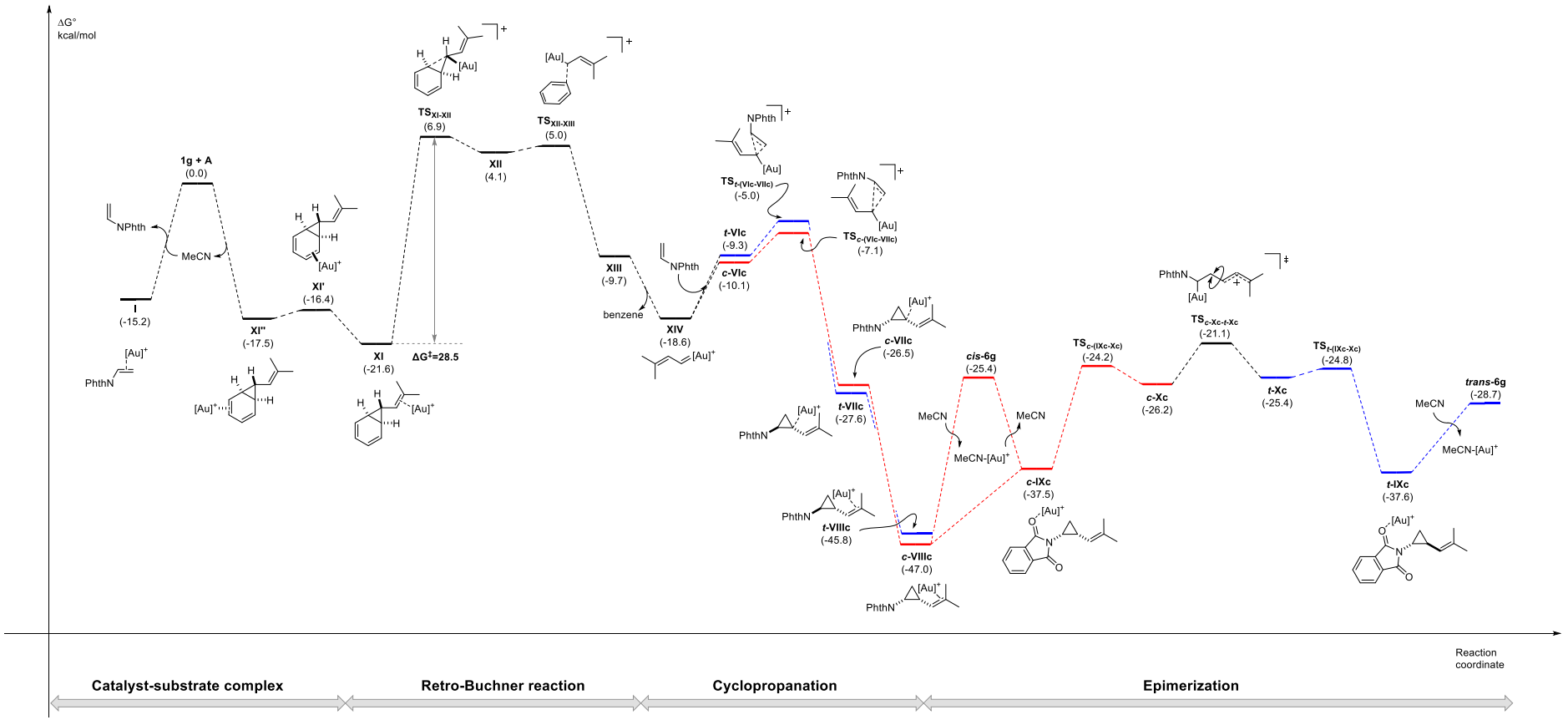
6	0.463289000	1.353654000	-0.275694000
6	-0.603494000	0.989265000	0.733493000
6	0.090383000	2.323404000	0.791703000
1	0.130114000	1.557641000	-1.294173000
1	0.806742000	2.482456000	1.595109000
1	-0.469244000	3.206662000	0.488012000
7	1.719481000	0.680461000	-0.178999000
6	2.963070000	1.332327000	-0.138024000
6	1.863473000	-0.715869000	-0.227284000
6	3.980547000	0.253472000	-0.097580000
8	3.127330000	2.531980000	-0.141483000
6	3.322033000	-0.971374000	-0.150001000
8	0.956628000	-1.513273000	-0.316021000
6	5.359384000	0.331718000	-0.029032000
6	4.013498000	-2.168368000	-0.137224000
1	5.867104000	1.293900000	0.010898000
6	6.068658000	-0.872189000	-0.014070000
1	3.489969000	-3.121818000	-0.181401000
6	5.407161000	-2.101091000	-0.066488000
1	7.155546000	-0.853951000	0.038851000
1	5.989751000	-3.020341000	-0.054475000
6	-1.993055000	0.887322000	0.271326000
1	-2.306670000	1.644037000	-0.455024000
6	-2.847222000	-0.062385000	0.678497000
1	-2.486573000	-0.801029000	1.401172000
6	-4.235895000	-0.237705000	0.251939000
6	-4.968866000	-1.318704000	0.761408000
6	-4.876174000	0.625236000	-0.651836000
6	-6.289503000	-1.536033000	0.383335000
1	-4.485510000	-1.997773000	1.465037000
6	-6.194367000	0.409195000	-1.029641000
1	-4.335731000	1.476382000	-1.065247000
6	-6.909250000	-0.672282000	-0.515119000

1	-6.835966000	-2.384230000	0.793600000
1	-6.670042000	1.091777000	-1.732778000
1	-7.943239000	-0.838563000	-0.813363000
1	-0.296298000	0.254422000	1.478560000

Zero-point correction= 0.292519
(Hartree/Particle)
Thermal correction to Energy= 0.310294
Thermal correction to Enthalpy= 0.311238
Thermal correction to Gibbs Free Energy= 0.244902
Sum of electronic and zero-point Energies= -937.303110
Sum of electronic and thermal Energies= -937.285334
Sum of electronic and thermal Enthalpies= -937.284390
Sum of electronic and thermal Free Energies= -937.350726

E(M06/6-311+G(2d,p))= -937.864197858

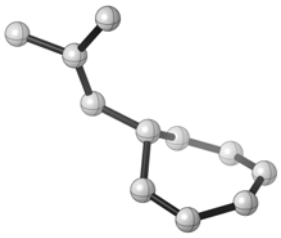
Calculated free energy profile for the formation and isomerization of 6g



Computational details:
SMD(CH_2Cl_2)-M06/6-311+G(2d,p), SDD(Au, f=1.05)//SMD(CH_2Cl_2)-M06/6-31G(d), SDD(Au)
Gibbs free energies given in kcal/mol at the standard state (298.15 K, 1 atm)
[Au] = Au-JohnPhos

Cartesian coordinates (in Å) and energies (in h) for reactants, intermediates and transition states involved in the formation and isomerization of 6g

Reactant 1g

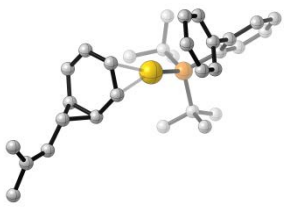


6	-0.071919000	0.000236000	-0.189094000
1	-0.145850000	-0.000062000	0.911715000
6	-0.831144000	-1.193944000	-0.704932000
1	-0.349042000	-1.820716000	-1.458480000
6	-2.056239000	-1.515544000	-0.238503000
1	-2.501411000	-2.461884000	-0.553249000
6	-2.858210000	-0.682403000	0.619797000
1	-3.629505000	-1.182662000	1.208728000
6	-2.858377000	0.681777000	0.620050000
1	-3.629780000	1.181631000	1.209189000
6	-2.056581000	1.515513000	-0.237841000
1	-2.502010000	2.461896000	-0.552114000
6	-0.831347000	1.194513000	-0.704335000
1	-0.349370000	1.821849000	-1.457487000
6	1.357251000	0.000280000	-0.637631000
1	1.482621000	0.000609000	-1.727081000
6	2.465303000	-0.000073000	0.114837000
6	2.494384000	-0.000379000	1.612381000
1	3.041269000	-0.880084000	1.984923000
1	3.041016000	0.879360000	1.985270000
1	1.502327000	-0.000556000	2.076783000
6	3.823188000	0.000076000	-0.520675000
1	4.406464000	0.879989000	-0.207500000
1	4.406223000	-0.880295000	-0.208360000
1	3.769201000	0.000627000	-1.616661000

Zero-point correction= 0.216277
(Hartree/Particle)
Thermal correction to Energy= 0.227338
Thermal correction to Enthalpy= 0.228282
Thermal correction to Gibbs Free Energy= 0.179136
Sum of electronic and zero-point Energies= -426.968784
Sum of electronic and thermal Energies= -426.957723
Sum of electronic and thermal Enthalpies= -426.956778
Sum of electronic and thermal Free Energies= -427.005925

E(M06/6-311+G(2d,p))= -427.315116865

Intermediate XI''



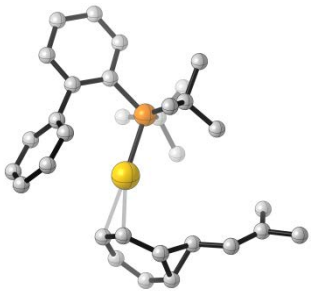
6	2.333874000	0.965282000	-0.191964000
6	1.996615000	1.432855000	1.062891000
6	2.374353000	0.703278000	2.268876000
6	3.070155000	-0.448221000	2.187343000
1	2.091290000	1.557144000	-1.077211000
1	1.507707000	2.403892000	1.161306000
1	2.006033000	1.068686000	3.225504000
1	3.233945000	-1.051717000	3.079767000
79	0.124725000	0.237121000	0.200972000
15	-1.808357000	-1.095508000	-0.080208000
6	-1.568006000	-2.096654000	-1.665198000
6	-1.989370000	-2.162470000	1.483352000
6	-3.366569000	-0.139470000	-0.277941000
6	-0.379824000	-3.037301000	-1.473847000
6	-1.234247000	-1.082890000	-2.761555000
6	-2.791955000	-2.896706000	-2.106099000
6	-2.788176000	-3.451595000	1.306199000
6	-2.648741000	-1.280480000	2.544446000
6	-0.585639000	-2.530232000	1.977329000
6	-4.577998000	-0.850241000	-0.309549000
6	-3.413026000	1.270972000	-0.314514000
1	-0.592373000	-3.836553000	-0.751775000
1	-0.151997000	-3.516374000	-2.437726000
1	0.523868000	-2.502571000	-1.144525000
1	-0.312679000	-0.523285000	-2.539897000
1	-1.083886000	-1.620948000	-3.709299000
1	-2.049303000	-0.361536000	-2.918288000
1	-2.520334000	-3.470212000	-3.004975000
1	-3.132102000	-3.614789000	-1.350630000
1	-3.633288000	-2.247345000	-2.378462000
1	-2.829204000	-3.964535000	2.278754000
1	-3.825209000	-3.279194000	0.994991000
1	-2.315748000	-4.140820000	0.594026000
1	-3.704654000	-1.076597000	2.327460000
1	-2.599928000	-1.800376000	3.512562000
1	-2.128328000	-0.317004000	2.661003000
1	-0.687157000	-3.153915000	2.878054000
1	-0.007572000	-3.103409000	1.240882000
1	-0.003388000	-1.638601000	2.251713000
6	-5.806108000	-0.206257000	-0.365886000
1	-4.568181000	-1.936308000	-0.276961000
6	-4.663748000	1.902904000	-0.359739000
6	-2.244660000	2.196171000	-0.317300000
6	-5.849065000	1.182881000	-0.385647000
1	-6.723336000	-0.791523000	-0.386699000
1	-4.691282000	2.991936000	-0.383398000
6	-1.522256000	2.441886000	-1.490731000
6	-1.962396000	2.957752000	0.822520000
1	-6.802714000	1.706328000	-0.423214000
6	-0.533129000	3.422558000	-1.520343000
1	-1.757470000	1.875333000	-2.392228000
6	-0.969027000	3.933766000	0.794423000
1	-2.540768000	2.788716000	1.731933000
6	-0.253683000	4.170418000	-0.377930000
1	0.008786000	3.613901000	-2.445774000
1	-0.764217000	4.522471000	1.687546000
1	0.509973000	4.946317000	-0.406055000
6	3.231084000	-0.187792000	-0.356085000
1	3.121066000	-0.767703000	-1.273379000
6	4.638477000	-0.097463000	0.184775000
1	4.884270000	0.843768000	0.679345000
6	3.623426000	-0.945079000	0.921773000
1	3.768836000	-2.022210000	0.836211000
6	6.975405000	-0.370319000	-0.727583000
6	5.708018000	-0.778447000	-0.564035000
1	5.406527000	-1.722212000	-1.031938000
6	7.944170000	-1.184089000	-1.529746000
1	8.820217000	-1.465395000	-0.924981000
1	7.491789000	-2.103483000	-1.922080000
1	8.335131000	-0.605681000	-2.381238000
6	7.551557000	0.888892000	-0.159160000
1	6.845581000	1.469312000	0.444773000
1	8.424416000	0.661025000	0.471521000

1	7.920676000	1.542051000	-0.964732000

Zero-point correction= 0.637000
(Hartree/Particle)
Thermal correction to Energy= 0.673030
Thermal correction to Enthalpy= 0.673974
Thermal correction to Gibbs Free Energy= 0.568698
Sum of electronic and zero-point Energies= -1681.345878
Sum of electronic and thermal Energies= -1681.309848
Sum of electronic and thermal Enthalpies= -1681.308904
Sum of electronic and thermal Free Energies= -1681.414181

E(M06/6-311+G(2d,p))= -1682.35502229

Intermediate XI'

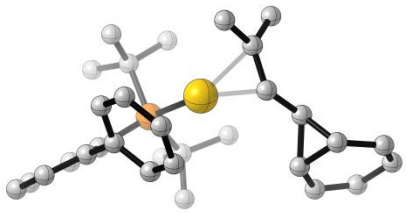


6	-1.912779000	-2.338362000	-0.568897000
6	-3.667058000	-0.455598000	-0.077057000
6	-1.422604000	-2.674263000	0.679770000
6	-3.238812000	-1.732794000	-0.742323000
6	-2.260518000	-2.564468000	1.862525000
6	-4.165013000	-1.758280000	0.505669000
6	-3.568369000	-2.248534000	1.745918000
1	-1.431263000	-2.754626000	-1.455096000
1	-0.521737000	-3.290366000	0.744148000
1	-3.715750000	-1.921717000	-1.704316000
1	-1.855301000	-2.901896000	2.814297000
1	-5.221320000	-1.972257000	0.340638000
1	-4.232852000	-2.379021000	2.599654000
1	-2.896343000	0.039765000	0.520037000
6	-4.884396000	1.698005000	-0.589640000
79	-0.242995000	-0.738913000	0.073623000
15	1.037092000	1.257622000	0.115495000
6	0.411723000	2.342876000	-1.302131000
6	0.806789000	2.002804000	1.850999000
6	2.849697000	1.044249000	-0.121508000
6	-1.052556000	2.682285000	-1.033222000
6	0.505280000	1.483003000	-2.563512000
6	1.193690000	3.633408000	-1.540889000
6	1.116589000	3.492514000	1.967509000
6	1.717566000	1.204711000	2.785660000
6	-0.643384000	1.785389000	2.293326000
6	3.654487000	2.192049000	-0.030331000
6	3.482489000	-0.208931000	-0.281259000
1	-1.660401000	1.784733000	-0.840054000
1	-1.163547000	3.373779000	-0.187573000
1	-1.470767000	3.178552000	-1.922185000
1	-0.105778000	0.570877000	-2.489322000
1	0.133877000	2.067897000	-3.418262000
1	1.541173000	1.191902000	-2.788475000
1	0.692868000	4.188258000	-2.348245000
1	1.222478000	4.289719000	-0.662026000
1	2.221617000	3.439939000	-1.871090000
1	0.931193000	3.802022000	3.007195000
1	2.162623000	3.732513000	1.746193000
1	0.467990000	4.102286000	1.325060000
1	2.782046000	1.398227000	2.601930000
1	1.497880000	1.496630000	3.823250000
1	1.543182000	0.120321000	2.706840000
1	-0.753898000	2.173308000	3.316964000
1	-1.361970000	2.321966000	1.661404000
1	-0.919236000	0.720689000	2.309575000
6	5.039995000	2.125759000	-0.077604000
1	3.192613000	3.168126000	0.088382000
6	4.883621000	-0.256562000	-0.304863000
6	2.799750000	-1.519528000	-0.455666000
6	5.660239000	0.888725000	-0.205445000
1	5.627807000	3.038874000	-0.007102000
1	5.363742000	-1.227704000	-0.424321000
6	2.137119000	-1.835761000	-1.648202000
6	2.931385000	-2.509040000	0.524775000
1	6.745650000	0.813482000	-0.234476000
6	1.614646000	-3.110950000	-1.851405000
1	2.054125000	-1.081212000	-2.430809000
6	2.396216000	-3.779831000	0.327510000
1	3.468409000	-2.277582000	1.445549000
6	1.738280000	-4.084995000	-0.862113000
1	1.116136000	-3.345320000	-2.791373000
1	2.509608000	-4.539331000	1.099806000
1	1.333846000	-5.083212000	-1.023210000
6	-4.616712000	0.402431000	-0.813019000
1	-5.156136000	-0.101583000	-1.622108000
6	-5.861059000	2.438417000	-1.450512000
1	-6.304500000	1.796646000	-2.221978000
1	-6.676805000	2.864982000	-0.847197000
1	-5.375040000	3.289094000	-1.953498000
6	-4.273740000	2.518867000	0.502739000
1	-3.740625000	3.389191000	0.088760000
1	-5.061190000	2.928278000	1.154270000
1	-3.579540000	1.957983000	1.139275000

Zero-point correction= 0.638873
(Hartree/Particle)
Thermal correction to Energy= 0.674142
Thermal correction to Enthalpy= 0.675086
Thermal correction to Gibbs Free Energy= 0.572980
Sum of electronic and zero-point Energies= -1681.346266
Sum of electronic and thermal Energies= -1681.310997
Sum of electronic and thermal Enthalpies= -1681.310053
Sum of electronic and thermal Free Energies= -1681.412158

E(M06/6-311+G(2d,p))= -1682.35752425

Intermediate XI



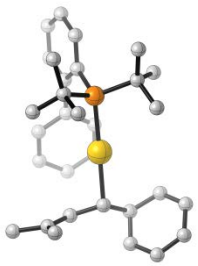
6	-3.443020000	-1.616843000	-2.028669000
6	-3.413809000	0.025750000	-0.052736000
6	-4.575114000	-2.321889000	-1.824391000
6	-3.294218000	-0.244388000	-1.535496000
6	-5.764772000	-1.693023000	-1.284636000
6	-4.557825000	0.424269000	-0.963081000
6	-5.781337000	-0.381868000	-0.966831000
1	-2.614754000	-2.048675000	-2.591453000
1	-4.645854000	-3.351093000	-2.174080000
1	-2.581570000	0.396018000	-2.060181000
1	-6.686315000	-2.272595000	-1.248741000
1	-4.666592000	1.498883000	-1.114412000
1	-6.718483000	0.118921000	-0.725830000
1	-3.597410000	-0.852046000	0.568669000
6	-2.211184000	1.222826000	1.853004000
79	-0.416787000	0.294044000	0.576297000
15	1.513799000	-1.032874000	0.233872000
6	2.267141000	-1.363583000	1.939417000
6	0.914854000	-2.590083000	-0.672905000
6	2.857534000	-0.272332000	-0.765346000
6	1.285564000	-2.199525000	2.757697000
6	2.432168000	0.008538000	2.595732000
6	3.626172000	-2.060675000	1.919123000

6	1.851940000	-3.793387000	-0.601997000
6	0.707295000	-2.173075000	-2.129832000
6	-0.439150000	-3.014543000	-0.093041000
6	3.984022000	-1.057006000	-1.063534000
6	2.848966000	1.075978000	-1.183619000
1	1.227677000	-3.234107000	2.396544000
1	1.637154000	-2.233183000	3.799556000
1	0.271531000	-1.773291000	2.763847000
1	1.464578000	0.516786000	2.732640000
1	2.889341000	-0.123850000	3.587799000
1	3.091458000	0.669337000	2.014278000
1	3.921277000	-2.265258000	2.959089000
1	3.606319000	-3.021446000	1.389497000
1	4.408337000	-1.431532000	1.477125000
1	1.380772000	-4.627842000	-1.142917000
1	2.822967000	-3.615604000	-1.078534000
1	2.017091000	-4.127154000	0.430848000
1	1.651233000	-1.931581000	-2.636033000
1	0.239132000	-3.007098000	-2.673686000
1	0.038912000	-1.301876000	-2.214926000
1	-0.822523000	-3.854235000	-0.692204000
1	-0.367160000	-3.358445000	0.946291000
1	-1.185603000	-2.207361000	-0.134463000
6	5.082855000	-0.540032000	-1.735309000
1	4.015959000	-2.097439000	-0.752971000
6	3.978677000	1.586587000	-1.838115000
6	1.726684000	2.041454000	-1.019460000
6	5.085303000	0.797049000	-2.114797000
1	5.935989000	-1.180047000	-1.951680000
1	3.968063000	2.631743000	-2.146385000
6	1.827720000	3.083500000	-0.092029000
6	0.632205000	2.016332000	-1.892591000
1	5.943075000	1.225560000	-2.630018000
6	0.850883000	4.074348000	-0.028989000
1	2.692055000	3.125116000	0.571495000
6	-0.336978000	3.016472000	-1.838636000
1	0.558340000	1.222874000	-2.638774000
6	-0.230723000	4.046641000	-0.906491000
1	0.945892000	4.879497000	0.698332000
1	-1.172678000	2.997036000	-2.537643000
1	-0.984941000	4.831632000	-0.869745000
6	-2.608396000	1.109871000	0.533537000
1	-2.493934000	2.000052000	-0.097749000
6	-1.693692000	2.529378000	2.380932000
1	-1.492693000	3.249300000	1.579093000
1	-2.444114000	2.965475000	3.058879000
1	-0.776557000	2.394808000	2.972035000
6	-2.517529000	0.198924000	2.906917000
1	-2.692015000	-0.807340000	2.508939000
1	-1.699421000	0.143504000	3.638600000
1	-3.418714000	0.506231000	3.460373000

Zero-point correction= 0.636432
(Hartree/Particle)
Thermal correction to Energy= 0.672272
Thermal correction to Enthalpy= 0.673216
Thermal correction to Gibbs Free Energy= 0.569580
Sum of electronic and zero-point Energies= -1681.353299
Sum of electronic and thermal Energies= -1681.317459
Sum of electronic and thermal Enthalpies= -1681.316515
Sum of electronic and thermal Free Energies= -1681.420152

E(M06/6-311+G(2d,p))= -1682.36240346

Transition state TS_{XI-XII}



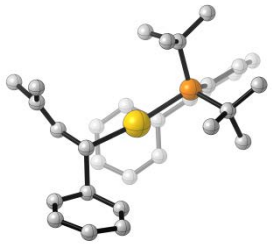
6	-2.783455000	-0.855021000	-2.275683000
6	-2.729219000	0.015574000	0.215019000
6	-3.423664000	-2.041273000	-2.397695000
6	-3.255480000	0.162550000	-1.334450000
6	-4.623310000	-2.297509000	-1.654541000
6	-4.541701000	-0.078736000	-0.735139000
6	-5.178923000	-1.335483000	-0.855469000
1	-1.886016000	-0.638975000	-2.857659000
1	-3.052551000	-2.801508000	-3.081959000
1	-3.011756000	1.194599000	-1.599074000
1	-5.111930000	-3.264331000	-1.762225000
1	-5.023814000	0.727055000	-0.186911000
1	-6.114916000	-1.512739000	-0.331126000
1	-3.014633000	-0.929435000	0.688646000
6	-3.074259000	1.247967000	2.378005000
79	-0.564615000	-0.266032000	0.060293000
15	1.720554000	-0.869540000	0.246941000
6	2.034657000	-1.071247000	2.105332000
6	1.976477000	-2.461833000	-0.757641000
6	2.979132000	0.353153000	-0.311771000
6	1.140086000	-2.193891000	2.628673000
6	1.609097000	0.257102000	2.738868000
6	3.480154000	-1.351297000	2.512235000
6	3.152247000	-3.334013000	-0.321966000
6	2.150501000	-2.032950000	-2.215094000
6	0.703055000	-3.307686000	-0.658848000
6	4.332113000	-0.019853000	-0.249857000
6	2.664626000	1.666816000	-0.719103000
1	1.471026000	-3.180631000	2.277613000
1	1.187543000	-2.201568000	3.727924000
1	0.087465000	-2.056187000	2.340789000
1	0.549723000	0.488646000	2.548218000
1	1.753604000	0.193904000	3.827933000
1	2.214187000	1.099502000	2.372548000
1	3.506076000	-1.481576000	3.604691000
1	3.886031000	-2.266784000	2.064340000
1	4.148477000	-0.515754000	2.270738000
1	3.192536000	-4.213047000	-0.982982000
1	4.124118000	-2.832988000	-0.401167000
1	3.030173000	-3.705081000	0.704172000
1	3.089700000	-1.491768000	-2.386389000
1	2.161203000	-2.931482000	-2.850135000
1	1.317193000	-1.398627000	-2.556454000
1	0.851588000	-4.230046000	-1.240354000
1	0.467182000	-3.600000000	0.372075000
1	-0.170532000	-2.784636000	-1.074006000
6	5.355202000	0.865764000	-0.557547000
1	4.601260000	-1.026993000	0.055559000
6	3.712183000	2.556063000	-0.999220000
6	1.296853000	2.217214000	-0.925786000
6	5.042605000	2.170052000	-0.921943000
1	6.391147000	0.537049000	-0.502219000
1	3.458787000	3.571954000	-1.301696000
6	0.785351000	3.180138000	-0.050263000
6	0.575643000	1.902685000	-2.083519000
1	5.830714000	2.884627000	-1.152525000
6	-0.423321000	3.815589000	-0.324115000
1	1.352807000	3.441302000	0.844090000
6	-0.626762000	2.547857000	-2.363759000
1	0.980241000	1.168525000	-2.782369000
6	-1.128246000	3.506743000	-1.485523000
1	-0.806736000	4.566876000	0.365304000

1	-1.166217000	2.312307000	-3.281136000
1	-2.063148000	4.019251000	-1.709983000
6	-2.862742000	1.220448000	1.045911000
1	-2.668222000	2.170311000	0.535655000
6	-2.976706000	2.526461000	3.147030000
1	-2.749831000	3.383528000	2.499860000
1	-3.911174000	2.739319000	3.689149000
1	-2.187983000	2.464414000	3.914429000
6	-3.323579000	0.017490000	3.193229000
1	-3.818228000	-0.780803000	2.624018000
1	-2.380342000	-0.398234000	3.586711000
1	-3.950186000	0.246436000	4.066404000

Zero-point correction= 0.636358
(Hartree/Particle)
Thermal correction to Energy= 0.671806
Thermal correction to Enthalpy= 0.672750
Thermal correction to Gibbs Free Energy= 0.570179
Sum of electronic and zero-point Energies= -1681.309276
Sum of electronic and thermal Energies= -1681.273829
Sum of electronic and thermal Enthalpies= -1681.272884
Sum of electronic and thermal Free Energies= -1681.375455

E(M06/6-311+G(2d,p))= -1682.31755483

Intermediate XII

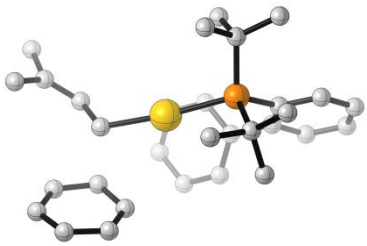


6	-2.857111000	-0.839564000	-2.172261000
6	-2.655152000	-0.021096000	0.275437000
6	-3.570083000	-1.966193000	-2.450293000
6	-3.351509000	0.160760000	-1.235908000
6	-4.849975000	-2.146868000	-1.866308000
6	-4.712200000	-0.015969000	-0.789326000
6	-5.420129000	-1.181805000	-1.050738000
1	-1.869007000	-0.686687000	-2.610336000
1	-3.174827000	-2.724798000	-3.121673000
1	-3.059752000	1.188277000	-1.484752000
1	-5.398438000	-3.064486000	-2.074454000
1	-5.144004000	0.757055000	-0.155293000
1	-6.410020000	-1.330878000	-0.626971000
1	-3.043516000	-0.954590000	0.705771000
6	-3.115874000	1.136421000	2.457827000
79	-0.536763000	-0.283614000	0.081072000
15	1.773332000	-0.854215000	0.229698000
6	2.107237000	-1.073290000	2.083133000
6	2.048742000	-2.434704000	-0.789855000
6	3.013972000	0.386678000	-0.334620000
6	1.229838000	-2.212851000	2.600272000
6	1.665017000	0.239815000	2.737239000
6	3.558759000	-1.337635000	2.477960000
6	3.231859000	-3.301430000	-0.363832000
6	2.220884000	-1.991704000	-2.243503000
6	0.781959000	-3.292974000	-0.702789000
6	4.373621000	0.035550000	-0.291630000
6	2.672943000	1.691662000	-0.748934000
1	1.565624000	-3.192082000	2.232965000
1	1.289288000	-2.235188000	3.698845000
1	0.172872000	-2.080219000	2.325503000
1	0.600796000	0.457838000	2.555298000
1	1.815628000	0.163571000	3.824791000
1	2.256140000	1.096245000	2.380929000
1	3.595569000	-1.478726000	3.568877000
1	3.974319000	-2.242440000	2.017240000
1	4.213876000	-0.490497000	2.239950000
1	3.287132000	-4.167888000	-1.040395000
1	4.197920000	-2.786916000	-0.427319000
1	3.108888000	-3.692767000	0.654654000
1	3.159996000	-1.449262000	-2.411074000
1	2.230681000	-2.883907000	-2.887589000
1	1.387849000	-1.353523000	-2.578348000
1	0.939053000	-4.207286000	-1.294862000
1	0.547611000	-3.598858000	0.324573000
1	-0.096885000	-2.772395000	-1.111150000
6	5.377534000	0.932663000	-0.628357000
1	4.662255000	-0.964733000	0.019216000
6	3.701385000	2.592463000	-1.061271000
6	1.292700000	2.223662000	-0.923010000
6	5.038616000	2.226811000	-1.005257000
1	6.419353000	0.620712000	-0.587046000
1	3.427783000	3.601556000	-1.369046000
6	0.781374000	3.159028000	-0.017897000
6	0.552097000	1.916747000	-2.070106000
1	5.811640000	2.949378000	-1.260802000
6	-0.448655000	3.769894000	-0.248580000
1	1.363871000	3.416865000	0.867651000
6	-0.673278000	2.536192000	-2.306559000
1	0.955246000	1.203682000	-2.791252000
6	-1.175771000	3.465134000	-1.397487000
1	-0.833512000	4.497281000	0.465322000
1	-1.230017000	2.303215000	-3.214326000
1	-2.129445000	3.956854000	-1.587435000
6	-2.867591000	1.155116000	1.131338000
1	-2.688168000	2.127250000	0.657154000
6	-3.082709000	2.392854000	3.268306000
1	-2.879265000	3.278782000	2.652751000
1	-4.034569000	2.551093000	3.798902000
1	-2.305597000	2.337979000	4.048051000
6	-3.327809000	-0.127524000	3.232021000
1	-3.801304000	-0.919807000	2.636455000
1	-2.369918000	-0.531171000	3.603207000
1	-3.954973000	0.053138000	4.115824000

Zero-point correction= 0.635640
(Hartree/Particle)
Thermal correction to Energy= 0.672094
Thermal correction to Enthalpy= 0.673038
Thermal correction to Gibbs Free Energy= 0.566411
Sum of electronic and zero-point Energies= -1681.310798
Sum of electronic and thermal Energies= -1681.274344
Sum of electronic and thermal Enthalpies= -1681.273400
Sum of electronic and thermal Free Energies= -1681.380027

E(M06/6-311+G(2d,p))= -1682.31828441

Transition state $TS_{XII\text{-}XIII}$



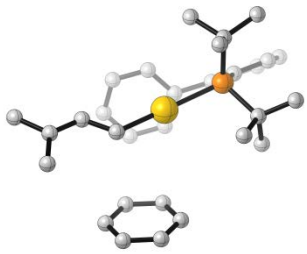
6	2.307202000	0.398882000	2.380961000
6	2.580385000	-0.292657000	-0.213813000
6	2.819778000	-0.485506000	3.299239000
6	3.089567000	0.829566000	1.262166000
6	4.158725000	-0.902304000	3.189934000
6	4.466472000	0.470664000	1.248500000
6	4.985313000	-0.412894000	2.182760000
1	1.279986000	0.754182000	2.464678000
1	2.205858000	-0.846031000	4.121920000
1	2.784429000	1.757100000	0.768134000

1	4.556959000	-1.610480000	3.915001000
1	5.092817000	0.843274000	0.439334000
1	6.025672000	-0.724300000	2.126112000
1	3.050433000	-1.229584000	0.106293000
6	4.121606000	-0.277670000	-2.192394000
79	0.472292000	-0.363676000	-0.130417000
15	-1.875240000	-0.851132000	-0.096452000
6	-2.261331000	-1.789442000	-1.695372000
6	-2.207912000	-1.862384000	1.484694000
6	-3.051575000	0.568300000	-0.018956000
6	-1.456677000	-3.089036000	-1.699893000
6	-1.764915000	-0.891309000	-2.831334000
6	-3.731737000	-2.111304000	-1.952975000
6	-3.457206000	-2.738651000	1.462859000
6	-2.304247000	-0.853939000	2.631811000
6	-1.001467000	-2.767320000	1.752474000
6	-4.426013000	0.291308000	0.077186000
6	-2.636609000	1.915665000	0.062092000
1	-1.843550000	-3.818563000	-0.976491000
1	-1.534557000	-3.546157000	-2.697860000
1	-0.389667000	-2.921154000	-1.492728000
1	-0.687734000	-0.682225000	-2.751497000
1	-1.941638000	-1.399910000	-3.791258000
1	-2.304964000	0.065895000	-2.860893000
1	-3.791675000	-2.711365000	-2.873796000
1	-4.194231000	-2.699297000	-1.151027000
1	-4.331707000	-1.208668000	-2.121030000
1	-3.546229000	-3.238613000	2.439575000
1	-4.382647000	-2.172110000	1.310003000
1	-3.395516000	-3.526076000	0.700744000
1	-3.210896000	-0.237513000	2.578666000
1	-2.330062000	-1.405594000	3.583570000
1	-1.432529000	-0.181708000	2.665639000
1	-1.180465000	-3.315929000	2.689630000
1	-0.840954000	-3.511043000	0.961962000
1	-0.072014000	-2.191857000	1.871262000
6	-5.369984000	1.292132000	0.261223000
1	-4.776538000	-0.734959000	0.016390000
6	-3.602948000	2.911419000	0.265797000
6	-1.241837000	2.413536000	-0.079242000
6	-4.954042000	2.613995000	0.366353000
1	-6.425236000	1.034103000	0.328119000
1	-3.271104000	3.947742000	0.326958000
6	-0.608556000	2.428571000	-1.327622000
6	-0.602248000	3.017571000	1.008664000
1	-5.678764000	3.411987000	0.517751000
6	0.632923000	3.038197000	-1.484577000
1	-1.111107000	1.984521000	-2.187172000
6	0.646991000	3.614557000	0.855279000
1	-1.099781000	3.030085000	1.979354000
6	1.265186000	3.631925000	-0.393373000
1	1.101892000	3.060421000	-2.467781000
1	1.131317000	4.082794000	1.711565000
1	2.232778000	4.116840000	-0.519124000
6	3.151577000	0.277145000	-1.423093000
1	2.683201000	1.193513000	-1.796494000
6	4.461519000	0.310019000	-3.522342000
1	3.862914000	1.199290000	-3.753505000
1	5.526701000	0.584854000	-3.560750000
1	4.309017000	-0.426760000	-4.325729000
6	4.894294000	-1.503065000	-1.833688000
1	4.787906000	-1.802815000	-0.784949000
1	4.583380000	-2.355631000	-2.457099000
1	5.962423000	-1.346703000	-2.043656000

Zero-point correction= 0.634645
(Hartree/Particle)
Thermal correction to Energy= 0.670811
Thermal correction to Enthalpy= 0.671755
Thermal correction to Gibbs Free Energy= 0.567128
Sum of electronic and zero-point Energies= -1681.311017
Sum of electronic and thermal Energies= -1681.274851
Sum of electronic and thermal Enthalpies= -1681.273907
Sum of electronic and thermal Free Energies= -1681.378534

E(M06/6-311+G(2d,p))= -1682.31746465

Intermediate XIII



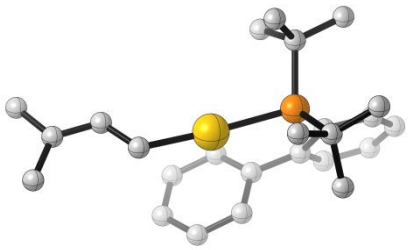
6	2.072148000	-0.797945000	2.579915000
6	2.458480000	-0.178345000	-0.874707000
6	2.138836000	-2.188430000	2.640352000
6	3.202933000	-0.058332000	2.234292000
6	3.337091000	-2.840859000	2.354273000
6	4.404072000	-0.710989000	1.961877000
6	4.471176000	-2.102033000	2.021095000
1	1.136407000	-0.285740000	2.804700000
1	1.256045000	-2.766154000	2.914830000
1	3.143909000	1.029554000	2.180462000
1	3.390799000	-3.927468000	2.404090000
1	5.291789000	-0.132506000	1.706324000
1	5.410533000	-2.611901000	1.809848000
1	3.049138000	-1.060220000	-0.596031000
6	4.543305000	0.785799000	-1.767720000
79	0.437654000	-0.244445000	-0.569734000
15	-1.943863000	-0.646694000	-0.446359000
6	-2.574930000	-0.778387000	-2.226968000
6	-2.175050000	-2.247604000	0.560427000
6	-2.983947000	0.622515000	0.396603000
6	-1.880551000	-1.961751000	-2.899994000
6	-2.139454000	0.513648000	-2.922610000
6	-4.086103000	-0.921590000	-2.388923000
6	-3.477798000	-3.010470000	0.331451000
6	-2.067236000	-1.844628000	2.032633000
6	-1.013779000	-3.191874000	0.231827000
6	-4.352276000	0.354169000	0.569107000
6	-2.453179000	1.790412000	0.988637000
1	-2.244507000	-2.926672000	-2.523264000
1	-2.096089000	-1.929782000	-3.978696000
1	-0.788101000	-1.927707000	-2.777603000
1	-1.047084000	0.642395000	-2.908900000
1	-2.462696000	0.476482000	-3.973930000
1	-2.600515000	1.402186000	-2.467343000
1	-4.307187000	-1.027054000	-3.461986000
1	-4.490660000	-1.807051000	-1.883879000
1	-4.625879000	-0.034871000	-2.034111000
1	-3.483772000	-3.888997000	0.994927000
1	-4.373493000	-2.426839000	0.572154000
1	-3.567046000	-3.384487000	-0.696686000
1	-2.945017000	-1.282403000	2.376696000
1	-1.987690000	-2.754644000	2.646269000
1	-1.172479000	-1.233868000	2.229242000
1	-1.126900000	-4.107024000	0.832894000
1	-0.997784000	-3.490774000	-0.823873000
1	-0.036859000	-2.749982000	0.474016000
6	-5.178297000	1.180444000	1.318298000
1	-4.790027000	-0.531453000	0.117084000
6	-3.298190000	2.600455000	1.761076000
6	-1.058166000	2.286691000	0.845833000
6	-4.642958000	2.306730000	1.932065000
1	-6.233281000	0.936054000	1.427252000
1	-2.877693000	3.495871000	2.218567000
6	-0.596540000	2.795482000	-0.374245000
6	-0.234110000	2.389597000	1.972109000
1	-5.270605000	2.960179000	2.535498000
6	0.658955000	3.390279000	-0.464620000
1	-1.242332000	2.749187000	-1.251365000
6	1.026571000	2.974275000	1.879302000
1	-0.595033000	2.015565000	2.931361000
6	1.475556000	3.478901000	0.661302000
1	0.995975000	3.795915000	-1.418156000

1	1.653421000	3.046199000	2.767662000
1	2.456237000	3.947922000	0.589993000
6	3.183034000	0.846515000	-1.470410000
1	2.666214000	1.766439000	-1.756524000
6	5.196043000	1.940604000	-2.419888000
1	4.482365000	2.679247000	-2.797435000
1	5.849612000	2.430797000	-1.679794000
1	5.862185000	1.609008000	-3.228315000
6	5.421485000	-0.370846000	-1.494952000
1	4.997643000	-1.122557000	-0.824030000
1	5.657504000	-0.856010000	-2.455401000
1	6.383533000	-0.019876000	-1.096801000

Zero-point correction= 0.635216
(Hartree/Particle)
Thermal correction to Energy= 0.671978
Thermal correction to Enthalpy= 0.672922
Thermal correction to Gibbs Free Energy= 0.567139
Sum of electronic and zero-point Energies= -1681.331335
Sum of electronic and thermal Energies= -1681.294573
Sum of electronic and thermal Enthalpies= -1681.293629
Sum of electronic and thermal Free Energies= -1681.399412

E(M06/6-311+G(2d,p))= -1682.34090845

Intermediate XIV

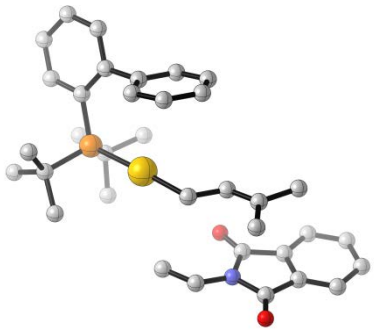


79	-0.828228000	-0.631236000	-0.232858000
15	1.571602000	-0.706593000	0.017243000
6	1.887434000	-1.510710000	1.704938000
6	2.312180000	-1.661185000	-1.445838000
6	-2.862277000	-0.699456000	-0.385274000
1	-3.321994000	-0.827990000	-1.373389000
6	-3.756124000	-0.538874000	0.662217000
1	-3.371753000	-0.422587000	1.678521000
6	-5.142722000	-0.465076000	0.516541000
6	2.424204000	0.925910000	0.107254000
6	3.820490000	0.948449000	0.260173000
6	1.730396000	2.156335000	0.124888000
6	4.520690000	2.130443000	0.460496000
1	4.384771000	0.019830000	0.232803000
6	2.450548000	3.336330000	0.359658000
6	3.827362000	3.333166000	0.529214000
1	5.603082000	2.105451000	0.570861000
1	1.904932000	4.279546000	0.380686000
1	4.356449000	4.268998000	0.700654000
6	0.278009000	2.342807000	-0.140730000
6	-0.571810000	2.814059000	0.865550000
6	-0.228801000	2.195514000	-1.438024000
6	-1.900487000	3.123977000	0.583633000
1	-0.177932000	2.952665000	1.873151000
6	-1.554703000	2.516469000	-1.722190000
1	0.434641000	1.855550000	-2.234778000
6	-2.393152000	2.982482000	-0.711725000
1	-2.547525000	3.496535000	1.376598000
1	-1.927848000	2.414327000	-2.740454000
1	-3.426913000	3.242370000	-0.936138000
6	3.669559000	-2.308492000	-1.192051000
1	3.984711000	-2.824602000	-2.111782000
1	4.455168000	-1.583153000	-0.948806000
1	3.627267000	-3.062092000	-0.395163000
6	2.416687000	-0.671545000	-2.607006000
1	3.171628000	0.106242000	-2.433830000
1	2.705976000	-1.222374000	-3.514544000
1	1.454112000	-0.179460000	-2.813112000
6	1.321407000	-2.758071000	-1.847020000
1	1.723558000	-3.290613000	-2.722082000
1	1.162595000	-3.498454000	-1.053290000
1	0.342308000	-2.342173000	-2.125171000
6	1.326159000	-2.931589000	1.671657000
1	1.919205000	-3.595136000	1.027280000
1	1.357609000	-3.347879000	2.689929000
1	0.280172000	-2.958389000	1.332181000
6	1.087571000	-0.670113000	2.704678000
1	0.012105000	-0.661134000	2.471577000
1	1.213568000	-1.095682000	3.711797000
1	1.439102000	0.371471000	2.737098000
6	3.339856000	-1.554019000	2.173503000
1	3.369895000	-2.068815000	3.145712000
1	3.997302000	-2.106606000	1.491415000
1	3.756048000	-0.550462000	2.324416000
6	-5.986457000	-0.270246000	1.711783000
1	-6.773797000	0.472107000	1.520859000
1	-6.515863000	-1.216794000	1.912338000
1	-5.413597000	0.002954000	2.603047000
6	-5.863010000	-0.545125000	-0.770633000
1	-6.142515000	0.479981000	-1.063583000
1	-5.290628000	-0.987513000	-1.589267000
1	-6.807942000	-1.088230000	-0.642513000

Zero-point correction= 0.532776
(Hartree/Particle)
Thermal correction to Energy= 0.563814
Thermal correction to Enthalpy= 0.564758
Thermal correction to Gibbs Free Energy= 0.471453
Sum of electronic and zero-point Energies= -1449.365928
Sum of electronic and thermal Energies= -1449.334889
Sum of electronic and thermal Enthalpies= -1449.333945
Sum of electronic and thermal Free Energies= -1449.427250

E(M06/6-311+G(2d,p))= -1450.20559366

Intermediate *c*-VIc



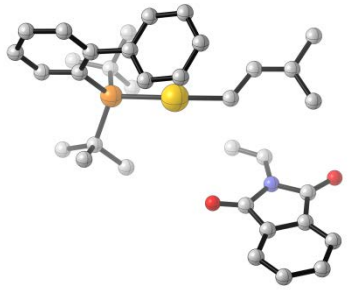
79	0.642664000	-0.043778000	-0.649787000
15	2.747463000	-0.924096000	0.126996000
6	2.380380000	-1.859361000	1.734493000
6	3.474247000	-2.026403000	-1.238778000
6	-1.204476000	0.591483000	-1.260732000
1	-1.491387000	0.535329000	-2.318077000
6	-1.839405000	-2.375505000	-1.349996000
1	-1.403406000	-2.492888000	-0.363341000
1	-1.251744000	-2.672759000	-2.215685000
6	-3.083374000	-1.925211000	-1.543428000
1	-3.526607000	-1.852862000	-2.536317000
6	-2.132227000	1.206576000	-0.421301000
1	-1.904226000	1.292405000	0.644626000
6	-3.299611000	1.821826000	-0.854523000
6	4.035178000	0.313713000	0.585930000
6	5.302023000	-0.147169000	0.982774000
6	3.790273000	1.703322000	0.621621000
6	6.295580000	0.716165000	1.423115000
1	5.523805000	-1.210679000	0.957257000
6	4.797438000	2.558353000	1.090792000

6	6.036896000	2.080096000	1.490724000
1	7.264144000	0.319154000	1.721189000
1	4.592277000	3.628293000	1.122244000
1	6.798578000	2.771814000	1.846221000
6	2.545477000	2.384511000	0.169251000
6	1.666030000	2.940808000	1.103445000
6	2.318551000	2.612488000	-1.193122000
6	0.572013000	3.694465000	0.685021000
1	1.853227000	2.790441000	2.167381000
6	1.231750000	3.377659000	-1.611079000
1	3.017837000	2.206825000	-1.925813000
6	0.354215000	3.916420000	-0.672790000
1	-0.104274000	4.122218000	1.424283000
1	1.077876000	3.561189000	-2.673822000
1	-0.492880000	4.519284000	-0.998529000
6	4.453363000	-3.103675000	-0.780009000
1	4.794960000	-3.659199000	-1.666835000
1	5.349524000	-2.699679000	-0.294305000
1	3.985038000	-3.830475000	-0.104118000
6	4.163409000	-1.090312000	-2.232618000
1	5.070039000	-0.631324000	-1.817292000
1	4.456857000	-1.669498000	-3.120908000
1	3.493321000	-0.285486000	-2.571461000
6	2.309952000	-2.712746000	-1.960928000
1	2.717772000	-3.333548000	-2.773143000
1	1.726962000	-3.370271000	-1.302812000
1	1.621766000	-1.981584000	-2.408942000
6	1.454253000	-3.029067000	1.409378000
1	1.968906000	-3.830762000	0.862676000
1	1.081207000	-3.459326000	2.351083000
1	0.581738000	-2.709447000	0.821417000
6	1.634612000	-0.865409000	2.629031000
1	0.703302000	-0.506380000	2.164645000
1	1.370146000	-1.366741000	3.572389000
1	2.254529000	0.006754000	2.881871000
6	3.599275000	-2.370153000	2.497762000
1	3.246396000	-2.920748000	3.382970000
1	4.218750000	-3.056847000	1.908322000
1	4.234404000	-1.550412000	2.856761000
7	-3.964024000	-1.484896000	-0.553171000
6	-5.285569000	-1.085641000	-0.874223000
6	-3.687383000	-1.280733000	0.817484000
6	-5.874199000	-0.585642000	0.383205000
6	-4.919091000	-0.693186000	1.390646000
8	-5.768015000	-1.142687000	-1.981796000
8	-2.640687000	-1.532456000	1.371684000
6	-7.123625000	-0.041608000	0.618972000
1	-7.863140000	0.040152000	-0.175495000
6	-5.173074000	-0.258706000	2.678327000
1	-4.421519000	-0.344439000	3.461010000
6	-7.390661000	0.400258000	1.918044000
1	-8.360943000	0.836140000	2.147500000
6	-6.432607000	0.294227000	2.928255000
1	-6.672924000	0.648758000	3.928587000
6	-4.120841000	2.591775000	0.105271000
1	-4.334903000	3.592796000	-0.298245000
1	-5.104328000	2.102931000	0.212834000
1	-3.657004000	2.682882000	1.093159000
6	-3.786449000	1.808245000	-2.254187000
1	-3.420918000	2.714989000	-2.762177000
1	-3.449744000	0.942975000	-2.834591000
1	-4.882002000	1.864145000	-2.280106000

Zero-point correction= 0.684999
(Hartree/Particle)
Thermal correction to Energy= 0.726889
Thermal correction to Enthalpy= 0.727833
Thermal correction to Gibbs Free Energy= 0.610755
Sum of electronic and zero-point Energies= -2039.332630
Sum of electronic and thermal Energies= -2039.290740
Sum of electronic and thermal Enthalpies= -2039.289796
Sum of electronic and thermal Free Energies= -2039.406874

E(M06/6-311+G(2d,p))= -2040.49425754

Intermediate *t*-VIc



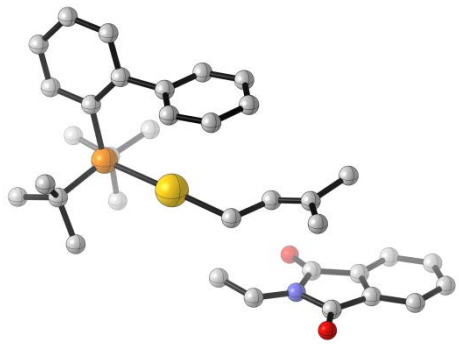
79	0.527067000	0.294793000	0.345170000
15	2.578575000	-0.967841000	0.406617000
6	3.302629000	-0.695776000	2.137255000
6	2.193749000	-2.787270000	0.012116000
6	-1.221525000	1.346631000	0.490628000
1	-2.112367000	0.995997000	-0.046673000
6	-2.105627000	-0.917786000	2.395163000
1	-1.628253000	-0.541722000	3.297329000
1	-1.583645000	-1.670274000	1.812298000
6	-3.317342000	-0.454310000	2.079305000
6	-1.383502000	2.543487000	1.184200000
1	-0.528083000	2.963110000	1.719752000
6	-2.563522000	3.277693000	1.235656000
6	3.911039000	-0.417838000	-0.745271000
6	5.103188000	-1.159533000	-0.787038000
6	3.826887000	0.755296000	-1.527286000
6	6.191531000	-0.765989000	-1.553364000
1	5.194185000	-2.067818000	-0.197714000
6	4.945341000	1.150766000	-2.275186000
6	6.116301000	0.407211000	-2.294645000
1	7.095660000	-1.371814000	-1.560308000
1	4.873962000	2.062538000	-2.867829000
1	6.962843000	0.738949000	-2.893251000
6	2.633772000	1.634850000	-1.668378000
6	2.657323000	2.933559000	-1.148877000
6	1.539238000	1.239599000	-2.446669000
6	1.609635000	3.816883000	-1.397872000
1	3.516487000	3.255499000	-0.559119000
6	0.496869000	2.127496000	-2.706615000
1	1.523197000	0.237806000	-2.877899000
6	0.530754000	3.418730000	-2.184198000
1	1.648256000	4.827017000	-0.992683000
1	-0.338142000	1.810783000	-3.330549000
1	-0.278115000	4.116278000	-2.396795000
6	3.178004000	-3.822676000	0.550677000
1	2.838122000	-4.817383000	0.224095000
1	4.199496000	-3.698557000	0.173376000
1	3.206424000	-3.837344000	1.647616000
6	2.115813000	-2.892712000	-1.511710000
1	3.093219000	-2.757135000	-1.992101000
1	1.745050000	-3.893725000	-1.778239000
1	1.415847000	-2.159470000	-1.939728000
6	0.809816000	-3.107288000	0.585818000
1	0.560078000	-4.150152000	0.336702000
1	0.773997000	-3.012916000	1.679101000
1	0.027873000	-2.465463000	0.156500000
6	2.322757000	-1.254798000	3.167937000
1	2.296703000	-2.352507000	3.165885000
1	2.645230000	-0.937124000	4.171080000
1	1.300529000	-0.878716000	3.012942000
6	3.395530000	0.822934000	2.310106000
1	2.413095000	1.311622000	2.222764000
1	3.796208000	1.042245000	3.311428000
1	4.075177000	1.278787000	1.576032000
6	4.686977000	-1.291390000	2.380716000
1	4.964874000	-1.097887000	3.427965000
1	4.719919000	-2.376756000	2.226579000
1	5.455498000	-0.826300000	1.750695000
1	-3.831539000	0.282672000	2.695418000

7	-4.086518000	-0.810165000	0.965527000
6	-3.715695000	-1.645472000	-0.110509000
6	-5.388630000	-0.286705000	0.779466000
6	-4.880097000	-1.665266000	-1.022863000
6	-5.877625000	-0.850935000	-0.493913000
8	-2.647010000	-2.201354000	-0.236277000
8	-5.934029000	0.480538000	1.540763000
6	-7.084798000	-0.665657000	-1.142188000
1	-7.858664000	-0.026485000	-0.721533000
6	-5.046557000	-2.328808000	-2.224180000
1	-4.262550000	-2.964411000	-2.631516000
6	-6.263081000	-2.149121000	-2.887892000
1	-6.435892000	-2.654262000	-3.836269000
6	-7.263642000	-1.332257000	-2.357255000
1	-8.199284000	-1.214146000	-2.900096000
6	-3.841798000	2.865069000	0.619919000
1	-4.527917000	2.542807000	1.420802000
1	-4.325823000	3.728226000	0.143252000
1	-3.758210000	2.050759000	-0.105956000
6	-2.591312000	4.561511000	1.969128000
1	-2.722139000	5.381823000	1.245696000
1	-3.469280000	4.607183000	2.629365000
1	-1.679413000	4.744153000	2.546290000

Zero-point correction= 0.683947
(Hartree/Particle)
Thermal correction to Energy= 0.726342
Thermal correction to Enthalpy= 0.727286
Thermal correction to Gibbs Free Energy= 0.608462
Sum of electronic and zero-point Energies= -2039.330645
Sum of electronic and thermal Energies= -2039.288250
Sum of electronic and thermal Enthalpies= -2039.287305
Sum of electronic and thermal Free Energies= -2039.406130

E(M06/6-311+G(2d,p))= -2040.49067587

Transition state $TS_{c\text{-}(VIc\text{-}VIIc)}$

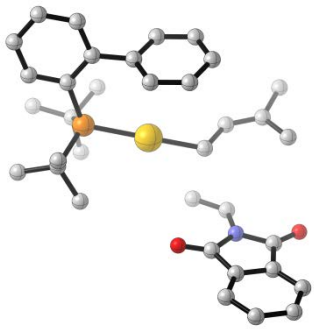


79	0.739210000	-0.320577000	-0.433892000
15	3.003755000	-0.845680000	0.140916000
6	2.937879000	-1.608738000	1.873095000
6	3.704334000	-2.018007000	-1.182435000
6	-1.248115000	0.069243000	-0.887614000
1	-1.543947000	0.120636000	-1.941190000
6	-1.813863000	-2.159111000	-0.621556000
1	-1.648938000	-2.190705000	0.450358000
1	-1.059268000	-2.602989000	-1.266288000
6	-3.024437000	-1.871923000	-1.163825000
1	-3.198935000	-1.945822000	-2.237281000
6	-2.077798000	0.781517000	0.014904000
1	-1.826790000	0.744872000	1.078910000
6	-3.113304000	1.602901000	-0.351309000
6	4.165681000	0.576537000	0.298996000
6	5.522109000	0.302708000	0.540674000
6	3.752772000	1.926460000	0.259448000
6	6.452710000	1.310611000	0.751642000
1	5.866828000	-0.727712000	0.569800000
6	4.702347000	2.929930000	0.500875000
6	6.036141000	2.636672000	0.743770000
1	7.495611000	1.056145000	0.931248000
1	4.372360000	3.968281000	0.476549000
1	6.748576000	3.441176000	0.917418000
6	2.381931000	2.425186000	-0.042364000
6	1.626604000	3.034039000	0.965340000
6	1.892046000	2.437848000	-1.354054000
6	0.404121000	3.634369000	0.672854000
1	2.013099000	3.048285000	1.985043000
6	0.675422000	3.050954000	-1.649350000
1	2.484659000	1.986008000	-2.151018000
6	-0.069395000	3.650725000	-0.636627000
1	-0.170559000	4.107369000	1.468373000
1	0.314156000	3.065193000	-2.677380000
1	-1.014508000	4.140995000	-0.868057000
6	4.825490000	-2.953232000	-0.734229000
1	5.146469000	-3.544347000	-1.605585000
1	5.712952000	-2.427400000	-0.362840000
1	4.494140000	-3.664578000	0.033253000
6	4.193546000	-1.137755000	-2.332893000
1	5.092321000	-0.564634000	-2.071775000
1	4.442014000	-1.780488000	-3.190618000
1	3.419040000	-0.429639000	-2.664928000
6	2.546574000	-2.878826000	-1.699698000
1	2.933170000	-3.569746000	-2.464197000
1	2.082498000	-3.485372000	-0.910343000
1	1.762741000	-2.264575000	-2.165739000
6	2.080386000	-2.872001000	1.814394000
1	2.573891000	-3.685167000	1.265904000
1	1.903419000	-3.228674000	2.840241000
1	1.098415000	-2.686340000	1.352410000
6	2.239473000	-0.568013000	2.752512000
1	1.230855000	-0.324116000	2.385282000
1	2.140234000	-0.971221000	3.771733000
1	2.817435000	0.364827000	2.820571000
6	4.289632000	-1.937070000	2.500469000
1	4.112759000	-2.389099000	3.488210000
1	4.872566000	-2.654544000	1.911117000
1	4.899286000	-1.038351000	2.657967000
7	-4.115325000	-1.381955000	-0.485476000
6	-5.274838000	-0.919531000	-1.179202000
6	-4.282008000	-1.255162000	0.923478000
6	-6.201029000	-0.442863000	-0.138840000
6	-5.613290000	-0.644925000	1.108205000
8	-5.392422000	-0.932815000	-2.380354000
8	-3.476650000	-1.595165000	1.757148000
6	-7.440735000	0.157594000	-0.269288000
1	-7.891759000	0.315198000	-1.247258000
6	-6.245033000	-0.265174000	2.277981000
1	-5.778605000	-0.425979000	3.248085000
6	-8.085487000	0.548159000	0.906991000
1	-9.062137000	1.024147000	0.849299000
6	-7.499292000	0.338476000	2.157515000
1	-8.031006000	0.653487000	3.052998000
6	-3.785427000	2.445723000	0.672790000
1	-3.629796000	3.512938000	0.447821000
1	-4.875606000	2.290593000	0.642041000
1	-3.423444000	2.245453000	1.688256000
6	-3.570944000	1.802641000	-1.755070000
1	-3.034101000	2.652642000	-2.205569000
1	-3.401217000	0.931297000	-2.398789000
1	-4.638175000	2.060464000	-1.781803000

Zero-point correction= 0.684364
(Hartree/Particle)
Thermal correction to Energy= 0.725354
Thermal correction to Enthalpy= 0.726299
Thermal correction to Gibbs Free Energy= 0.611867
Sum of electronic and zero-point Energies= -2039.330507
Sum of electronic and thermal Energies= -2039.289516
Sum of electronic and thermal Enthalpies= -2039.288572
Sum of electronic and thermal Free Energies= -2039.403004

E(M06/6-311+G(2d,p))= -2040.49055673
E(PBE/6-311+G(2d,p))= -2039.512107
E(PBE-D3(BJ)/6-311+G(2d,p))= -2039.6536124

Transition state $TS_{t\text{-(VIc-VIIc)}}$

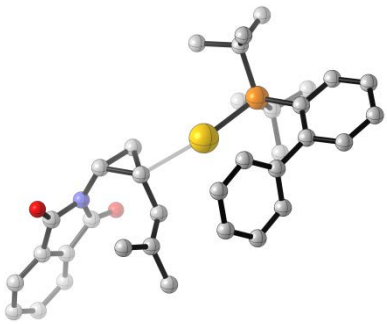


79	0.509907000	0.127030000	0.380585000
15	2.592058000	-1.055115000	0.334887000
6	3.301007000	-0.862229000	2.082114000
6	2.262152000	-2.860251000	-0.163891000
6	-1.261161000	1.191359000	0.619698000
1	-2.055828000	1.043663000	-0.118842000
6	-2.024013000	-0.280867000	2.143095000
1	-1.519492000	0.207156000	2.973577000
1	-1.632068000	-1.232471000	1.797556000
6	-3.263827000	0.152814000	1.799785000
6	-1.240157000	2.472312000	1.253130000
1	-0.400486000	2.688613000	1.920784000
6	-2.099615000	3.500604000	0.988456000
6	3.908442000	-0.397426000	-0.774672000
6	5.122102000	-1.100079000	-0.855410000
6	3.788751000	0.815911000	-1.487465000
6	6.197417000	-0.631801000	-1.597844000
1	5.238602000	-2.038496000	-0.319598000
6	4.894935000	1.287177000	-2.209164000
6	6.086885000	0.579871000	-2.269833000
1	7.119181000	-1.208986000	-1.639299000
1	4.795883000	2.229468000	-2.747788000
1	6.922593000	0.970733000	-2.847651000
6	2.566316000	1.661406000	-1.581965000
6	2.540643000	2.927632000	-0.987479000
6	1.486187000	1.269628000	-2.381219000
6	1.460133000	3.783651000	-1.186672000
1	3.387850000	3.247784000	-0.379632000
6	0.408951000	2.128890000	-2.587586000
1	1.508370000	0.294556000	-2.869677000
6	0.394445000	3.388511000	-1.992202000
1	1.458683000	4.768940000	-0.721825000
1	-0.416436000	1.815660000	-3.226067000
1	-0.440628000	4.066559000	-2.165561000
6	3.264934000	-3.899248000	0.331721000
1	2.957899000	-4.881589000	-0.058615000
1	4.289312000	-3.726010000	-0.017933000
1	3.275417000	-3.978462000	1.426261000
6	2.204976000	-2.887488000	-1.691534000
1	3.185521000	-2.712944000	-2.152524000
1	1.854697000	-3.879309000	-2.014610000
1	1.497770000	-2.144649000	-2.090095000
6	0.878577000	-3.241479000	0.372243000
1	0.663962000	-4.282802000	0.087618000
1	0.816253000	-3.178293000	1.466764000
1	0.089871000	-2.606166000	-0.054289000
6	2.326387000	-1.497839000	3.073026000
1	2.310324000	-2.593101000	2.999301000
1	2.643330000	-1.242588000	4.095600000
1	1.299653000	-1.123201000	2.940726000
6	3.361839000	0.646615000	2.337795000
1	2.368997000	1.118421000	2.277706000
1	3.760301000	0.820533000	3.348913000
1	4.027828000	1.157502000	1.627474000
6	4.696785000	-1.441028000	2.300708000
1	4.963796000	-1.305010000	3.359684000
1	4.756049000	-2.514242000	2.082630000
1	5.458881000	-0.921750000	1.706422000
1	-3.683317000	1.063611000	2.227939000
7	-4.114197000	-0.424818000	0.881243000
6	-3.879651000	-1.573996000	0.079711000
6	-5.393475000	0.143035000	0.600838000
6	-5.111082000	-1.760426000	-0.711819000
6	-6.008521000	-0.739650000	-0.404361000
8	-2.856584000	-2.217874000	0.069823000
8	-5.812890000	1.148395000	1.120970000
6	-7.248906000	-0.655580000	-1.011191000
1	-7.942683000	0.146341000	-0.767120000
6	-5.416044000	-2.739002000	-1.640581000
1	-4.709880000	-3.532654000	-1.876099000
6	-6.667663000	-2.664776000	-2.256272000
1	-6.949295000	-3.416556000	-2.990558000
6	-7.567082000	-1.641561000	-1.947731000
1	-8.532806000	-1.613599000	-2.447985000
6	-3.327153000	3.390905000	0.156544000
1	-4.205205000	3.646236000	0.769663000
1	-3.302588000	4.129623000	-0.658008000
1	-3.492960000	2.399561000	-0.276889000
6	-1.823501000	4.859563000	1.529578000
1	-1.641302000	5.564311000	0.703387000
1	-2.700086000	5.246694000	2.069774000
1	-0.954443000	4.876871000	2.196995000

Zero-point correction= 0.684228
(Hartree/Particle)
Thermal correction to Energy= 0.725522
Thermal correction to Enthalpy= 0.726467
Thermal correction to Gibbs Free Energy= 0.608977
Sum of electronic and zero-point Energies= -2039.325340
Sum of electronic and thermal Energies= -2039.284046
Sum of electronic and thermal Enthalpies= -2039.283101
Sum of electronic and thermal Free Energies= -2039.400591

E(M06/6-311+G(2d,p))= -2040.48432812
E(PBE/6-311+G(2d,p))= -2039.511041
E(PBE-D3(BJ)/6-311+G(2d,p))= -2039.6477209

Intermediate *c*-VIIc



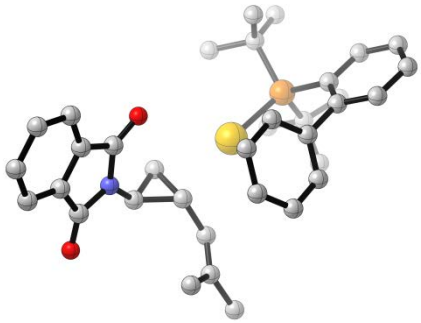
79	0.737804000	-0.338877000	-0.381201000
15	2.949068000	-0.903518000	0.108273000
6	2.903560000	-1.656119000	1.842241000
6	3.533579000	-2.094519000	-1.255505000
6	-1.699351000	-0.200254000	-0.874723000
1	-1.231945000	0.220565000	-1.776416000
6	-1.601033000	-1.735328000	-0.602227000
1	-1.677117000	-2.021267000	0.443787000
1	-0.940107000	-2.349069000	-1.212405000
6	-2.798055000	-1.214087000	-1.269976000
1	-2.902974000	-1.392221000	-2.337750000
6	-2.009634000	0.713728000	0.261128000
1	-1.671065000	0.402830000	1.254919000
6	-2.726060000	1.845282000	0.153705000
6	4.143484000	0.488658000	0.207409000
6	5.498534000	0.159854000	0.378634000
6	3.776259000	1.851545000	0.205001000
6	6.475152000	1.130452000	0.549383000
1	5.803893000	-0.882993000	0.388320000
6	4.775080000	2.815586000	0.404182000
6	6.108113000	2.470710000	0.571831000

1	7.515418000	0.835592000	0.671995000
1	4.483746000	3.865567000	0.406864000
1	6.857503000	3.247374000	0.713304000
6	2.408288000	2.399007000	-0.002563000
6	1.766663000	3.061001000	1.048614000
6	1.810674000	2.401455000	-1.270264000
6	0.555755000	3.715151000	0.841086000
1	2.236339000	3.079180000	2.032547000
6	0.602554000	3.064491000	-1.479596000
1	2.318097000	1.911514000	-2.102934000
6	-0.022820000	3.725578000	-0.424783000
1	0.071108000	4.232192000	1.668264000
1	0.154642000	3.073152000	-2.473413000
1	-0.958605000	4.257677000	-0.592393000
6	4.643998000	-3.062288000	-0.847224000
1	4.906192000	-3.666732000	-1.728540000
1	5.563903000	-2.562980000	-0.522628000
1	4.326112000	-3.758544000	-0.060722000
6	4.002862000	-1.228238000	-2.424824000
1	4.929924000	-0.685379000	-2.201981000
1	4.194398000	-1.880974000	-3.289131000
1	3.239208000	-0.495673000	-2.727001000
6	2.331377000	-2.922561000	-1.721102000
1	2.672469000	-3.625357000	-2.495693000
1	1.880109000	-3.514273000	-0.913670000
1	1.549910000	-2.289480000	-2.165570000
6	2.014690000	-2.897233000	1.811702000
1	2.463938000	-3.718912000	1.238681000
1	1.870883000	-3.254763000	2.841881000
1	1.020255000	-2.681643000	1.391905000
6	2.266780000	-0.596526000	2.744435000
1	1.251306000	-0.324381000	2.417004000
1	2.195400000	-0.999362000	3.765709000
1	2.872821000	0.319358000	2.792379000
6	4.273951000	-2.014387000	2.412165000
1	4.125242000	-2.462649000	3.405812000
1	4.814053000	-2.744647000	1.798952000
1	4.909184000	-1.129906000	2.545116000
7	-4.067708000	-1.097040000	-0.636455000
6	-5.132803000	-0.483512000	-1.329585000
6	-4.397960000	-1.327247000	0.710764000
6	-6.232654000	-0.348795000	-0.352378000
6	-5.791288000	-0.847395000	0.868887000
8	-5.092805000	-0.149321000	-2.492405000
8	-3.676492000	-1.815839000	1.553758000
6	-7.500097000	0.180960000	-0.507273000
1	-7.835713000	0.570199000	-1.466638000
6	-6.601018000	-0.841415000	1.989482000
1	-6.247494000	-1.232818000	2.941522000
6	-8.326308000	0.194549000	0.619633000
1	-9.331557000	0.604144000	0.542719000
6	-7.884330000	-0.307371000	1.845462000
1	-8.553192000	-0.281445000	2.703481000
6	-3.041572000	2.675523000	1.356600000
1	-2.769430000	3.729911000	1.196132000
1	-4.125211000	2.666934000	1.553724000
1	-2.526269000	2.316877000	2.256401000
6	-3.291153000	2.352932000	-1.134197000
1	-2.887240000	3.350910000	-1.363525000
1	-3.091736000	1.699402000	-1.990694000
1	-4.381951000	2.481613000	-1.051912000

Zero-point correction= 0.688112
(Hartree/Particle)
Thermal correction to Energy= 0.729191
Thermal correction to Enthalpy= 0.730135
Thermal correction to Gibbs Free Energy= 0.614912
Sum of electronic and zero-point Energies= -2039.362131
Sum of electronic and thermal Energies= -2039.321052
Sum of electronic and thermal Enthalpies= -2039.320108
Sum of electronic and thermal Free Energies= -2039.435330

E(M06/6-311+G(2d,p))= -2040.52451993

Intermediate *t*-VIIc



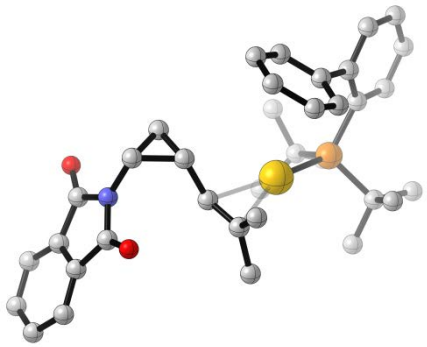
79	-0.608535000	0.154623000	-0.645383000
15	-2.835874000	-0.512419000	-0.607190000
6	-3.796918000	0.858723000	-1.486545000
6	-2.926797000	-2.211462000	-1.449248000
6	1.656689000	1.260401000	-0.705332000
1	1.614717000	0.745576000	0.266715000
6	1.591470000	0.390572000	-2.020867000
1	1.222394000	0.912176000	-2.903081000
1	1.395145000	-0.679560000	-1.980302000
6	2.885688000	0.847571000	-1.473948000
6	1.239493000	2.690192000	-0.760525000
1	0.378073000	2.936622000	-1.389505000
6	1.866181000	3.673641000	-0.096673000
6	-3.579517000	-0.645752000	1.066925000
6	-4.903845000	-1.106650000	1.156629000
6	-2.931040000	-0.228052000	2.249268000
6	-5.590729000	-1.139604000	2.361925000
1	-5.425023000	-1.441933000	0.263757000
6	-3.650421000	-0.247594000	3.452617000
6	-4.962612000	-0.693072000	3.518280000
1	-6.615366000	-1.504716000	2.390273000
1	-3.145945000	0.085380000	4.359374000
1	-5.488065000	-0.698176000	4.471466000
6	-1.518433000	0.228179000	2.370410000
6	-1.244706000	1.570787000	2.652454000
6	-0.464265000	-0.694441000	2.374222000
6	0.056548000	1.987338000	2.920811000
1	-2.065956000	2.288337000	2.675042000
6	0.834998000	-0.278981000	2.657866000
1	-0.673676000	-1.748348000	2.184424000
6	1.099105000	1.062566000	2.927719000
1	0.253227000	3.036231000	3.141162000
1	1.640912000	-1.011112000	2.682394000
1	2.114173000	1.383274000	3.159782000
6	-4.284644000	-2.559312000	-2.056206000
1	-4.212002000	-3.567019000	-2.491817000
1	-5.096211000	-2.588717000	-1.320265000
1	-4.566307000	-1.874457000	-2.866283000
6	-2.547372000	-3.247168000	-0.391233000
1	-3.305702000	-3.340986000	0.396475000
1	-2.447797000	-4.227326000	-0.880591000
1	-1.580737000	-3.018335000	0.083157000
6	-1.879221000	-2.258632000	-2.566043000
1	-1.943176000	-3.240069000	-3.058870000
1	-2.038180000	-1.491250000	-3.334795000
1	-0.858698000	-2.146809000	-2.171522000
6	-3.297910000	0.951038000	-2.927412000
1	-3.585142000	0.078094000	-3.528593000
1	-3.746718000	1.838004000	-3.398918000
1	-2.204025000	1.064131000	-2.978770000
6	-3.452592000	2.153698000	-0.746963000
1	-2.374457000	2.371798000	-0.773232000
1	-3.979357000	2.988181000	-1.233312000
1	-3.773034000	2.126247000	0.304213000
6	-5.314771000	0.687363000	-1.474718000
1	-5.757491000	1.526025000	-2.032171000
1	-5.646502000	-0.239352000	-1.957301000
1	-5.724649000	0.719479000	-0.457578000
1	3.400234000	1.655500000	-1.992238000

7	3.825706000	-0.062564000	-0.894158000
6	3.568871000	-1.314056000	-0.320396000
6	5.182979000	0.297520000	-0.767444000
6	4.875796000	-1.809508000	0.170589000
6	5.841907000	-0.843452000	-0.095764000
8	2.481565000	-1.851494000	-0.243262000
8	5.654723000	1.345194000	-1.147441000
6	7.165927000	-1.022714000	0.257006000
1	7.914596000	-0.261347000	0.046729000
6	5.192016000	-2.995882000	0.805120000
1	4.431439000	-3.746963000	1.010015000
6	6.528752000	-3.188846000	1.165446000
1	6.820796000	-4.109540000	1.666722000
6	7.497640000	-2.220035000	0.897228000
1	8.529085000	-2.403044000	1.191836000
6	3.072417000	3.442450000	0.758180000
1	3.298639000	2.379896000	0.911866000
1	3.959220000	3.911528000	0.304288000
1	2.948099000	3.915517000	1.743906000
6	1.395311000	5.090063000	-0.171662000
1	1.074792000	5.444841000	0.819986000
1	2.209419000	5.758175000	-0.490309000
1	0.555448000	5.212142000	-0.866617000

Zero-point correction= 0.688574
(Hartree/Particle)
Thermal correction to Energy= 0.729282
Thermal correction to Enthalpy= 0.730226
Thermal correction to Gibbs Free Energy= 0.616433
Sum of electronic and zero-point Energies= -2039.366147
Sum of electronic and thermal Energies= -2039.325440
Sum of electronic and thermal Enthalpies= -2039.324496
Sum of electronic and thermal Free Energies= -2039.438289

E(M06/6-311+G(2d,p))= -2040.52784353

Intermediate *c*-VIIIc



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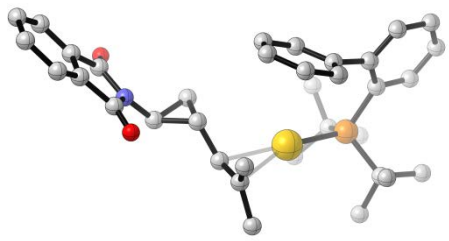
6	3.139552000	-1.993538000	1.589341000
6	2.075172000	-2.379480000	-1.397806000
6	-1.861946000	1.705109000	-0.321010000
1	-1.398204000	2.639237000	-0.002473000
6	-1.966531000	1.465837000	-1.799133000
1	-1.921059000	0.428039000	-2.131129000
1	-1.529363000	2.186954000	-2.486073000
6	-1.691960000	0.535494000	0.566527000
1	-2.094895000	-0.406168000	0.173860000
6	-1.374596000	0.553023000	1.908530000
6	3.960947000	-0.174622000	-0.651433000
6	5.113180000	-0.862633000	-1.069562000
6	3.905328000	1.221605000	-0.848798000
6	6.175632000	-0.213126000	-1.681814000
1	5.187570000	-1.936221000	-0.922798000
6	4.981947000	1.857106000	-1.483913000
6	6.105176000	1.157721000	-1.900322000
1	7.051115000	-0.781538000	-1.989750000
1	4.928814000	2.935058000	-1.634637000
1	6.924191000	1.683288000	-2.387994000
6	2.807914000	2.128196000	-0.416865000
6	2.650090000	2.471326000	0.930935000
6	2.031522000	2.785060000	-1.377308000
6	1.737220000	3.452560000	1.308372000
1	3.273244000	1.986935000	1.682934000
6	1.111986000	3.760195000	-0.998264000
1	2.167023000	2.538537000	-2.431321000
6	0.966678000	4.100206000	0.344622000
1	1.639030000	3.722229000	2.359346000
1	0.519957000	4.268869000	-1.758125000
1	0.260762000	4.875416000	0.640542000
6	2.992905000	-3.590279000	-1.553155000
1	2.624554000	-4.193053000	-2.396911000
1	4.030303000	-3.323681000	-1.785362000
1	2.984411000	-4.236933000	-0.665871000
6	2.062746000	-1.564680000	-2.692700000
1	3.066483000	-1.249794000	-3.004865000
1	1.643497000	-2.189433000	-3.495198000
1	1.427983000	-0.667794000	-2.610860000
6	0.651086000	-2.889447000	-1.148731000
1	0.390681000	-3.590864000	-1.955464000
1	0.544693000	-3.426794000	-0.197617000
1	-0.085974000	-2.072707000	-1.169460000
6	2.063810000	-2.977336000	2.047241000
1	1.999297000	-3.857190000	1.393709000
1	2.320418000	-3.334865000	3.055532000
1	1.070104000	-2.507379000	2.101949000
6	3.266718000	-0.871492000	2.623958000
1	2.308584000	-0.356846000	2.799433000
1	3.595832000	-1.308685000	3.578451000
1	4.014473000	-0.121393000	2.328872000
6	4.482341000	-2.714001000	1.499351000
1	4.677038000	-3.192815000	2.470725000
1	4.497807000	-3.501387000	0.736537000
1	5.309997000	-2.020455000	1.307955000
7	-4.228814000	0.928869000	-0.832006000
6	-4.818122000	0.142426000	-1.839424000
6	-4.900370000	0.790267000	0.394760000
6	-5.914712000	-0.601190000	-1.174039000
6	-5.962488000	-0.215956000	0.162497000
8	-4.472949000	0.108041000	-2.998893000
8	-4.631315000	1.394815000	1.410025000
6	-6.802111000	-1.524404000	-1.695154000
1	-6.761447000	-1.815278000	-2.743204000
6	-6.897439000	-0.740257000	1.035968000
1	-6.929124000	-0.431526000	2.079200000
6	-7.751481000	-2.060721000	-0.821252000
1	-8.470069000	-2.789290000	-1.191798000
6	-7.797342000	-1.676827000	0.520628000
1	-8.549875000	-2.113325000	1.174489000
6	-3.184518000	1.879944000	-1.044772000
1	-3.529250000	2.907545000	-1.159189000
6	-1.588628000	-0.671588000	2.746718000
1	-0.759422000	-0.837778000	3.448681000
1	-2.494549000	-0.519909000	3.355550000
1	-1.733064000	-1.575814000	2.142029000
6	-1.083203000	1.799286000	2.681363000
1	-0.232430000	1.646584000	3.361088000
1	-0.876048000	2.669797000	2.050633000
1	-1.956550000	2.031080000	3.310956000

Zero-point correction= 0.688122
(Hartree/Particle)
Thermal correction to Energy= 0.729053
Thermal correction to Enthalpy= 0.729997
Thermal correction to Gibbs Free Energy= 0.614444
Sum of electronic and zero-point Energies= -2039.393452
Sum of electronic and thermal Energies= -2039.352522
Sum of electronic and thermal Enthalpies= -2039.351577
Sum of electronic and thermal Free Energies= -2039.467131

E(M06/6-311+G(2d,p))= -2040.55666388

Intermediate *t*-VIIIc



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15	-3.124010000	-0.309707000	0.474011000
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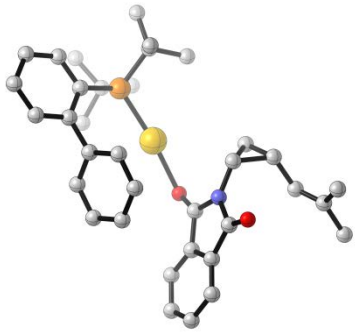
6	-3.175909000	-0.953707000	2.259911000
6	2.083991000	-0.763399000	0.122111000
1	2.286689000	0.124401000	-0.475789000
6	2.150990000	-0.575899000	1.609711000
1	1.496391000	-1.183900000	2.234911000
1	2.348389000	0.427901000	1.982011000
6	3.260291000	-1.288997000	0.909011000
1	3.327593000	-2.370497000	1.036011000
6	1.155692000	-1.755400000	-0.455789000
1	0.969293000	-2.633901000	0.175011000
6	-3.661713000	1.448392000	0.483411000
6	-4.925713000	1.750391000	1.018911000
6	-2.914614000	2.492894000	-0.099589000
6	-5.458115000	3.030590000	0.968611000
1	-5.521312000	0.968290000	1.481811000
6	-3.481316000	3.773793000	-0.166889000
6	-4.736617000	4.048291000	0.355911000
1	-6.438615000	3.224488000	1.399311000
1	-2.900817000	4.571394000	-0.629789000
1	-5.144418000	5.055490000	0.292811000
6	-1.527514000	2.395496000	-0.630289000
6	-1.292714000	2.499896000	-2.004989000
6	-0.436414000	2.385297000	0.246611000
6	0.006986000	2.600498000	-2.494389000
1	-2.141514000	2.526795000	-2.689589000
6	0.862186000	2.501099000	-0.243389000
1	-0.613614000	2.325697000	1.321911000
6	1.086586000	2.613199000	-1.613889000
1	0.175885000	2.686798000	-3.566889000
1	1.701586000	2.516800000	0.451511000
1	2.101785000	2.713701000	-1.995889000
6	-4.570209000	-1.255509000	2.805111000
1	-4.462008000	-1.618909000	3.838011000
1	-5.224010000	-0.376810000	2.847011000
1	-5.075408000	-2.045610000	2.234411000
6	-2.495011000	0.111594000	3.120211000
1	-3.070812000	1.044793000	3.168711000
1	-2.393610000	-0.275206000	4.144911000
1	-1.483011000	0.347796000	2.756411000
6	-2.348407000	-2.240906000	2.343611000
1	-2.364407000	-2.596506000	3.384811000
1	-2.747606000	-3.045006000	1.713611000
1	-1.297107000	-2.075904000	2.065411000
6	-4.052107000	-2.687308000	-0.648989000
1	-4.405606000	-3.128309000	0.292711000
1	-4.602206000	-3.176109000	-1.466889000
1	-2.986106000	-2.932207000	-0.771789000
6	-3.959510000	-0.658508000	-2.106389000
1	-2.917609000	-0.883806000	-2.384489000
1	-4.620109000	-1.136409000	-2.845189000
1	-4.106411000	0.428492000	-2.185889000
6	-5.797509000	-0.921711000	-0.464989000
1	-6.373608000	-1.527512000	-1.180289000
1	-6.124609000	-1.206811000	0.542311000
1	-6.068011000	0.126989000	-0.638089000
7	4.508890000	-0.624695000	0.729211000
6	5.146390000	-0.501395000	-0.516889000
6	5.311290000	-0.143994000	1.778111000
6	6.439689000	0.167907000	-0.240689000
6	6.537389000	0.382508000	1.131611000
8	4.691791000	-0.881395000	-1.573489000
8	5.022690000	-0.178095000	2.953111000
6	7.448789000	0.546809000	-1.106689000
1	7.366989000	0.373309000	-2.178189000
6	7.647588000	0.983109000	1.695411000
1	7.716288000	1.143809000	2.769711000
6	8.575488000	1.155711000	-0.547389000
1	9.393987000	1.466712000	-1.193789000
6	8.673287000	1.370211000	0.829011000
1	9.566087000	1.844312000	1.232211000
6	0.739392000	-1.833501000	-1.769289000
6	1.129991000	-0.857900000	-2.834089000
1	1.586489000	0.060400000	-2.451389000
1	1.852891000	-1.343399000	-3.507589000
1	0.258590000	-0.584102000	-3.447289000
6	0.060894000	-3.073002000	-2.275089000
1	-0.810506000	-2.832403000	-2.899889000
1	0.764995000	-3.624201000	-2.917789000
1	-0.253505000	-3.740603000	-1.463689000

Zero-point correction= 0.688852
(Hartree/Particle)
Thermal correction to Energy= 0.729363
Thermal correction to Enthalpy= 0.730307
Thermal correction to Gibbs Free Energy= 0.616866
Sum of electronic and zero-point Energies= -2039.393047
Sum of electronic and thermal Energies= -2039.352536
Sum of electronic and thermal Enthalpies= -2039.351592
Sum of electronic and thermal Free Energies= -2039.465033

E(M06/6-311+G(2d,p))= -2040.55725589

Intermediate *c*-IXc



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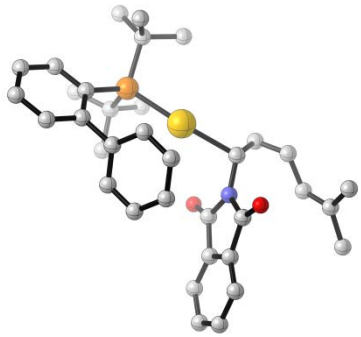
6	-3.739069000	0.725325000	-1.867486000
6	-2.976258000	2.407512000	0.741820000
6	2.284300000	1.455454000	0.747724000
1	1.669537000	1.388865000	1.647644000
6	1.982230000	2.534308000	-0.245121000
1	2.150603000	2.311790000	-1.298766000
1	1.124629000	3.172774000	-0.046744000
6	-3.671456000	-0.529854000	0.824492000
6	-5.018164000	-0.323326000	1.170974000
6	-3.052987000	-1.735080000	1.221779000
6	-5.751994000	-1.274567000	1.865417000
1	-5.517520000	0.601658000	0.893290000
6	-3.817847000	-2.691600000	1.904630000
6	-5.150247000	-2.474811000	2.223981000
1	-6.791691000	-1.075808000	2.117896000
1	-3.333447000	-3.621732000	2.200871000
1	-5.711804000	-3.238354000	2.759147000
6	-1.623012000	-2.107148000	1.025560000
6	-1.269605000	-3.083270000	0.087388000
6	-0.641758000	-1.618344000	1.897025000
6	0.039225000	-3.554235000	0.015889000

1	-2.033504000	-3.484643000	-0.579624000
6	0.663669000	-2.101608000	1.835682000
1	-0.916916000	-0.880835000	2.652424000
6	1.006241000	-3.072444000	0.895974000
1	0.300526000	-4.316929000	-0.716744000
1	1.406198000	-1.734520000	2.544483000
1	2.022110000	-3.465481000	0.857206000
6	-4.315405000	3.130230000	0.611662000
1	-4.267986000	4.046899000	1.218476000
1	-5.164940000	2.545867000	0.983524000
1	-4.523744000	3.436788000	-0.421564000
6	-2.688454000	2.100263000	2.211789000
1	-3.488442000	1.518654000	2.686712000
1	-2.594788000	3.051490000	2.756155000
1	-1.740432000	1.555255000	2.338189000
6	-1.875392000	3.334918000	0.224629000
1	-1.947812000	4.296005000	0.754871000
1	-1.954158000	3.541055000	-0.850784000
1	-0.881476000	2.912125000	0.423096000
6	-3.173883000	1.844205000	-2.740865000
1	-3.450978000	2.840031000	-2.370644000
1	-3.590146000	1.743941000	-3.754219000
1	-2.078203000	1.794147000	-2.825226000
6	-3.404048000	-0.631207000	-2.492176000
1	-2.324065000	-0.763517000	-2.651781000
1	-3.902002000	-0.700847000	-3.470738000
1	-3.767206000	-1.466004000	-1.876237000
6	-5.259495000	0.850181000	-1.796662000
1	-5.646538000	0.861969000	-2.826146000
1	-5.595909000	1.772099000	-1.310155000
1	-5.720614000	-0.004197000	-1.286817000
6	3.201962000	2.663427000	0.611529000
1	3.135406000	3.351169000	1.454091000
6	4.525777000	2.527618000	-0.038955000
1	4.504584000	2.269192000	-1.102893000
6	5.721120000	2.711649000	0.539675000
7	2.794739000	0.200383000	0.284628000
6	3.896546000	-0.451919000	0.915256000
6	2.354535000	-0.523663000	-0.792123000
6	4.206552000	-1.619784000	0.062193000
8	4.393374000	-0.095954000	1.953589000
6	3.283818000	-1.648892000	-0.981147000
8	1.349938000	-0.288796000	-1.476238000
6	5.162104000	-2.606704000	0.208203000
6	3.276998000	-2.660605000	-1.923583000
1	5.871777000	-2.587354000	1.032940000
6	5.174628000	-3.628851000	-0.746854000
1	2.541451000	-2.684155000	-2.725713000
6	4.251302000	-3.653960000	-1.793856000
1	5.915873000	-4.421815000	-0.670895000
1	4.289087000	-4.465972000	-2.517154000
6	6.985778000	2.591088000	-0.252537000
1	7.639437000	1.809668000	0.164802000
1	7.564909000	3.526658000	-0.215465000
1	6.794033000	2.351666000	-1.306052000
6	5.916315000	3.031048000	1.987581000
1	4.981938000	3.067917000	2.557758000
1	6.435638000	3.993796000	2.110844000
1	6.560882000	2.272020000	2.456296000

Zero-point correction= 0.687317
(Hartree/Particle)
Thermal correction to Energy= 0.728545
Thermal correction to Enthalpy= 0.729489
Thermal correction to Gibbs Free Energy= 0.612916
Sum of electronic and zero-point Energies= -2039.380959
Sum of electronic and thermal Energies= -2039.339731
Sum of electronic and thermal Enthalpies= -2039.338786
Sum of electronic and thermal Free Energies= -2039.455360

E(M06/6-311+G(2d,p))= -2040.54007102

Transition state $TS_{c\text{-}(IXc\text{-}Xc)}$



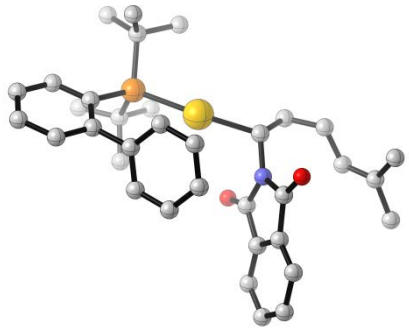
79	-0.500525000	0.788632000	0.189179000
15	-2.801333000	0.560331000	-0.292435000
6	-2.920512000	0.444540000	-2.177640000
6	-3.690582000	2.080398000	0.435990000
6	1.674499000	1.291087000	0.406471000
1	1.654607000	1.310729000	1.500366000
6	1.694557000	2.643613000	-0.400958000
1	1.797295000	2.458605000	-1.471501000
1	0.850951000	3.288173000	-0.156510000
6	-3.641936000	-0.956829000	0.325791000
6	-5.036003000	-1.037473000	0.178235000
6	-2.957543000	-2.077033000	0.848672000
6	-5.749488000	-2.178491000	0.517816000
1	-5.584421000	-0.189744000	-0.223198000
6	-3.692545000	-3.229368000	1.162007000
6	-5.069642000	-3.288739000	1.004204000
1	-6.830283000	-2.198400000	0.392501000
1	-3.155617000	-4.090828000	1.558909000
1	-5.609414000	-4.197141000	1.265913000
6	-1.498008000	-2.162655000	1.129134000
6	-0.687301000	-3.013575000	0.371496000
6	-0.941892000	-1.505987000	2.234167000
6	0.653206000	-3.197021000	0.703436000
1	-1.118522000	-3.544970000	-0.477534000
6	0.395517000	-1.698392000	2.572879000
1	-1.574593000	-0.863399000	2.847544000
6	1.195469000	-2.545345000	1.808297000
1	1.269977000	-3.869525000	0.107710000
1	0.813594000	-1.190660000	3.441740000
1	2.236926000	-2.707325000	2.083459000
6	-4.968859000	2.517421000	-0.278189000
1	-5.393815000	3.366698000	0.278173000
1	-5.744688000	1.744005000	-0.315010000
1	-4.776300000	2.867100000	-1.300626000
6	-3.996274000	1.762312000	1.900141000
1	-4.779857000	1.003239000	2.015170000
1	-4.347155000	2.681399000	2.392636000
1	-3.102081000	1.420925000	2.443089000
6	-2.712674000	3.261321000	0.401726000
1	-3.224413000	4.150116000	0.800778000
1	-2.372728000	3.503272000	-0.614048000
1	-1.827930000	3.074570000	1.026903000
6	-2.301127000	1.706620000	-2.777082000
1	-2.891742000	2.606379000	-2.559174000
1	-2.259186000	1.596268000	-3.870856000
1	-1.272531000	1.869843000	-2.418756000
6	-2.077265000	-0.768470000	-2.576935000
1	-1.035233000	-0.684018000	-2.234517000
1	-2.065974000	-0.843718000	-3.674761000
1	-2.501210000	-1.705020000	-2.187878000
6	-4.331429000	0.249318000	-2.726869000
1	-4.266937000	0.191843000	-3.823905000
1	-5.007430000	1.076127000	-2.481334000
1	-4.782549000	-0.688822000	-2.380109000
6	2.886174000	2.774529000	0.377106000
1	2.797932000	3.237844000	1.358344000
6	4.174260000	2.388744000	-0.122383000
1	4.226615000	2.147497000	-1.188004000
6	5.301041000	2.262982000	0.620568000

7	2.449828000	0.204442000	-0.084137000
6	3.408887000	-0.468047000	0.700458000
6	2.389564000	-0.315830000	-1.384205000
6	4.024406000	-1.474317000	-0.193117000
8	3.619688000	-0.249101000	1.873627000
6	3.422609000	-1.375670000	-1.445387000
8	1.630180000	0.058707000	-2.254373000
6	5.009641000	-2.407852000	0.068059000
6	3.787714000	-2.201856000	-2.491560000
1	5.468778000	-2.483749000	1.052519000
6	5.389774000	-3.245759000	-0.984962000
1	3.312230000	-2.120257000	-3.467273000
6	4.790123000	-3.144198000	-2.241304000
1	6.165054000	-3.992418000	-0.824673000
1	5.108655000	-3.812177000	-3.039094000
6	6.567406000	1.798548000	-0.012230000
1	6.896574000	0.861800000	0.465206000
1	7.378221000	2.524243000	0.148156000
1	6.460089000	1.621945000	-1.088733000
6	5.379385000	2.500094000	2.088148000
1	4.465367000	2.912595000	2.525745000
1	6.216083000	3.173365000	2.321913000
1	5.592500000	1.547005000	2.595147000

Zero-point correction= 0.685975
(Hartree/Particle)
Thermal correction to Energy= 0.726934
Thermal correction to Enthalpy= 0.727879
Thermal correction to Gibbs Free Energy= 0.612907
Sum of electronic and zero-point Energies= -2039.360210
Sum of electronic and thermal Energies= -2039.319251
Sum of electronic and thermal Enthalpies= -2039.318307
Sum of electronic and thermal Free Energies= -2039.433278

E(M06/6-311+G(2d,p))= -2040.51880997

Intermediate *c*-Xc

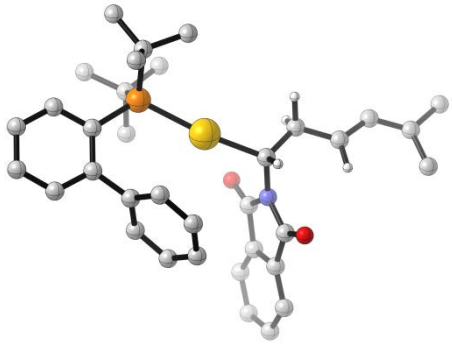


79	-0.519257000	0.803145000	0.211855000
15	-2.843152000	0.590877000	-0.284452000
6	-2.985154000	0.567233000	-2.174637000
6	-3.734180000	2.064966000	0.528812000
6	1.574905000	1.213552000	0.545088000
1	1.726882000	1.224048000	1.631913000
6	1.881346000	2.643947000	-0.074196000
1	1.835648000	2.599281000	-1.166856000
1	1.146095000	3.349696000	0.319702000
6	-3.699856000	-0.953411000	0.252225000
6	-5.090147000	-1.040346000	0.072793000
6	-3.018172000	-2.093137000	0.734914000
6	-5.799104000	-2.204377000	0.336289000
1	-5.641744000	-0.179101000	-0.293567000
6	-3.746577000	-3.269239000	0.966910000
6	-5.118464000	-3.334397000	0.773369000
1	-6.877090000	-2.226446000	0.188103000
1	-3.208985000	-4.144964000	1.330324000
1	-5.653341000	-4.261400000	0.972818000
6	-1.568684000	-2.174219000	1.060754000
6	-0.729546000	-3.010028000	0.317098000
6	-1.051345000	-1.530291000	2.191164000
6	0.599592000	-3.194088000	0.690457000
1	-1.131083000	-3.528340000	-0.554520000
6	0.275233000	-1.722290000	2.570711000
1	-1.705125000	-0.895586000	2.791244000
6	1.103271000	-2.555237000	1.820964000
1	1.236636000	-3.857406000	0.106048000
1	0.662014000	-1.223350000	3.459075000
1	2.137364000	-2.714790000	2.125273000
6	-5.044401000	2.505113000	-0.119782000
1	-5.452034000	3.341736000	0.467967000
1	-5.813252000	1.724305000	-0.133116000
1	-4.897481000	2.872162000	-1.143652000
6	-3.978695000	1.676530000	1.987754000
1	-4.743578000	0.896994000	2.094597000
1	-4.325782000	2.564416000	2.537280000
1	-3.057709000	1.324643000	2.477258000
6	-2.780111000	3.265078000	0.510605000
1	-3.285276000	4.120782000	0.983940000
1	-2.497829000	3.568070000	-0.506171000
1	-1.859778000	3.063175000	1.076761000
6	-2.376461000	1.858629000	-2.719008000
1	-2.983634000	2.740964000	-2.473692000
1	-2.321613000	1.790941000	-3.816001000
1	-1.354773000	2.021223000	-2.341960000
6	-2.135836000	-0.620485000	-2.635606000
1	-1.081659000	-0.520968000	-2.338172000
1	-2.170059000	-0.674282000	-3.734381000
1	-2.520211000	-1.574494000	-2.246466000
6	-4.395689000	0.392482000	-2.732038000
1	-4.334977000	0.406804000	-3.830822000
1	-5.080685000	1.194499000	-2.431914000
1	-4.836236000	-0.570280000	-2.444689000
6	3.209258000	2.806238000	0.473278000
1	3.280514000	3.152108000	1.506254000
6	4.347072000	2.351663000	-0.191857000
1	4.247921000	2.101978000	-1.251320000
6	5.569372000	2.131104000	0.410622000
7	2.412760000	0.169682000	0.023226000
6	3.396267000	-0.492309000	0.777426000
6	2.372226000	-0.307693000	-1.293938000
6	4.019333000	-1.478786000	-0.135190000
8	3.650303000	-0.266143000	1.943165000
6	3.417956000	-1.355167000	-1.385041000
8	1.620217000	0.088608000	-2.160739000
6	5.016377000	-2.405679000	0.103562000
6	3.794799000	-2.149517000	-2.451525000
1	5.474930000	-2.501692000	1.086620000
6	5.405891000	-3.214125000	-0.969228000
1	3.320122000	-2.048728000	-3.425927000
6	4.806783000	-3.087659000	-2.223387000
1	6.187541000	-3.957626000	-0.825592000
1	5.132370000	-3.732838000	-3.037035000
6	6.694940000	1.599192000	-0.387508000
1	7.139871000	0.728946000	0.118322000
1	7.496356000	2.353543000	-0.431868000
1	6.407229000	1.326789000	-1.408258000
6	5.823113000	2.305474000	1.858129000
1	5.173220000	3.038831000	2.343615000
1	6.872316000	2.563706000	2.044243000
1	5.640141000	1.331218000	2.342961000

Zero-point correction= 0.686547
(Hartree/Particle)
Thermal correction to Energy= 0.727867
Thermal correction to Enthalpy= 0.728812
Thermal correction to Gibbs Free Energy= 0.612774
Sum of electronic and zero-point Energies= -2039.362838
Sum of electronic and thermal Energies= -2039.321518
Sum of electronic and thermal Enthalpies= -2039.320573
Sum of electronic and thermal Free Energies= -2039.436611

E(M06/6-311+G(2d,p))= -2040.52185458

Transition state $TS_{c\text{-}Xc\text{-}t\text{-}Xc}$

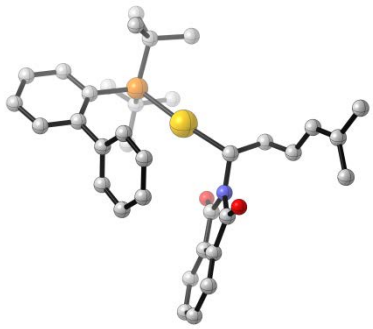


79	-0.325792000	0.688938000	0.241015000
15	-2.668193000	0.928228000	-0.255177000
6	-2.803810000	1.033803000	-2.143562000
6	-3.288891000	2.496542000	0.631884000
6	1.771740000	0.712044000	0.577405000
1	1.950961000	0.656357000	1.659874000
6	2.447647000	1.968922000	0.043877000
1	2.329375000	2.076882000	-1.048458000
1	1.944115000	2.869077000	0.447711000
6	-3.816765000	-0.445567000	0.199250000
6	-5.195503000	-0.262266000	0.001947000
6	-3.372572000	-1.707022000	0.653230000
6	-6.116871000	-1.276984000	0.222129000
1	-5.567202000	0.698235000	-0.344834000
6	-4.314668000	-2.728685000	0.845494000
6	-5.671023000	-2.526425000	0.636883000
1	-7.176969000	-1.090191000	0.060188000
1	-3.957696000	-3.699395000	1.189536000
1	-6.376307000	-3.338581000	0.804198000
6	-1.968861000	-2.075753000	0.985723000
6	-1.286658000	-3.014691000	0.204545000
6	-1.364655000	-1.605536000	2.156913000
6	-0.026113000	-3.470863000	0.583206000
1	-1.758803000	-3.401372000	-0.699450000
6	-0.109374000	-2.069685000	2.542204000
1	-1.899787000	-0.890539000	2.783222000
6	0.561409000	-3.004720000	1.756963000
1	0.490658000	-4.208813000	-0.030354000
1	0.342801000	-1.701923000	3.462927000
1	1.535173000	-3.380207000	2.070400000
6	-4.484502000	3.214522000	0.008755000
1	-4.737953000	4.075985000	0.646002000
1	-5.386555000	2.595133000	-0.056812000
1	-4.259056000	3.610130000	-0.990213000
6	-3.629092000	2.081507000	2.064239000
1	-4.523607000	1.447683000	2.116581000
1	-3.824797000	2.986503000	2.658920000
1	-2.798232000	1.544176000	2.545933000
6	-2.129176000	3.498074000	0.690881000
1	-2.471872000	4.398370000	1.224075000
1	-1.790914000	3.812754000	-0.305179000
1	-1.261562000	3.093642000	1.231604000
6	-1.977475000	2.227322000	-2.620825000
1	-2.427277000	3.186558000	-2.331269000
1	-1.924794000	2.206866000	-3.720039000
1	-0.945950000	2.194812000	-2.237096000
6	-2.166396000	-0.255879000	-2.668018000
1	-1.123776000	-0.368347000	-2.337328000
1	-2.172413000	-0.232902000	-3.768587000
1	-2.729033000	-1.146920000	-2.354399000
6	-4.214742000	1.131972000	-2.714335000
1	-4.139333000	1.190249000	-3.810973000
1	-4.756254000	2.022258000	-2.375942000
1	-4.817646000	0.246385000	-2.478655000
6	3.877836000	2.105188000	0.382550000
1	4.295178000	1.361689000	1.068813000
6	4.676523000	3.116816000	-0.089710000
1	4.244299000	3.847564000	-0.776084000
6	6.025297000	3.261543000	0.247525000
7	2.438415000	-0.474797000	0.036883000
6	3.223327000	-1.343358000	0.802369000
6	2.246813000	-0.970859000	-1.255187000
6	3.550920000	-2.494231000	-0.075731000
8	3.555768000	-1.158919000	1.957152000
6	2.970317000	-2.264860000	-1.318947000
8	1.604366000	-0.425551000	-2.131312000
6	4.262519000	-3.647918000	0.192540000
6	3.078834000	-3.179647000	-2.349157000
1	4.709140000	-3.819964000	1.170732000
6	4.376864000	-4.582654000	-0.841613000
1	2.617790000	-2.996930000	-3.318409000
6	3.794593000	-4.352956000	-2.089249000
1	4.924956000	-5.507487000	-0.671305000
1	3.899564000	-5.102526000	-2.871505000
6	6.778034000	4.401839000	-0.301701000
1	7.802892000	4.111757000	-0.568122000
1	6.882757000	5.146388000	0.506611000
1	6.278107000	4.885998000	-1.145608000
6	6.781455000	2.350408000	1.125189000
1	7.440244000	1.741661000	0.484477000
1	6.175104000	1.677059000	1.734858000
1	7.453267000	2.932058000	1.770515000

Zero-point correction= 0.685638
(Hartree/Particle)
Thermal correction to Energy= 0.726631
Thermal correction to Enthalpy= 0.727575
Thermal correction to Gibbs Free Energy= 0.610940
Sum of electronic and zero-point Energies= -2039.353205
Sum of electronic and thermal Energies= -2039.312212
Sum of electronic and thermal Enthalpies= -2039.311267
Sum of electronic and thermal Free Energies= -2039.427902

E(M06/6-311+G(2d,p))= -2040.51200344

Intermediate *t*-Xc



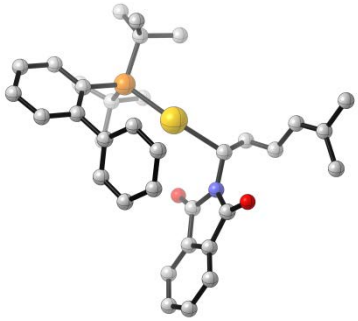
79	-0.285904000	0.705652000	-0.143962000
15	-2.667730000	0.687869000	-0.315059000
6	-3.058243000	0.233610000	-2.113266000
6	-3.289705000	2.415726000	0.184906000
6	1.862314000	0.889560000	-0.157824000
1	2.143638000	1.146163000	0.872379000
6	2.273506000	2.031401000	-1.163541000
1	2.283068000	1.617678000	-2.176179000
1	1.579241000	2.876297000	-1.104570000
6	-3.603725000	-0.556751000	0.672718000
6	-5.007356000	-0.512151000	0.638006000
6	-2.985250000	-1.618648000	1.369093000
6	-5.792143000	-1.482198000	1.246072000
1	-5.508814000	0.297612000	0.113825000
6	-3.794562000	-2.605652000	1.950832000
6	-5.179363000	-2.547491000	1.895511000
1	-6.876965000	-1.407675000	1.200624000
1	-3.307824000	-3.426723000	2.476911000
1	-5.775773000	-3.326403000	2.367334000
6	-1.522789000	-1.791159000	1.586955000
6	-0.852048000	-2.882117000	1.023703000
6	-0.830295000	-0.956363000	2.471980000
6	0.482223000	-3.133051000	1.336361000

1	-1.390390000	-3.545576000	0.345562000
6	0.501187000	-1.211351000	2.791139000
1	-1.352123000	-0.118848000	2.936671000
6	1.159113000	-2.302178000	2.226520000
1	0.990591000	-3.990368000	0.894368000
1	1.024536000	-0.558766000	3.489456000
1	2.196647000	-2.508999000	2.487912000
6	-4.609927000	2.859053000	-0.439177000
1	-4.853603000	3.859662000	-0.050195000
1	-5.454855000	2.207244000	-0.189853000
1	-4.541782000	2.944315000	-1.531226000
6	-3.406822000	2.418452000	1.709032000
1	-4.230972000	1.789186000	2.068326000
1	-3.598465000	3.447469000	2.048322000
1	-2.477604000	2.079427000	2.191130000
6	-2.219390000	3.437347000	-0.214899000
1	-2.569731000	4.441670000	0.068235000
1	-2.025886000	3.445531000	-1.295548000
1	-1.265651000	3.255401000	0.300812000
6	-2.392484000	1.260567000	-3.028665000
1	-2.874262000	2.246084000	-2.966664000
1	-2.479805000	0.915745000	-4.070127000
1	-1.320581000	1.379601000	-2.806502000
6	-2.409069000	-1.134677000	-2.337043000
1	-1.321760000	-1.109140000	-2.175241000
1	-2.588685000	-1.446724000	-3.377013000
1	-2.838999000	-1.905242000	-1.680633000
6	-4.539388000	0.123991000	-2.469392000
1	-4.615898000	-0.113597000	-3.541354000
1	-5.097761000	1.052759000	-2.300342000
1	-5.036085000	-0.687787000	-1.923563000
6	3.576596000	2.326841000	-0.607377000
1	4.354095000	1.575570000	-0.758384000
6	3.846579000	3.435042000	0.190385000
1	3.072004000	4.199516000	0.280795000
6	5.051666000	3.651719000	0.828367000
7	2.508763000	-0.360280000	-0.458690000
6	3.448775000	-0.975319000	0.383816000
6	2.175083000	-1.188338000	-1.541028000
6	3.701987000	-2.315907000	-0.192738000
8	3.929938000	-0.465663000	1.374748000
6	2.948539000	-2.438371000	-1.356805000
8	1.394781000	-0.902043000	-2.425784000
6	4.492536000	-3.348873000	0.273655000
6	2.957022000	-3.600018000	-2.106079000
1	5.071199000	-3.245993000	1.190186000
6	4.505948000	-4.530073000	-0.474540000
1	2.362951000	-3.690284000	-3.013616000
6	3.752498000	-4.652884000	-1.643383000
1	5.111614000	-5.370628000	-0.141359000
1	3.783418000	-5.586666000	-2.201395000
6	5.273868000	4.916316000	1.564465000
1	6.225179000	5.373714000	1.254919000
1	5.386780000	4.695919000	2.637562000
1	4.460593000	5.637081000	1.434731000
6	6.191108000	2.703361000	0.819307000
1	6.945498000	3.059355000	0.100370000
1	5.923838000	1.675533000	0.559225000
1	6.684694000	2.703467000	1.799740000

Zero-point correction= 0.686460
(Hartree/Particle)
Thermal correction to Energy= 0.728113
Thermal correction to Enthalpy= 0.729058
Thermal correction to Gibbs Free Energy= 0.612042
Sum of electronic and zero-point Energies= -2039.360906
Sum of electronic and thermal Energies= -2039.319252
Sum of electronic and thermal Enthalpies= -2039.318308
Sum of electronic and thermal Free Energies= -2039.435323

E(M06/6-311+G(2d,p))= -2040.51994525

Transition state $TS_{I\text{-}(IXc\text{-}Xc)}$



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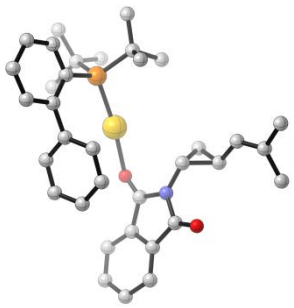
6	3.029853000	-0.034223000	-2.097371000
6	3.358637000	-2.256259000	0.156877000
6	-1.894622000	-1.021573000	-0.317574000
1	-2.001053000	-1.335032000	0.725246000
6	-1.977830000	-2.102274000	-1.459480000
1	-2.052741000	-1.610115000	-2.428520000
1	-1.176546000	-2.843319000	-1.420641000
6	3.480292000	0.724329000	0.723930000
6	4.884398000	0.764789000	0.715908000
6	2.783341000	1.731374000	1.428280000
6	5.596466000	1.768877000	1.357046000
1	5.443206000	-0.002195000	0.185677000
6	3.520243000	2.754319000	2.042565000
6	4.906994000	2.782140000	2.012280000
1	6.684419000	1.761414000	1.332469000
1	2.975120000	3.532553000	2.576227000
1	5.445079000	3.587144000	2.509628000
6	1.310001000	1.806104000	1.625449000
6	0.584947000	2.885275000	1.108686000
6	0.651528000	0.885288000	2.450460000
6	-0.767971000	3.039438000	1.404752000
1	1.093885000	3.620334000	0.484063000
6	-0.699547000	1.041828000	2.751330000
1	1.215077000	0.059989000	2.886651000
6	-1.411719000	2.120069000	2.230204000
1	-1.315193000	3.894039000	1.006932000
1	-1.194202000	0.324382000	3.405597000
1	-2.464011000	2.251349000	2.480961000
6	4.718536000	-2.600630000	-0.446641000
1	5.017077000	-3.592808000	-0.074981000
1	5.513799000	-1.902457000	-0.160599000
1	4.682993000	-2.662861000	-1.541715000
6	3.444530000	-2.292714000	1.682651000
1	4.211873000	-1.615575000	2.078250000
1	3.704943000	-3.314525000	1.996575000
1	2.483539000	-2.038793000	2.153863000
6	2.359444000	-3.328647000	-0.291156000
1	2.761861000	-4.316081000	-0.019083000
1	2.191792000	-3.327454000	-1.376143000
1	1.386066000	-3.213614000	0.207287000
6	2.451678000	-1.088287000	-3.041019000
1	3.006539000	-2.035119000	-2.994986000
1	2.522621000	-0.714552000	-4.073577000
1	1.389339000	-1.294142000	-2.834708000
6	2.292585000	1.291620000	-2.306015000
1	1.204931000	1.190060000	-2.181527000
1	2.483272000	1.641516000	-3.331826000
1	2.650540000	2.071861000	-1.618652000
6	4.505565000	0.184387000	-2.422952000
1	4.584682000	0.446444000	-3.488761000
1	5.122369000	-0.706233000	-2.258329000
1	4.935277000	1.017215000	-1.852695000
6	-3.178003000	-2.415444000	-0.753074000
1	-4.055854000	-1.811583000	-0.976648000
6	-3.284616000	-3.501964000	0.170991000
1	-2.407622000	-4.149410000	0.260517000
6	-4.387024000	-3.798628000	0.905218000

7	-2.578918000	0.203566000	-0.566637000
6	-3.600956000	0.700637000	0.266942000
6	-2.191091000	1.156700000	-1.524881000
6	-3.900478000	2.062831000	-0.226894000
8	-4.087982000	0.093332000	1.195368000
6	-3.067299000	2.329256000	-1.310030000
8	-1.295019000	1.011138000	-2.329937000
6	-4.793177000	3.003548000	0.251477000
6	-3.096058000	3.546513000	-1.965150000
1	-5.432982000	2.789382000	1.105800000
6	-4.830219000	4.238426000	-0.403110000
1	-2.438676000	3.750610000	-2.808309000
6	-3.997956000	4.504177000	-1.492045000
1	-5.517019000	5.008225000	-0.056831000
1	-4.051792000	5.476540000	-1.977670000
6	-4.396114000	-4.996932000	1.790819000
1	-3.432019000	-5.517235000	1.804903000
1	-5.171373000	-5.707102000	1.466400000
1	-4.658542000	-4.711029000	2.820228000
6	-5.648733000	-3.006046000	0.910445000
1	-5.678608000	-2.194341000	0.178488000
1	-5.798974000	-2.564780000	1.907157000
1	-6.509326000	-3.666830000	0.733349000

Zero-point correction= 0.684585
(Hartree/Particle)
Thermal correction to Energy= 0.725941
Thermal correction to Enthalpy= 0.726885
Thermal correction to Gibbs Free Energy= 0.609955
Sum of electronic and zero-point Energies= -2039.359998
Sum of electronic and thermal Energies= -2039.318642
Sum of electronic and thermal Enthalpies= -2039.317698
Sum of electronic and thermal Free Energies= -2039.434628

E(M06/6-311+G(2d,p))= -2040.51688529

Intermediate *t*-IXc



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15	-2.685448000	-0.523767000	0.358806000
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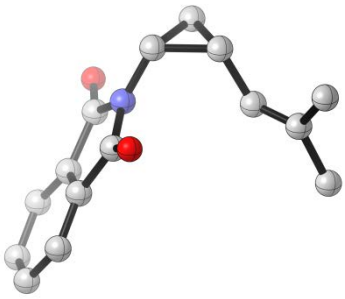
6	-2.655471000	-2.386885000	0.004782000
6	2.317858000	-1.331264000	0.220364000
1	1.524916000	-1.420401000	-0.526665000
6	2.195804000	-2.116137000	1.491580000
1	2.586807000	-1.653290000	2.396532000
1	1.293712000	-2.710848000	1.630735000
6	-3.377371000	0.325308000	-1.118149000
6	-4.687005000	-0.014949000	-1.496816000
6	-2.709845000	1.339846000	-1.838479000
6	-5.345256000	0.632501000	-2.532808000
1	-5.215844000	-0.800830000	-0.964856000
6	-3.401811000	1.997943000	-2.865308000
6	-4.701467000	1.659181000	-3.212662000
1	-6.359321000	0.339471000	-2.797313000
1	-2.886038000	2.788490000	-3.409780000
1	-5.204484000	2.189611000	-4.019184000
6	-1.298817000	1.784463000	-1.656173000
6	-1.025717000	3.039314000	-1.098580000
6	-0.243978000	1.044208000	-2.204635000
6	0.273452000	3.539027000	-1.080965000
1	-1.846935000	3.633426000	-0.695563000
6	1.055807000	1.546663000	-2.190348000
1	-0.451244000	0.080351000	-2.672333000
6	1.316308000	2.796775000	-1.631898000
1	0.469200000	4.519943000	-0.649495000
1	1.864966000	0.965072000	-2.633123000
1	2.327913000	3.202263000	-1.643508000
6	-4.012498000	-3.079546000	0.107435000
1	-3.866171000	-4.150409000	-0.098105000
1	-4.740966000	-2.712013000	-0.624775000
1	-4.444844000	-2.996063000	1.112718000
6	-2.092303000	-2.561710000	-1.405644000
1	-2.756122000	-2.153653000	-2.178694000
1	-1.971705000	-3.637347000	-1.601833000
1	-1.101691000	-2.095948000	-1.517363000
6	-1.697446000	-3.053063000	0.994222000
1	-1.631245000	-4.123731000	0.749961000
1	-2.033761000	-2.969890000	2.035127000
1	-0.687425000	-2.626387000	0.924325000
6	-3.342715000	-0.799258000	3.049618000
1	-3.638016000	-1.855657000	2.991282000
1	-3.835280000	-0.369285000	3.934331000
1	-2.256307000	-0.746183000	3.214274000
6	-3.506899000	1.479417000	2.037920000
1	-2.457652000	1.674579000	2.303962000
1	-4.137499000	1.834117000	2.866615000
1	-3.754922000	2.080301000	1.150779000
6	-5.284782000	-0.190992000	1.611963000
1	-5.786557000	0.076512000	2.553802000
1	-5.569394000	-1.222086000	1.371958000
1	-5.680754000	0.474010000	0.835127000
6	3.180888000	-2.550670000	0.446758000
1	4.223633000	-2.332131000	0.670373000
6	2.899841000	-3.742927000	-0.375687000
1	1.835255000	-3.988469000	-0.473282000
6	3.789680000	-4.523570000	-1.005074000
7	2.940202000	-0.043277000	0.281147000
6	4.152842000	0.298036000	-0.388225000
6	2.439181000	1.040080000	0.960316000
6	4.439967000	1.695901000	0.002606000
8	4.761346000	-0.440103000	-1.121368000
6	3.412704000	2.135057000	0.835284000
8	1.355888000	1.093534000	1.555537000
6	5.474936000	2.531458000	-0.370072000
6	3.375510000	3.423776000	1.334043000
1	6.268621000	2.188157000	-1.030652000
6	5.453127000	3.835852000	0.134491000
1	2.562505000	3.761444000	1.974432000
6	4.424591000	4.272745000	0.971447000
1	6.250809000	4.525775000	-0.132610000
1	4.439202000	5.295289000	1.342496000
6	3.341150000	-5.705887000	-1.807736000
1	2.249779000	-5.819236000	-1.808766000
1	3.780521000	-6.637238000	-1.418207000
1	3.678142000	-5.624330000	-2.852602000
6	5.272444000	-4.319884000	-0.980141000
1	5.591505000	-3.441329000	-0.409171000
1	5.660449000	-4.209210000	-2.004130000
1	5.776510000	-5.201848000	-0.556113000

Zero-point correction= 0.688642
(Hartree/Particle)
Thermal correction to Energy= 0.729609
Thermal correction to Enthalpy= 0.730553
Thermal correction to Gibbs Free Energy= 0.615136
Sum of electronic and zero-point Energies= -2039.381561
Sum of electronic and thermal Energies= -2039.340593
Sum of electronic and thermal Enthalpies= -2039.339649
Sum of electronic and thermal Free Energies= -2039.455067

E(M06/6-311+G(2d,p))= -2040.54238848

Product *cis*-6g



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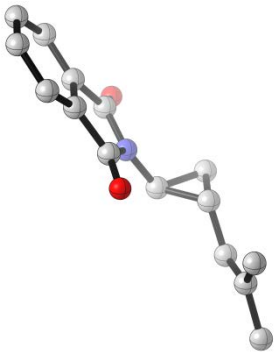
1	-1.353909000	2.445229000	1.149494000
1	-2.205856000	3.381767000	-0.176547000
6	-2.411778000	0.000976000	0.595675000
1	-1.626481000	-0.000529000	1.358932000
6	-3.289662000	-1.012877000	0.605849000
7	0.155520000	0.947660000	-0.530921000
6	1.202425000	1.466206000	0.247435000
6	0.480158000	-0.311382000	-1.063454000
6	2.242755000	0.407295000	0.276684000
6	1.812694000	-0.654452000	-0.512366000
8	1.229662000	2.558711000	0.769917000
8	-0.211313000	-0.941892000	-1.831616000
6	3.466877000	0.383674000	0.919254000
1	3.797464000	1.221026000	1.531398000
6	2.588181000	-1.784754000	-0.693832000
1	2.246282000	-2.610139000	-1.316035000
6	4.257243000	-0.755745000	0.746837000
1	5.227578000	-0.815740000	1.236190000
6	3.825943000	-1.821160000	-0.046424000
1	4.467036000	-2.693069000	-0.161476000
6	-1.047249000	1.636287000	-0.885128000
1	-1.058210000	1.997325000	-1.913497000
6	-3.194213000	-2.098585000	1.633794000
1	-4.121347000	-2.168495000	2.224188000
1	-3.060186000	-3.082898000	1.158421000
1	-2.360357000	-1.939926000	2.329085000
6	-4.422709000	-1.175949000	-0.358949000
1	-5.385624000	-1.201580000	0.174534000
1	-4.476970000	-0.384614000	-1.114611000
1	-4.340827000	-2.138137000	-0.887611000

Zero-point correction= 0.266974
(Hartree/Particle)
Thermal correction to Energy= 0.283235
Thermal correction to Enthalpy= 0.284179
Thermal correction to Gibbs Free Energy= 0.222145
Sum of electronic and zero-point Energies= -785.017675
Sum of electronic and thermal Energies= -785.001414
Sum of electronic and thermal Enthalpies= -785.000470
Sum of electronic and thermal Free Energies= -785.062504

E(M06/6-311+G(2d,p))= -785.507657060

Product *trans*-6g



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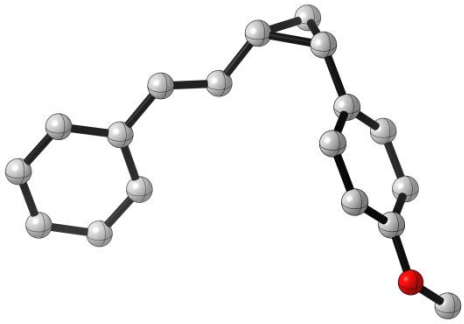
1	2.121950000	2.964339000	0.243388000
1	0.881246000	2.356123000	1.453006000
6	0.958487000	1.217205000	-0.446948000
1	1.224702000	1.406458000	-1.487775000
6	3.405323000	0.527379000	-0.105600000
1	3.764942000	1.337579000	-0.749963000
7	-0.345615000	0.664207000	-0.255554000
6	-0.625924000	-0.711142000	-0.310610000
6	-1.514599000	1.428089000	-0.111365000
6	-2.094283000	-0.830731000	-0.135946000
6	-2.624429000	0.449233000	-0.008405000
8	0.192579000	-1.589332000	-0.470958000
8	-1.567526000	2.637778000	-0.089278000
6	-2.897663000	-1.955622000	-0.097973000
1	-2.473826000	-2.952927000	-0.202617000
6	-3.979747000	0.659173000	0.165433000
1	-4.386468000	1.664174000	0.263170000
6	-4.269634000	-1.755358000	0.077249000
1	-4.937331000	-2.614186000	0.110558000
6	-4.800953000	-0.470557000	0.208245000
1	-5.874179000	-0.349711000	0.343092000
6	4.199751000	-0.538605000	0.068463000
6	3.846074000	-1.738236000	0.891785000
1	2.869335000	-1.664881000	1.382044000
1	3.834868000	-2.643235000	0.264813000
1	4.603763000	-1.914768000	1.670919000
6	5.545075000	-0.612896000	-0.586344000
1	6.344294000	-0.727469000	0.162689000
1	5.614978000	-1.492728000	-1.244955000
1	5.766923000	0.279722000	-1.184934000

Zero-point correction= 0.267869
(Hartree/Particle)
Thermal correction to Energy= 0.283864
Thermal correction to Enthalpy= 0.284808
Thermal correction to Gibbs Free Energy= 0.224162
Sum of electronic and zero-point Energies= -785.017893
Sum of electronic and thermal Energies= -785.001898
Sum of electronic and thermal Enthalpies= -785.000954
Sum of electronic and thermal Free Energies= -785.061601

E(M06/6-311+G(2d,p))= -785.514839058

Optimized structures of *cis*-3g and *trans*-3g

Product *cis*-3g

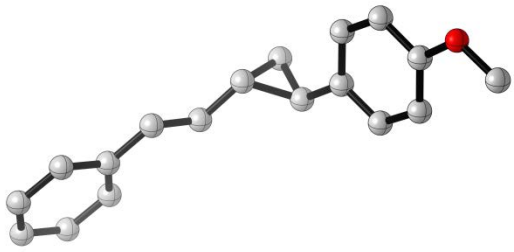


6	-4.474508000	0.025991000	0.451959000
6	-5.263958000	-1.106367000	0.283275000
6	-4.720849000	-2.258657000	-0.277730000
6	-3.380250000	-2.265358000	-0.663220000
6	-2.592640000	-1.134969000	-0.493811000
6	-3.127616000	0.038741000	0.061257000
1	-4.903067000	0.927348000	0.892639000
1	-6.308083000	-1.088181000	0.593087000
1	-5.333861000	-3.148903000	-0.409508000
1	-2.942836000	-3.165330000	-1.094111000
1	-1.542765000	-1.167763000	-0.784471000
6	-2.343361000	1.258437000	0.257192000
1	-2.842275000	2.045370000	0.831986000
6	-1.106737000	1.497292000	-0.205648000
1	-0.590221000	0.739736000	-0.802878000
6	-0.359294000	2.735566000	0.035733000
6	1.152653000	2.681954000	0.233546000
6	0.589306000	3.250826000	-1.021570000
1	-0.883494000	3.487470000	0.627438000
1	1.513191000	3.411968000	0.961776000
1	0.640200000	4.326225000	-1.180718000
1	0.670979000	2.653714000	-1.930520000
6	1.875439000	1.378956000	0.252194000
6	2.668361000	0.952102000	-0.809911000
6	1.781049000	0.543392000	1.374876000
6	3.352761000	-0.263750000	-0.773419000
1	2.762570000	1.583241000	-1.693980000
6	2.452675000	-0.665155000	1.430916000
1	1.158618000	0.851280000	2.216369000
6	3.246239000	-1.078629000	0.353095000
1	3.960932000	-0.560930000	-1.624524000
1	2.378260000	-1.316242000	2.300729000
8	3.861790000	-2.277188000	0.496753000
6	4.689107000	-2.721993000	-0.556349000
1	5.086330000	-3.692738000	-0.246851000
1	4.124019000	-2.847612000	-1.491680000
1	5.526907000	-2.031398000	-0.733122000

Zero-point correction= 0.309069
(Hartree/Particle)
Thermal correction to Energy= 0.325757
Thermal correction to Enthalpy= 0.326701
Thermal correction to Gibbs Free Energy= 0.263210
Sum of electronic and zero-point Energies= -771.038908
Sum of electronic and thermal Energies= -771.022219
Sum of electronic and thermal Enthalpies= -771.021275
Sum of electronic and thermal Free Energies= -771.084766

E(M06/6-311+G(2d,p))= -771.570294803

Product *trans*-3g



6	4.605818000	-1.269829000	-0.967522000
6	5.904058000	-1.626464000	-0.620212000
6	6.546480000	-0.983338000	0.433859000
6	5.875805000	0.020230000	1.133006000
6	4.579263000	0.375114000	0.786105000
6	3.915299000	-0.267132000	-0.271353000
1	4.105894000	-1.776282000	-1.794392000
1	6.416048000	-2.411334000	-1.175674000
1	7.563940000	-1.257602000	0.708298000
1	6.371590000	0.533738000	1.956089000
1	4.076979000	1.168886000	1.339126000
6	2.549261000	0.061309000	-0.678285000
1	2.197519000	-0.453522000	-1.577967000
6	1.703468000	0.902987000	-0.064613000
1	2.008541000	1.428494000	0.846665000
6	0.340954000	1.181530000	-0.527315000
6	-0.778884000	1.319446000	0.502171000
6	-0.289463000	2.516166000	-0.249019000
1	0.049083000	0.689262000	-1.457653000
1	-0.942273000	2.938524000	-1.012375000
1	0.305699000	3.248962000	0.295383000
6	-2.109546000	0.716070000	0.247560000
6	-2.788132000	0.069849000	1.280399000
6	-2.730236000	0.757260000	-1.010126000
6	-4.037793000	-0.518790000	1.090292000
1	-2.328204000	0.022803000	2.268381000
6	-3.970517000	0.177476000	-1.217232000
1	-2.237232000	1.249474000	-1.849748000
6	-4.636624000	-0.466285000	-0.168202000
1	-4.528035000	-1.011815000	1.926552000
1	-4.450753000	0.210901000	-2.194177000
1	-0.448732000	1.243778000	1.540058000
8	-5.844867000	-1.001431000	-0.471997000
6	-6.541503000	-1.673184000	0.554035000
1	-7.477580000	-2.026642000	0.112195000
1	-5.975040000	-2.538106000	0.929732000
1	-6.774766000	-1.002547000	1.394183000

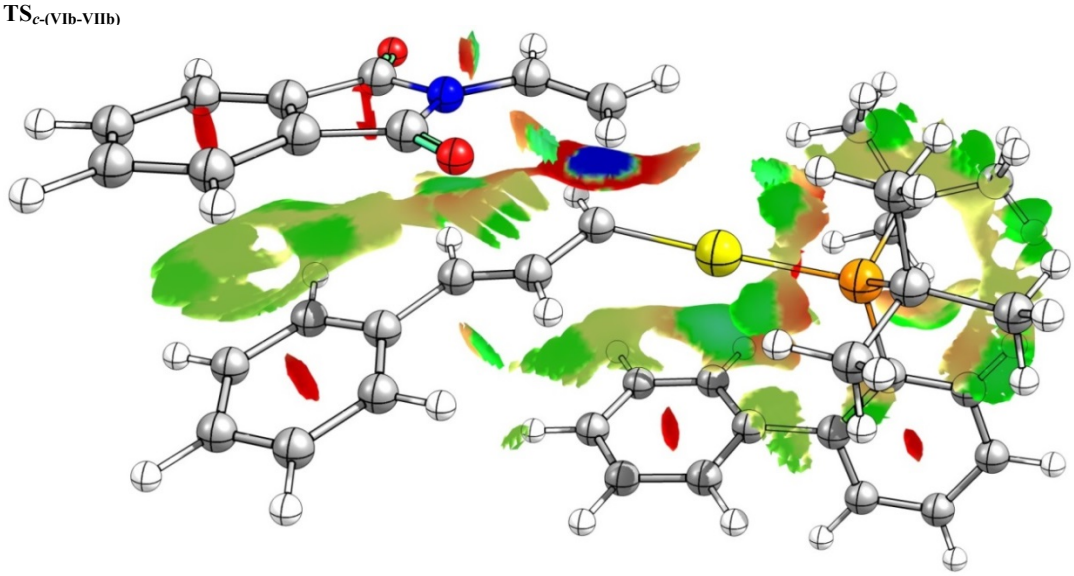
Zero-point correction= 0.309522
(Hartree/Particle)
Thermal correction to Energy= 0.326255
Thermal correction to Enthalpy= 0.327199
Thermal correction to Gibbs Free Energy= 0.263501
Sum of electronic and zero-point Energies= -771.040432
Sum of electronic and thermal Energies= -771.023699
Sum of electronic and thermal Enthalpies= -771.022755
Sum of electronic and thermal Free Energies= -771.086454

E(M06/6-311+G(2d,p))= -771.572360519

Reduced density gradient surface

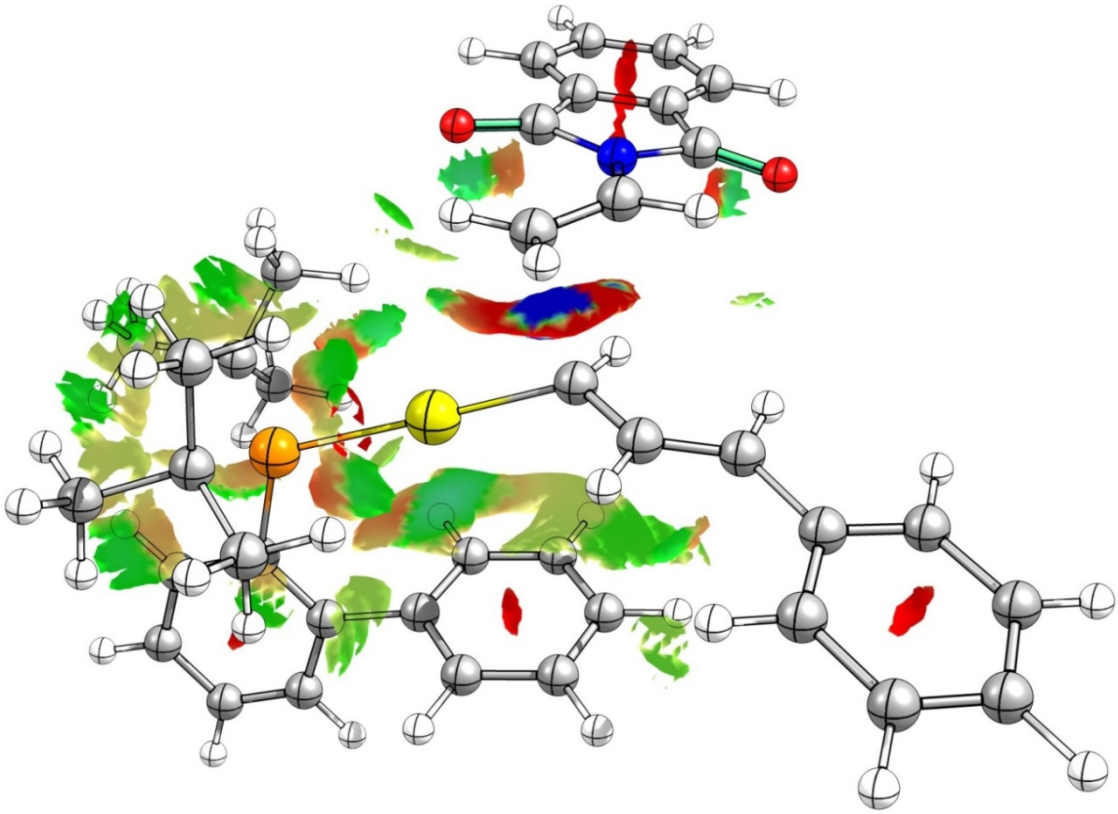
The Reduced density gradient surface was generated for the cyclopropanation transition states using Multiwfn.[21] The isosurface was visualized using ChemCraft, with the surface contour set at 0.5 and the color range fixed from -0.035 to 0.02.

$TS_{c\text{-(VIb-VIIb)}}$



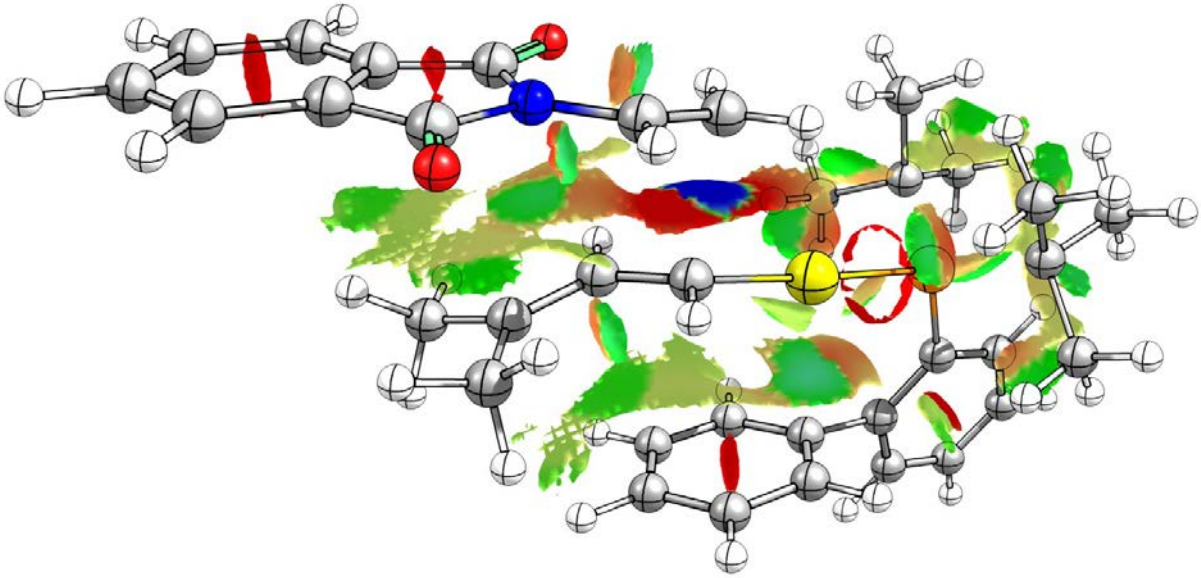
Color range:	-0.035		.02

$TS_{t\text{-(VIb-VIIIb)}}$



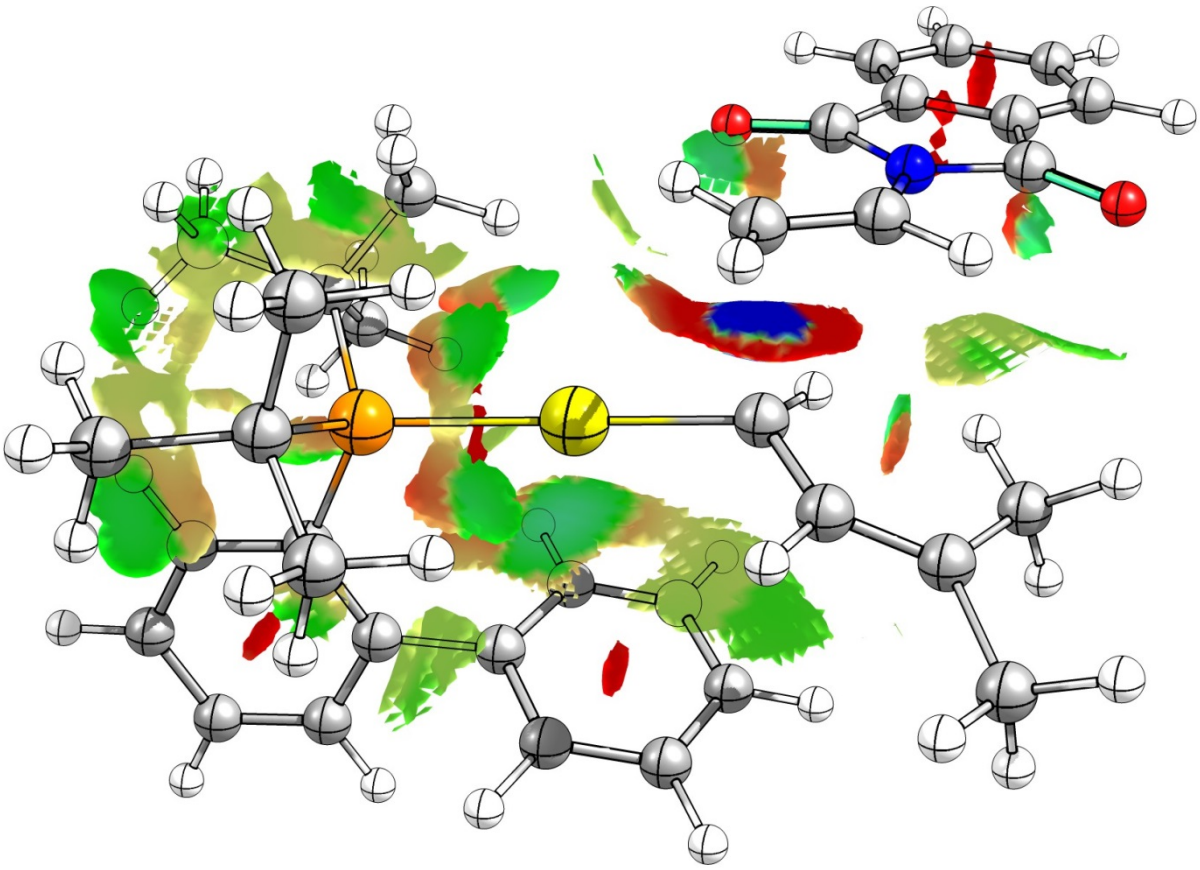
Color range:	-0.035		.02

$TS_{c\text{-(VIc-VIIc)}}$



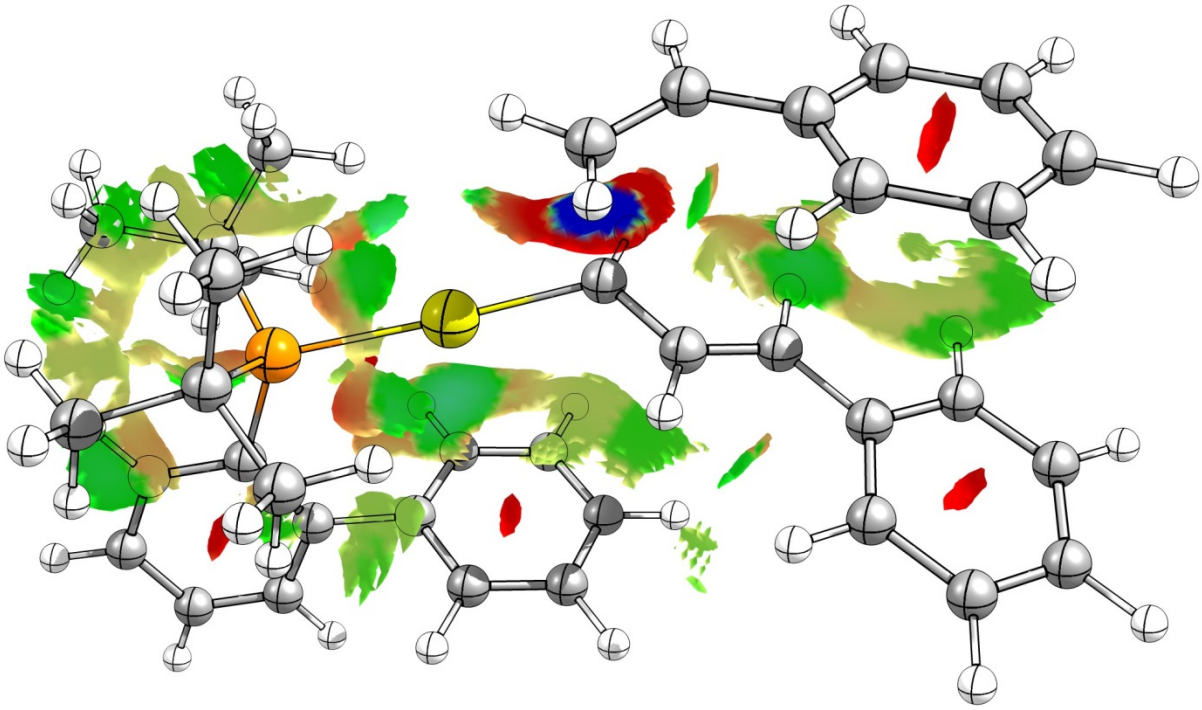
Color range: -0.035 .02

$TS_{t\text{-(VIc-VIIc)}}$



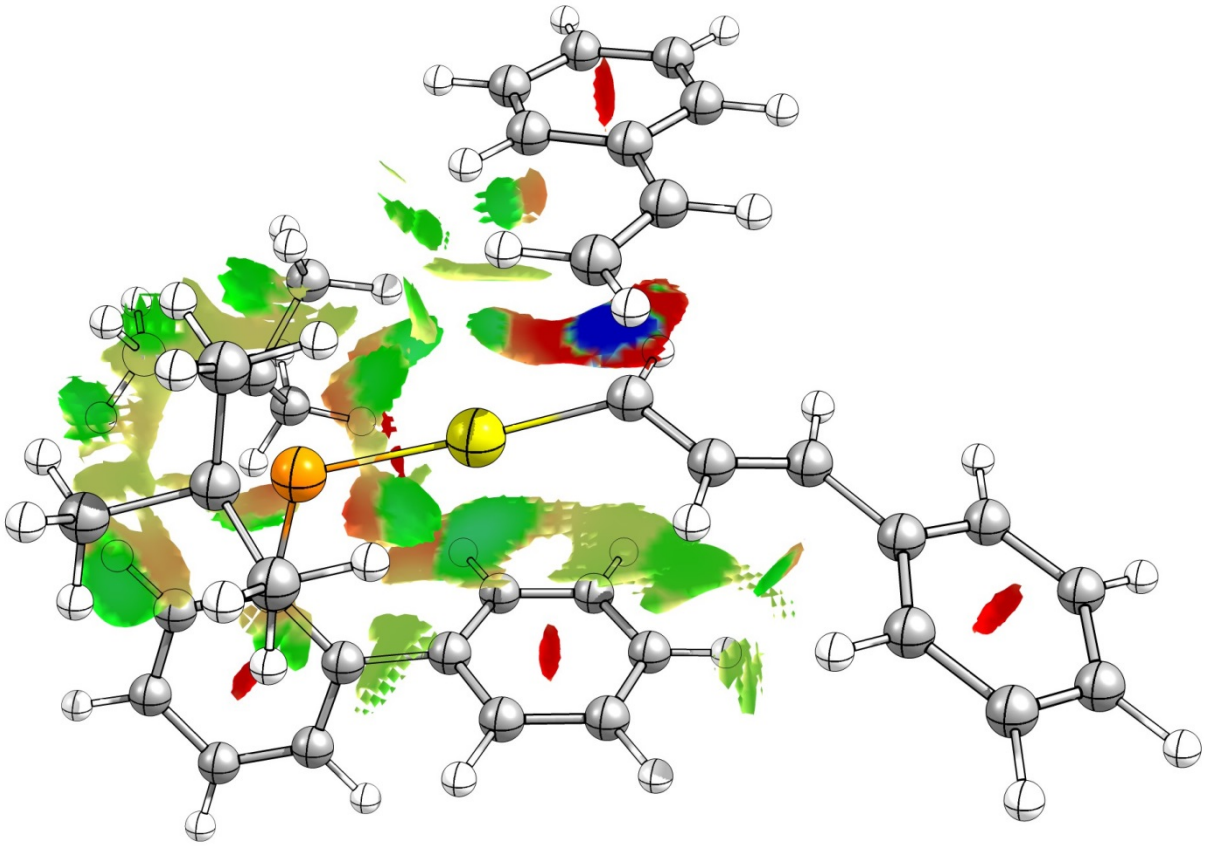
Color range: -0.035 .02

$TS_{c\text{-(VIa-VIIa)}}$



Color range: -0.035 .02

$TS_{t\text{-(VIa-VIIa)}}$

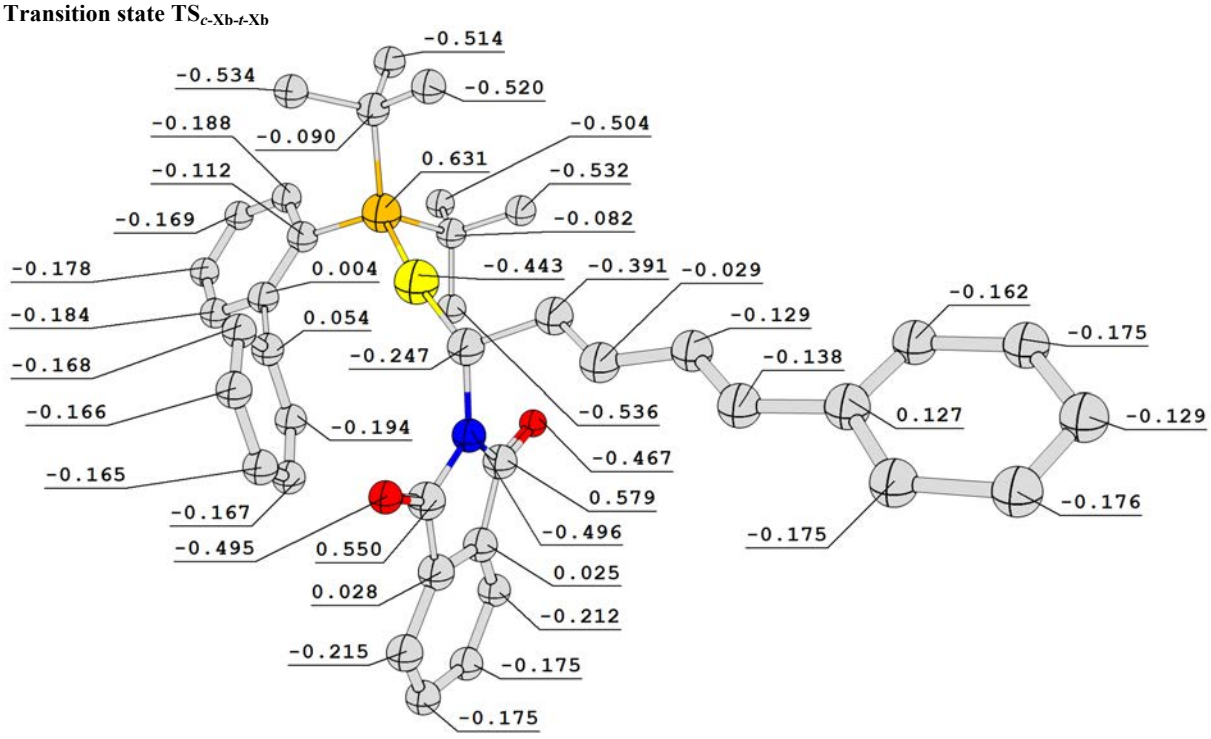


Color range: -0.035 .02

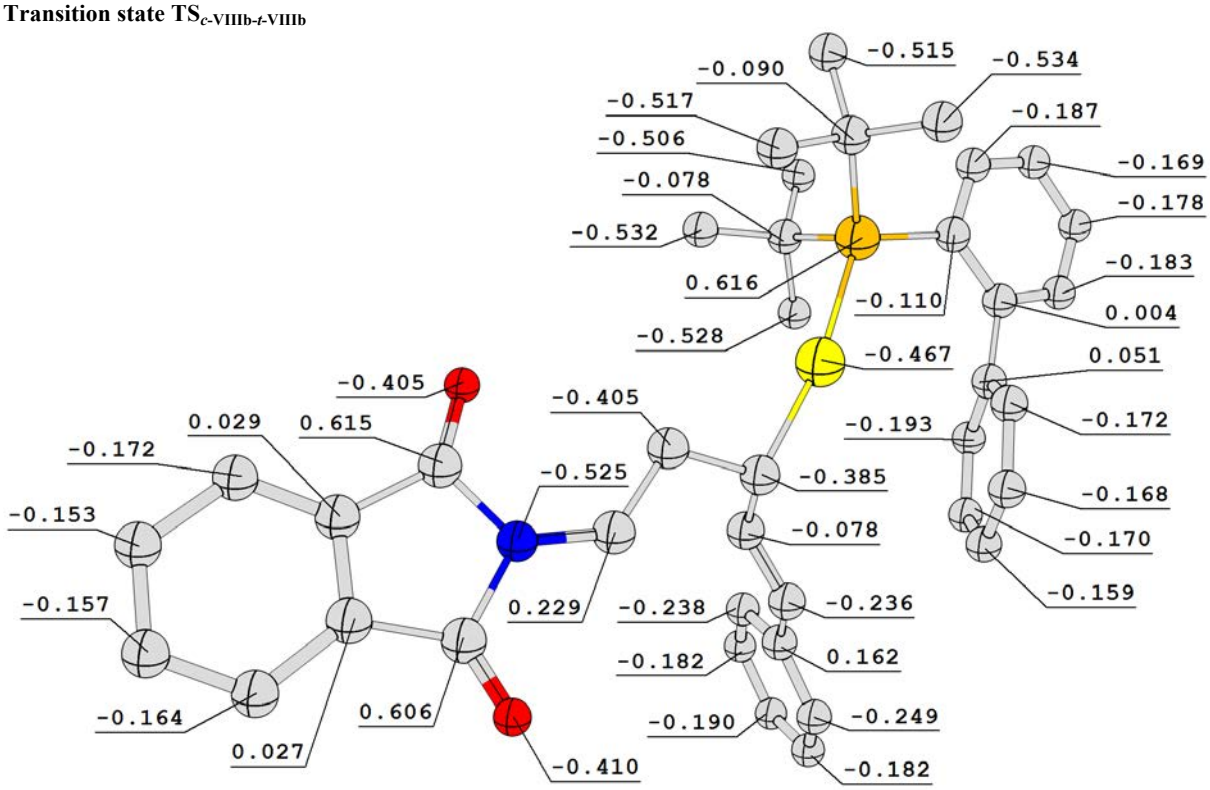
Natural bond orbital analysis

NBO charges were calculated from previously optimized geometries using NBO version 6.0.[22]

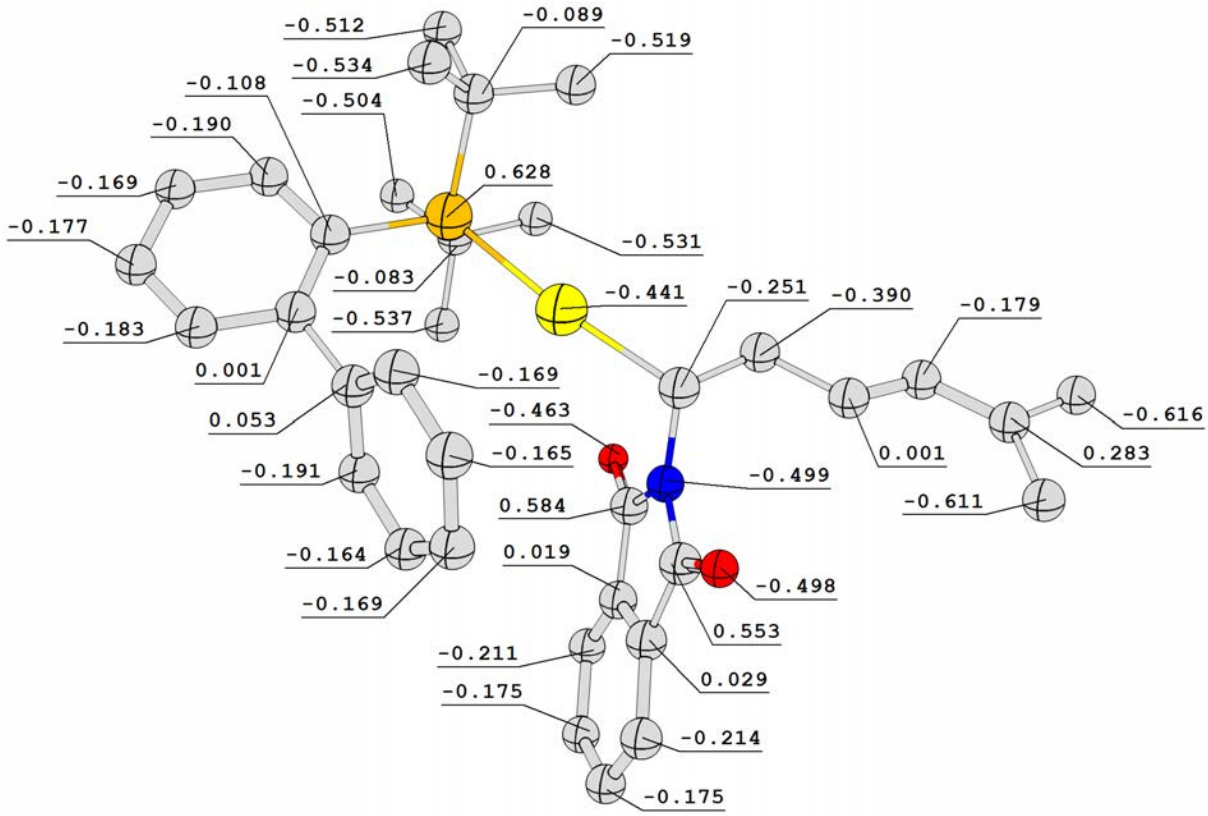
Transition state $TS_{c\text{-}Xb\text{-}t\text{-}Xb}$



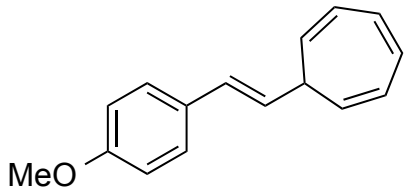
Transition state $TS_{c\text{-}VIIIb\text{-}t\text{-}VIIIb}$



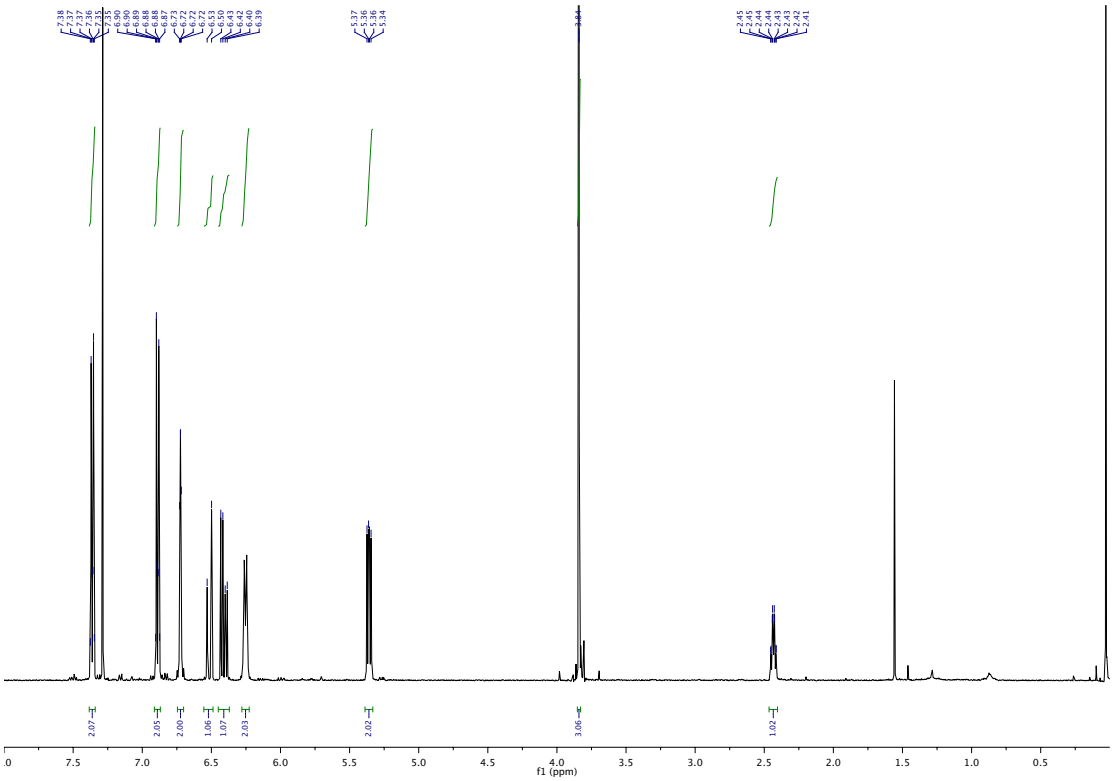
Transition state $TS_{c\text{-}Xc\text{-}t\text{-}Xc}$

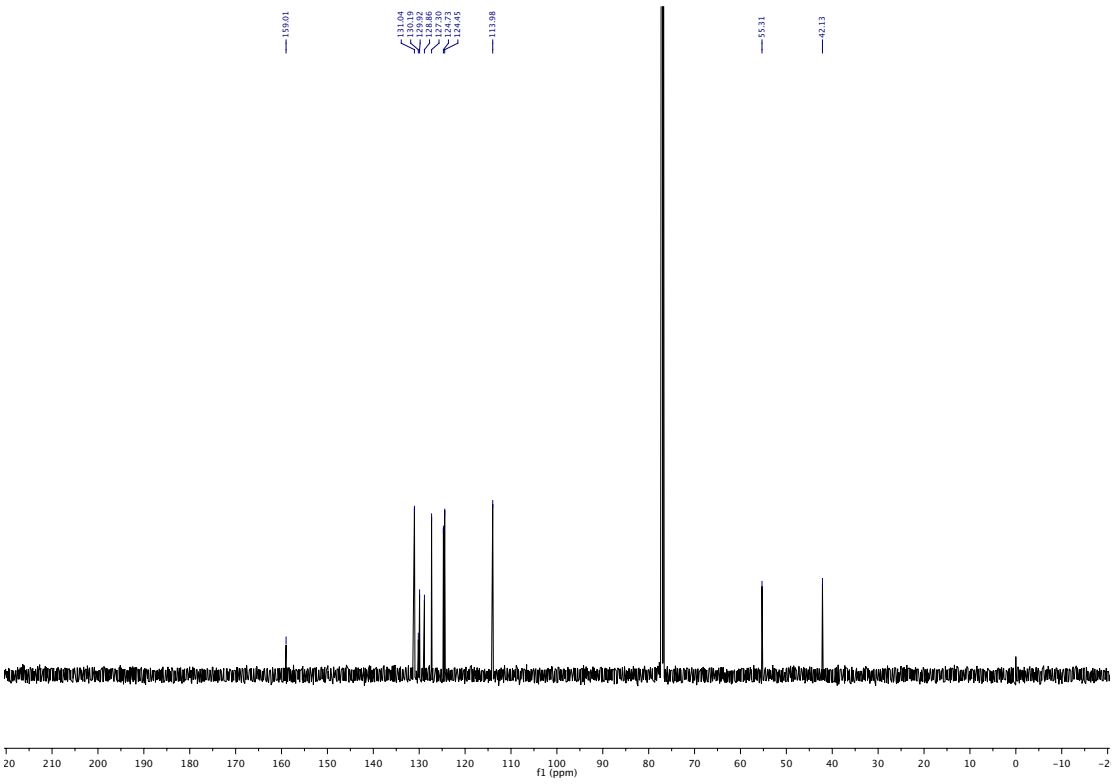


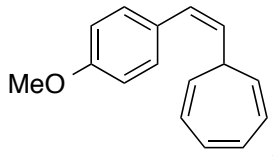
12. NMR spectra



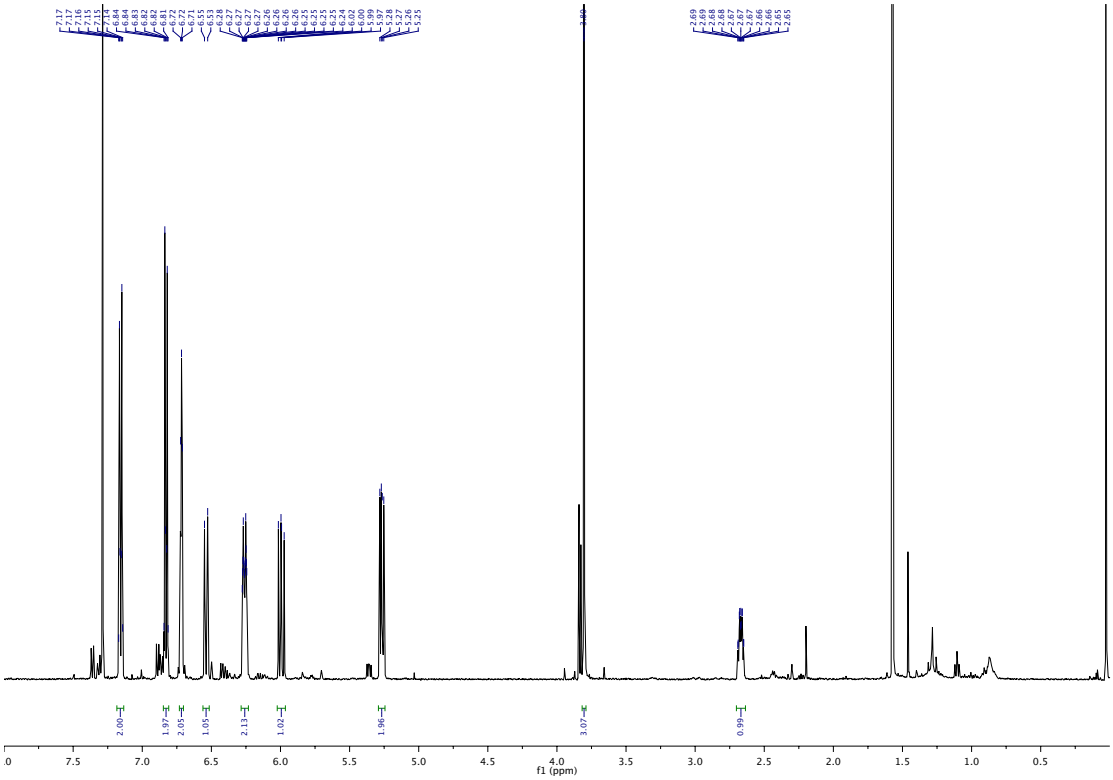
1b

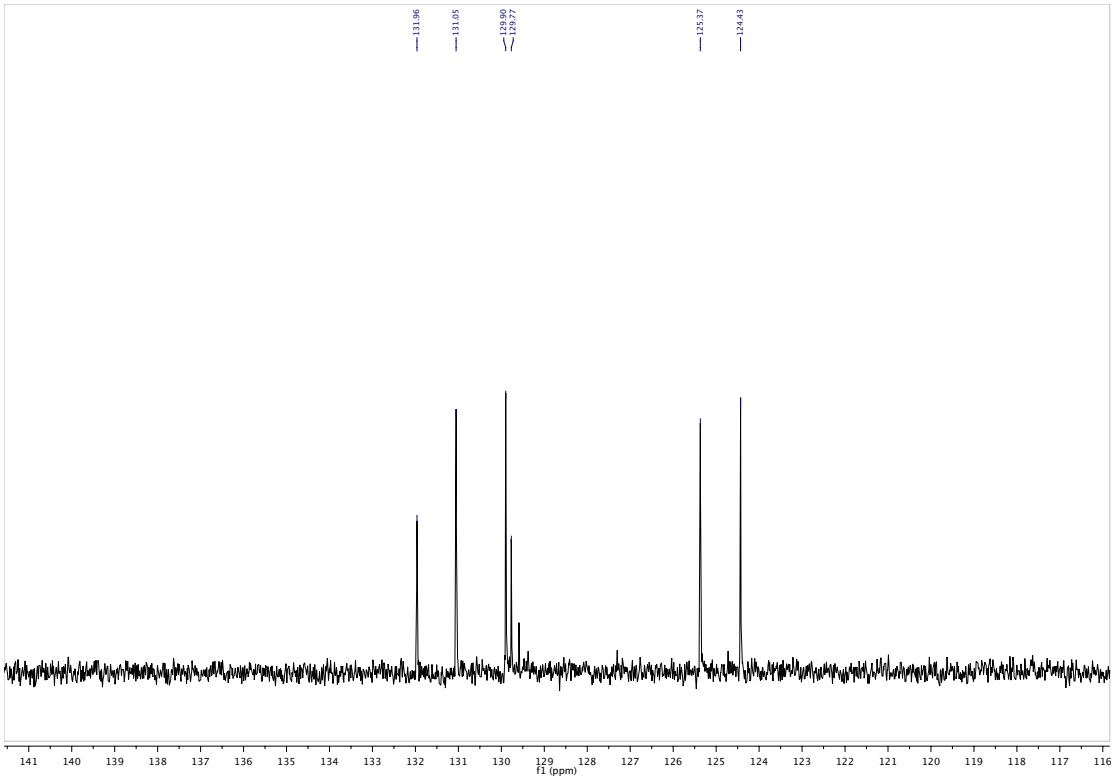


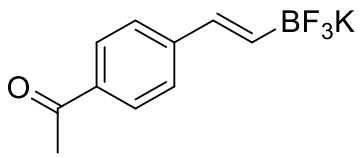




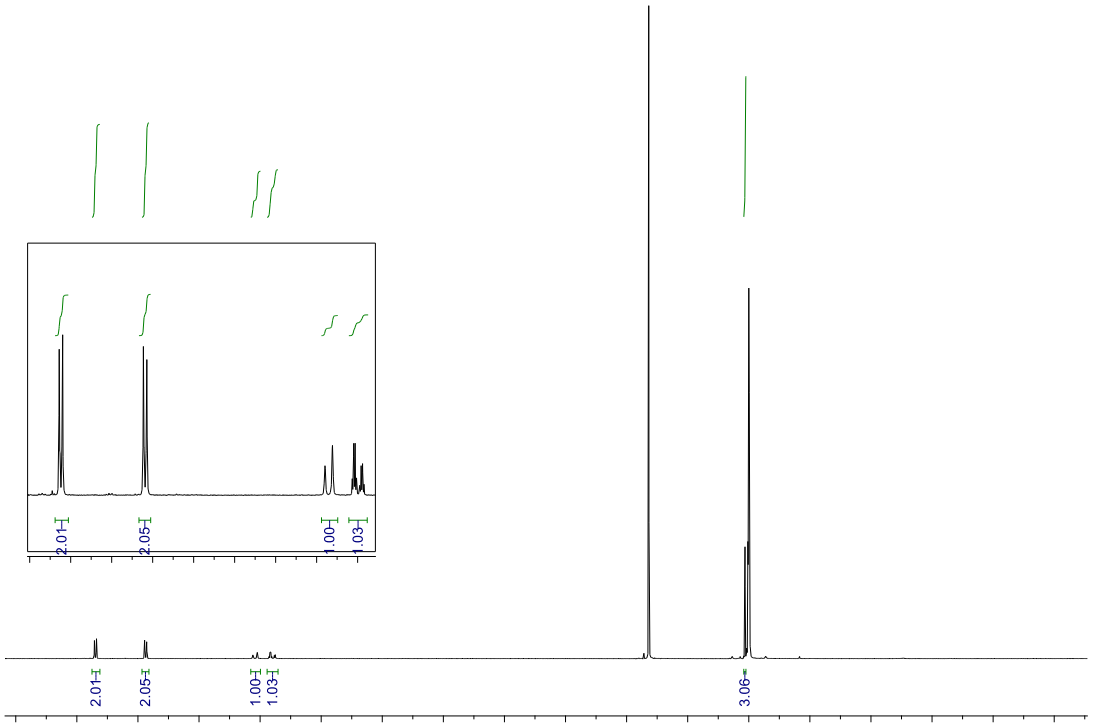
***Z*-1b**

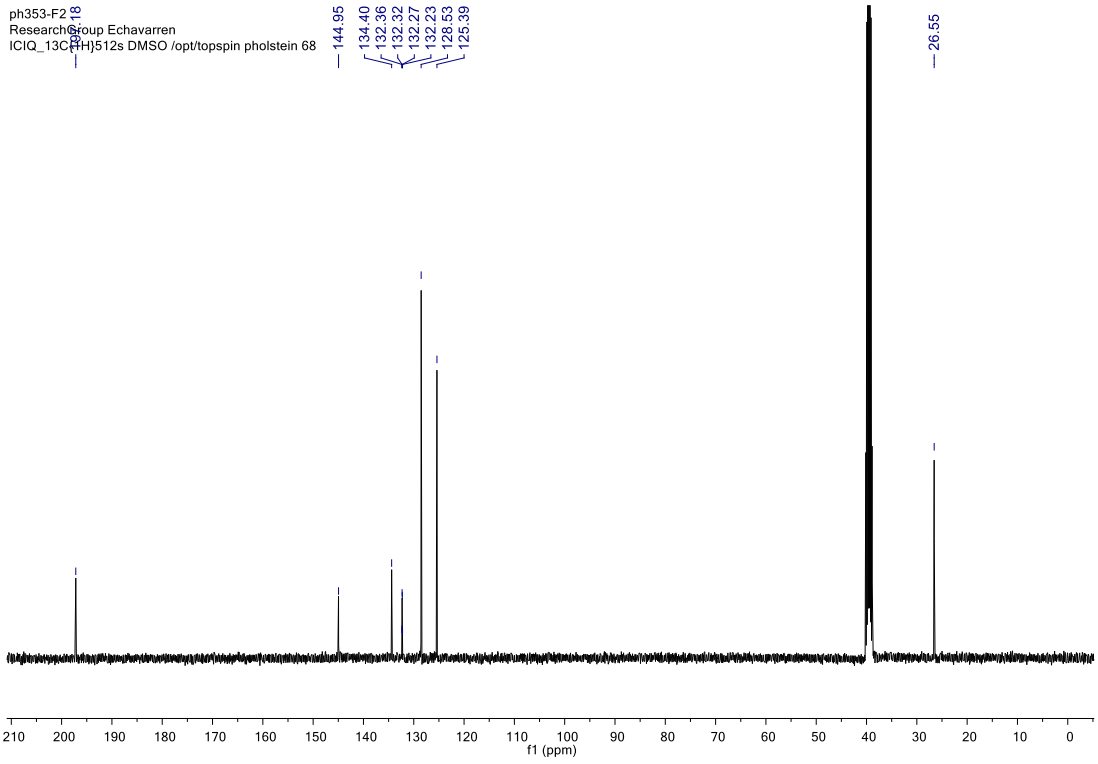


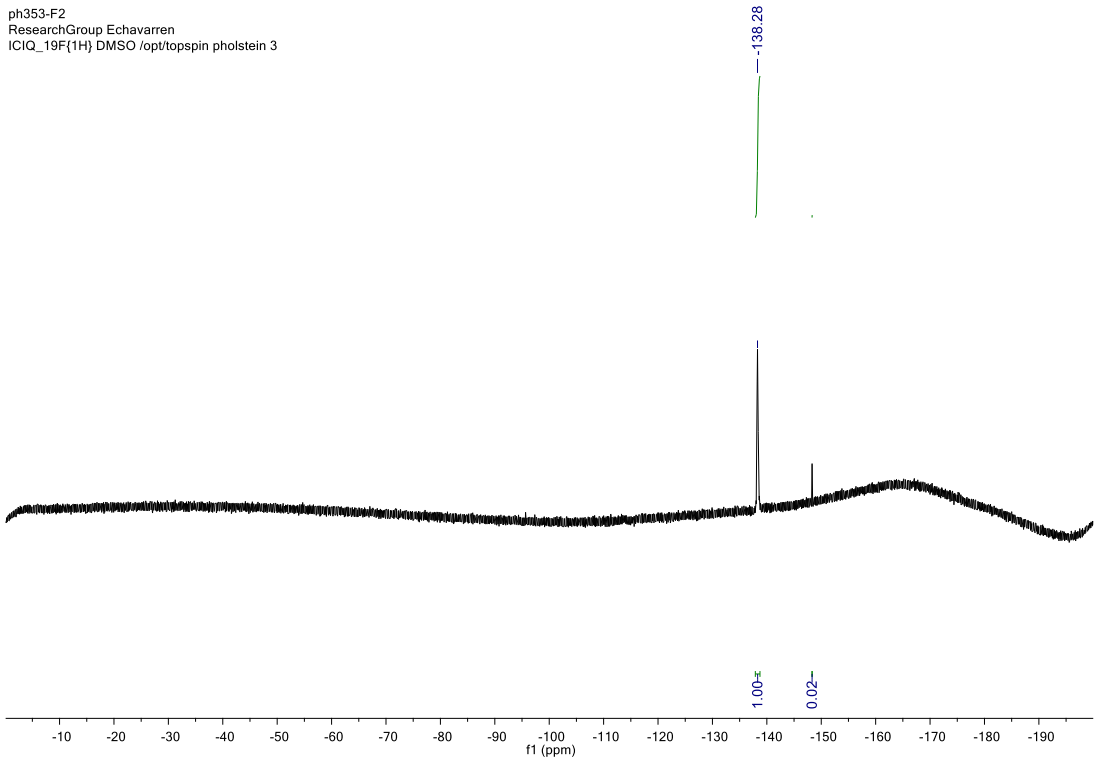


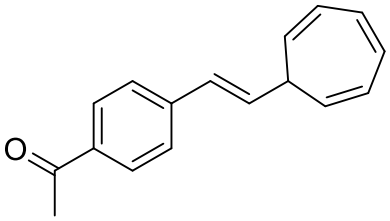

BF3K
O

1c

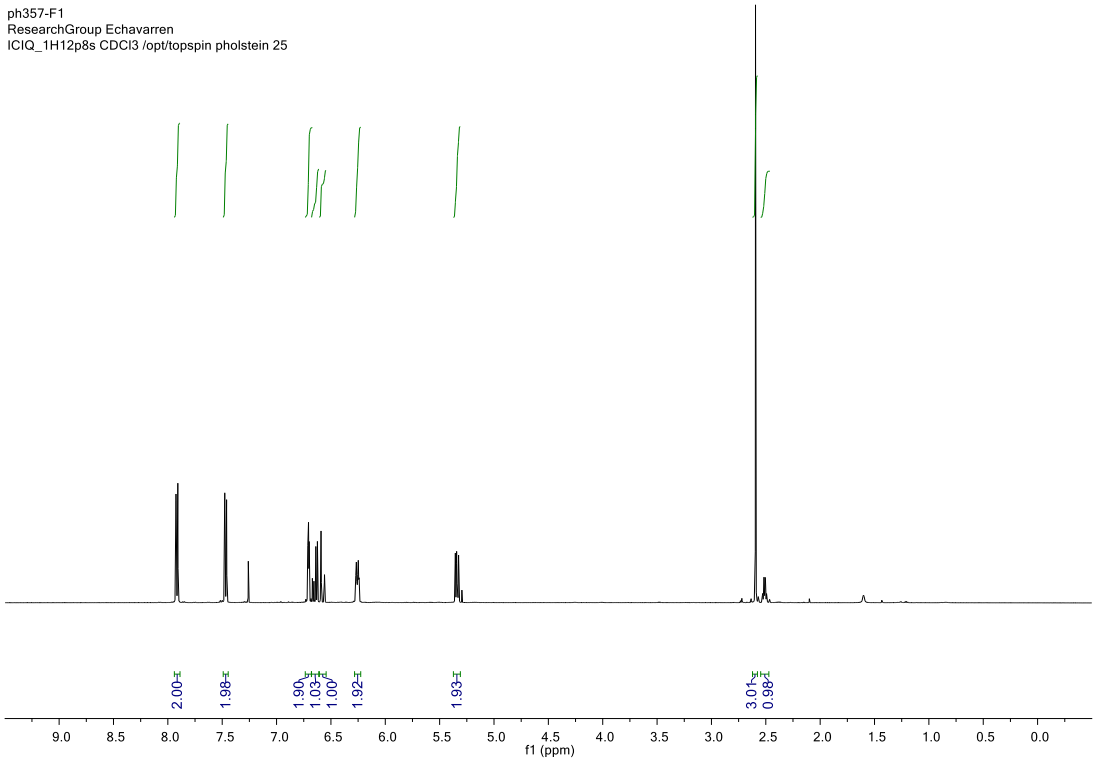

2.01
2.05
1.00
1.03
3.06

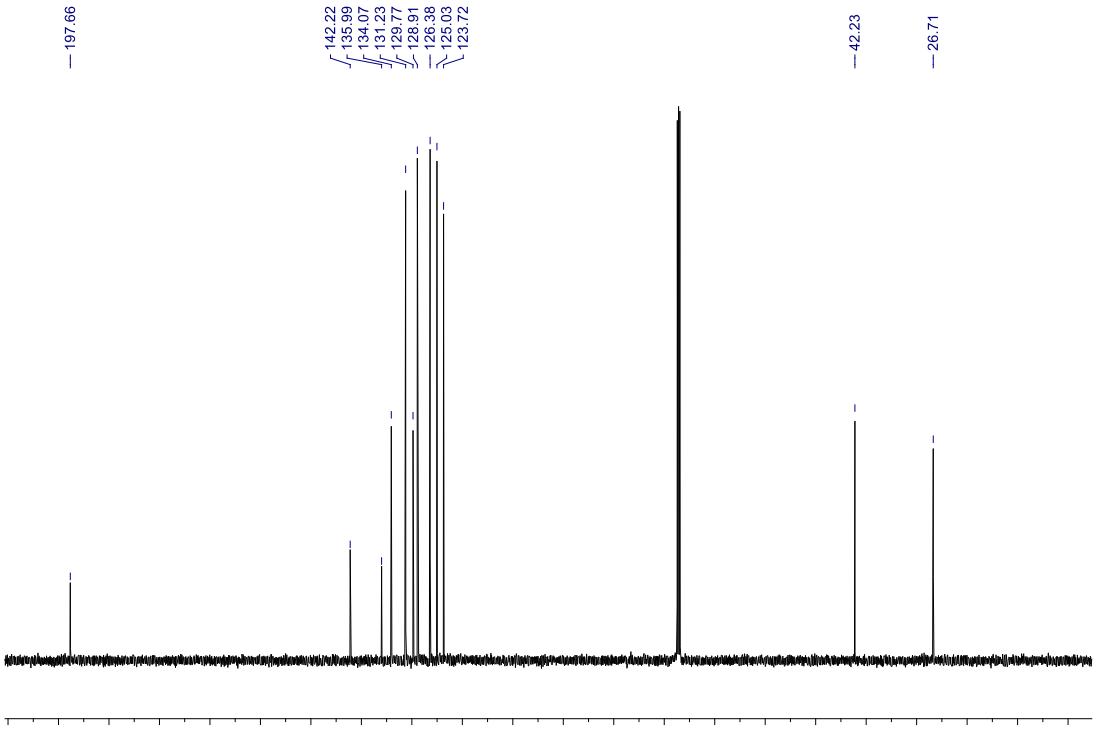

ph353-F2
Research Group Echavarren
ICIQ_13C{1H}512s DMSO /opt/topspin pholstein 68
144.95
134.40
132.36
132.32
132.27
132.23
128.53
125.39
26.55
f1 (ppm)

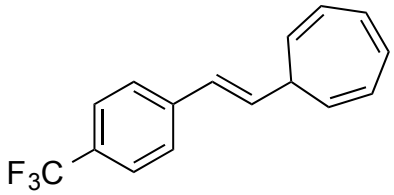

ph353-F2
ResearchGroup Echavarren
ICIQ_19F{1H} DMSO /opt/topspin pholstein 3
-138.28
1.00
0.02
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


O

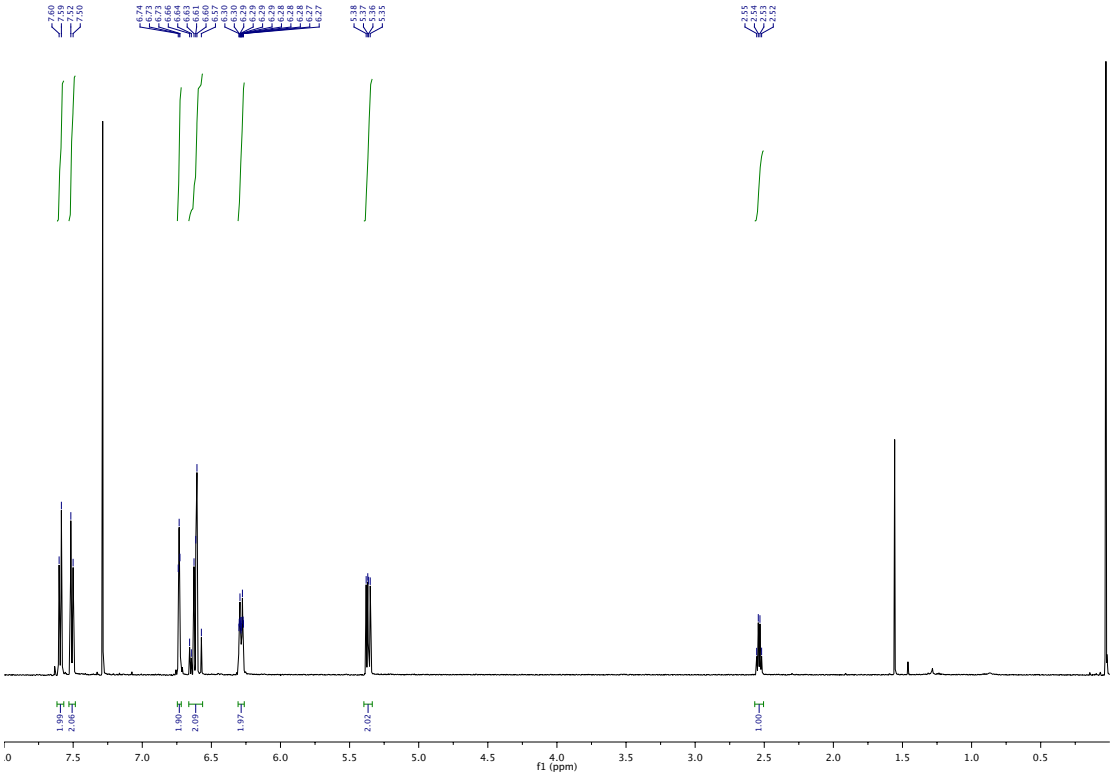
1c

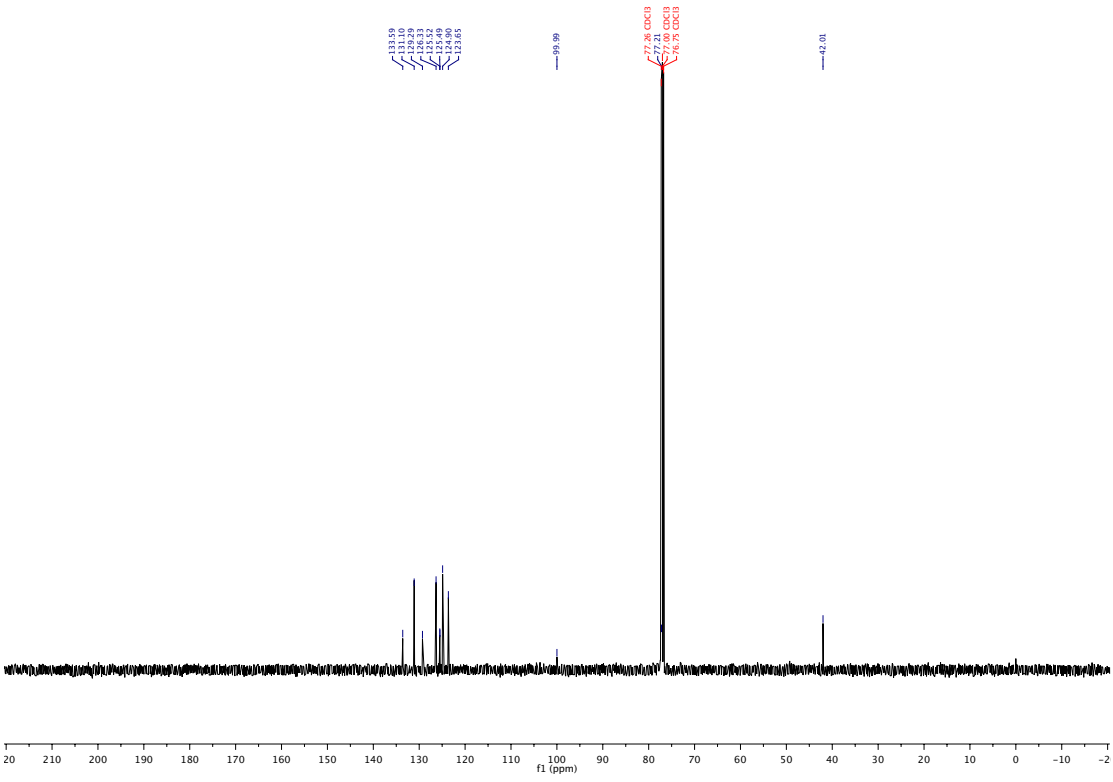

ph357-F1
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 25
2.00
1.98
1.90
1.05
1.00
1.92
1.93
3.01
0.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

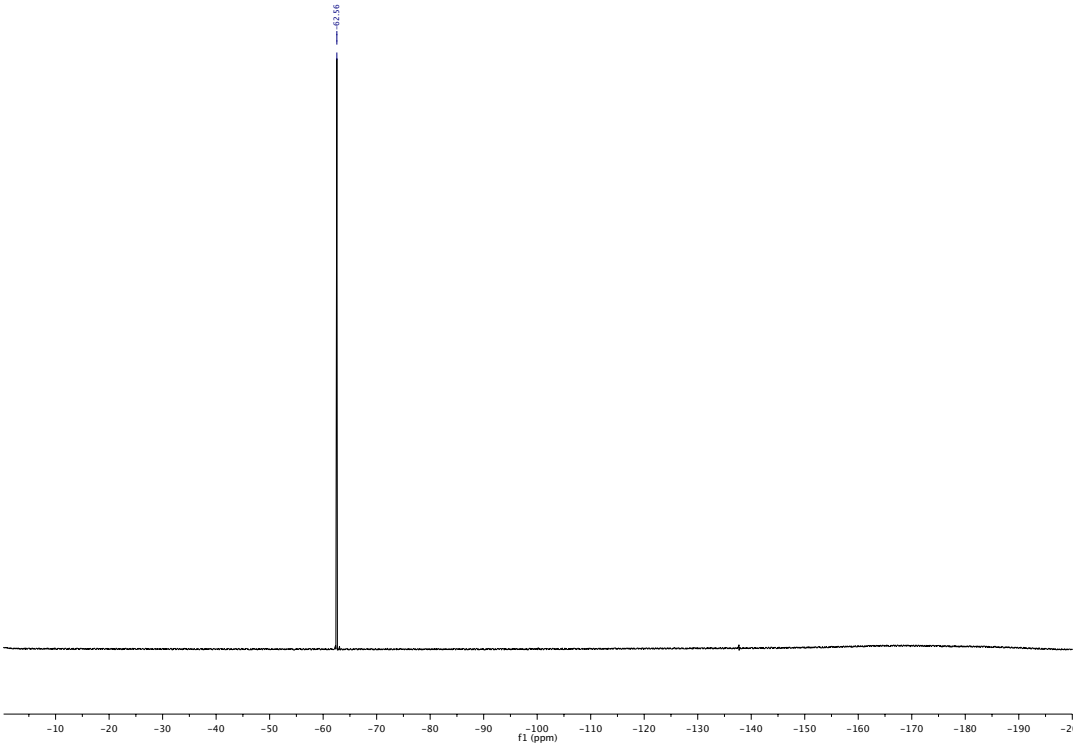

197.66
142.22
135.99
134.07
131.23
129.77
128.91
126.38
125.03
123.72
42.23
26.71

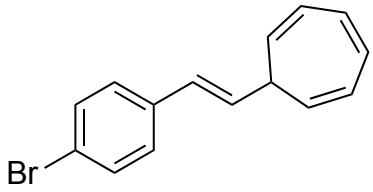

F3C

1d

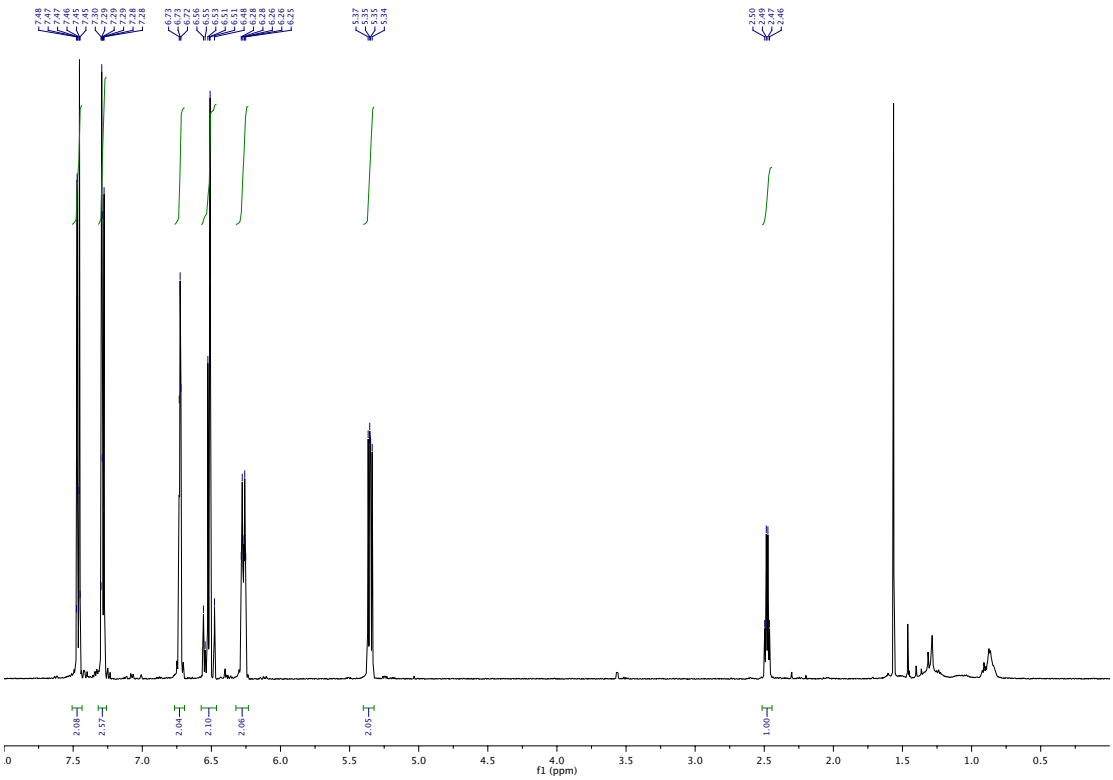

7.60
7.59
7.52
7.50
6.74
6.73
6.73
6.66
6.64
6.63
6.61
6.60
6.57
6.30
6.29
6.29
6.29
6.28
6.28
6.28
6.27
6.27
5.38
5.37
5.36
5.35
2.55
2.54
2.53
2.52
1.99
1.06
2.04
1.90
2.09
1.97
2.02
1.00
f1 (ppm)


133.59
131.10
129.39
128.31
125.52
125.49
124.90
123.65
99.99
77.36 CDCl3
77.20
77.00 CDCl3
76.75 CDCl3
42.01
f1 (ppm)


-62.56
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


Br

1e


7.48
7.47
7.47
7.46
7.45
7.45
7.30
7.29
7.29
7.29
7.29
7.28
7.28
6.73
6.73
6.72
6.72
6.56
6.55
6.53
6.53
6.51
6.51
6.48
6.48
6.28
6.26
6.26
6.25
6.25
5.37
5.35
5.35
5.34
2.50
2.49
2.47
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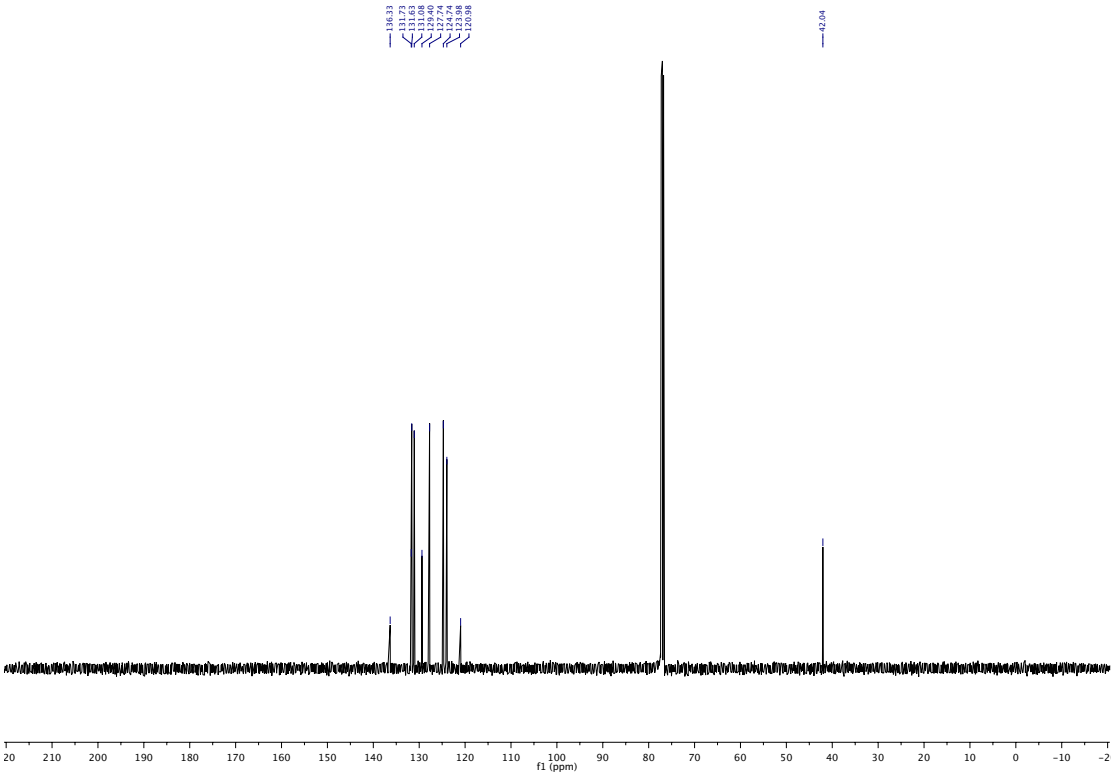
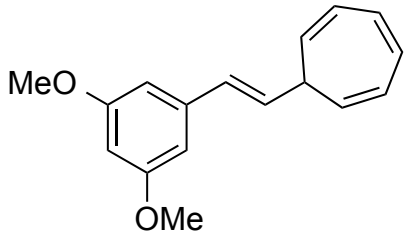
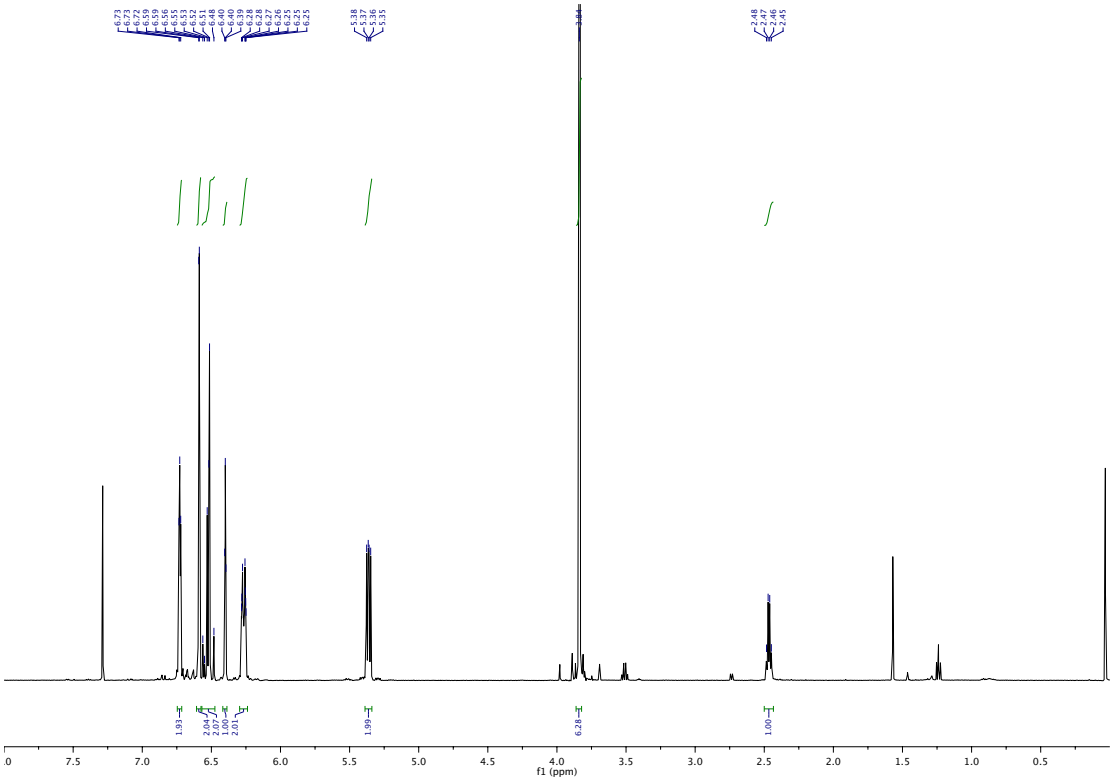
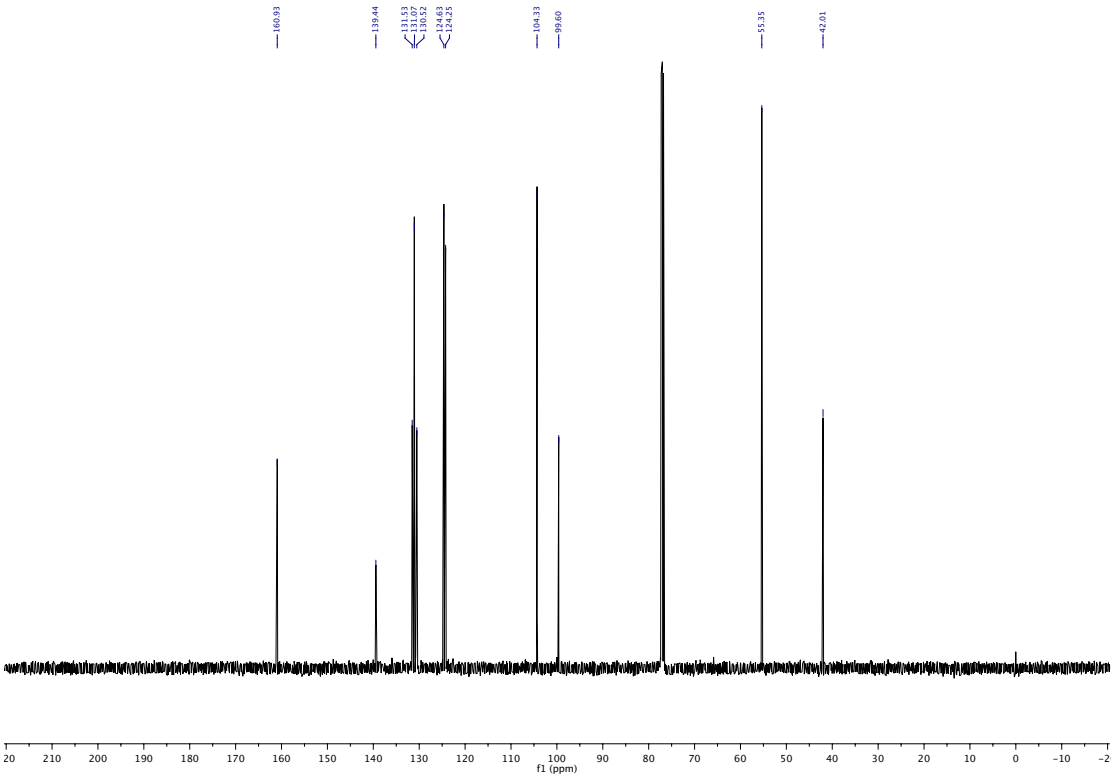
2.46
2.08
2.57
2.04
2.10
2.06
2.05
1.00
f1 (ppm)

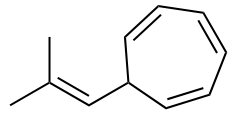

136.33
131.73
131.63
131.08
129.40
127.74
124.44
123.98
120.98
42.04
f1 (ppm)



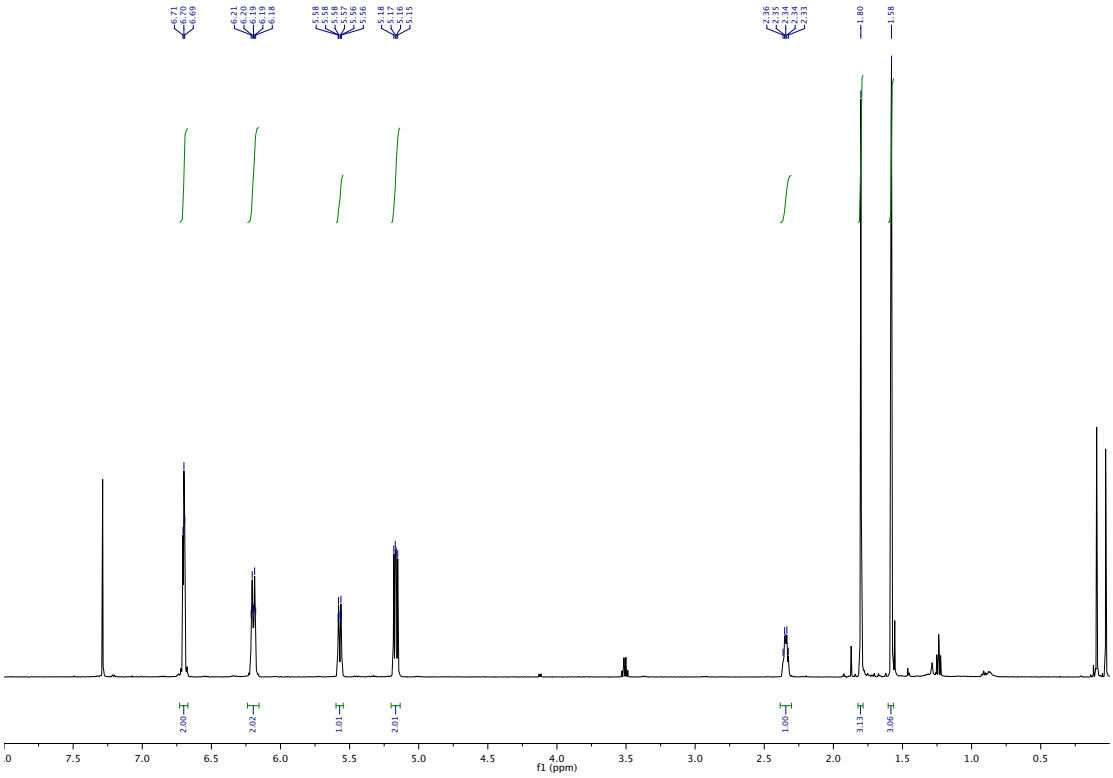
1f

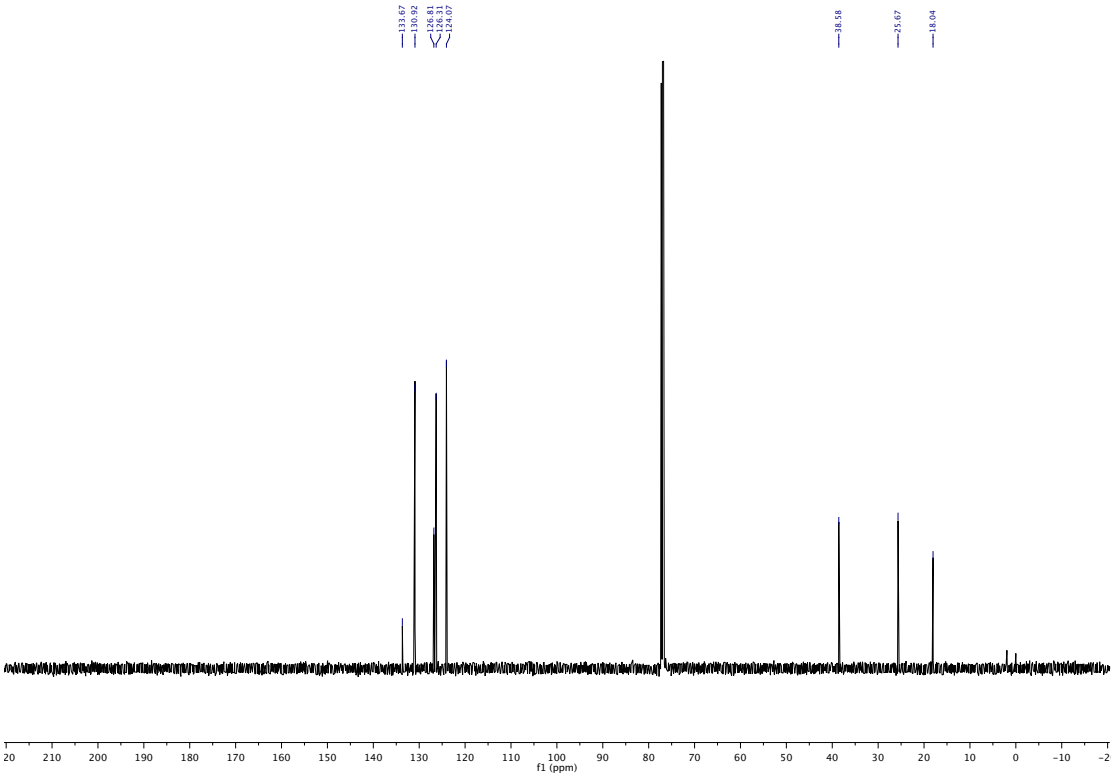


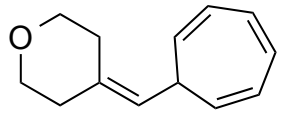




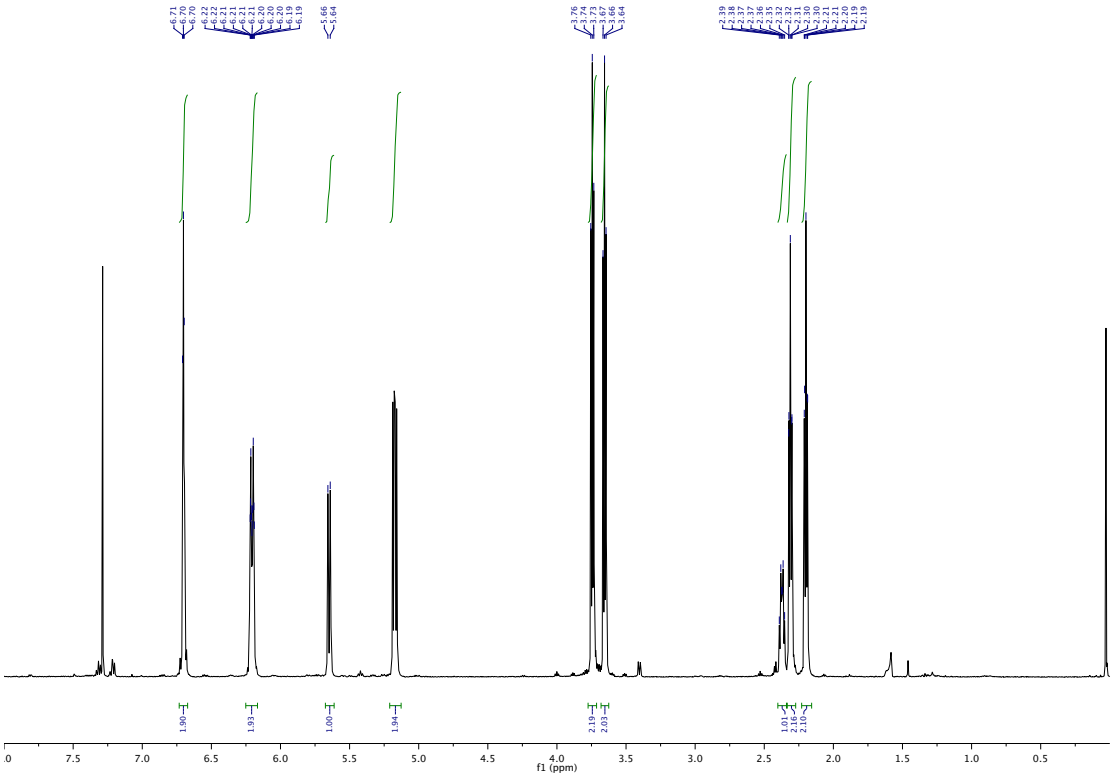
1g

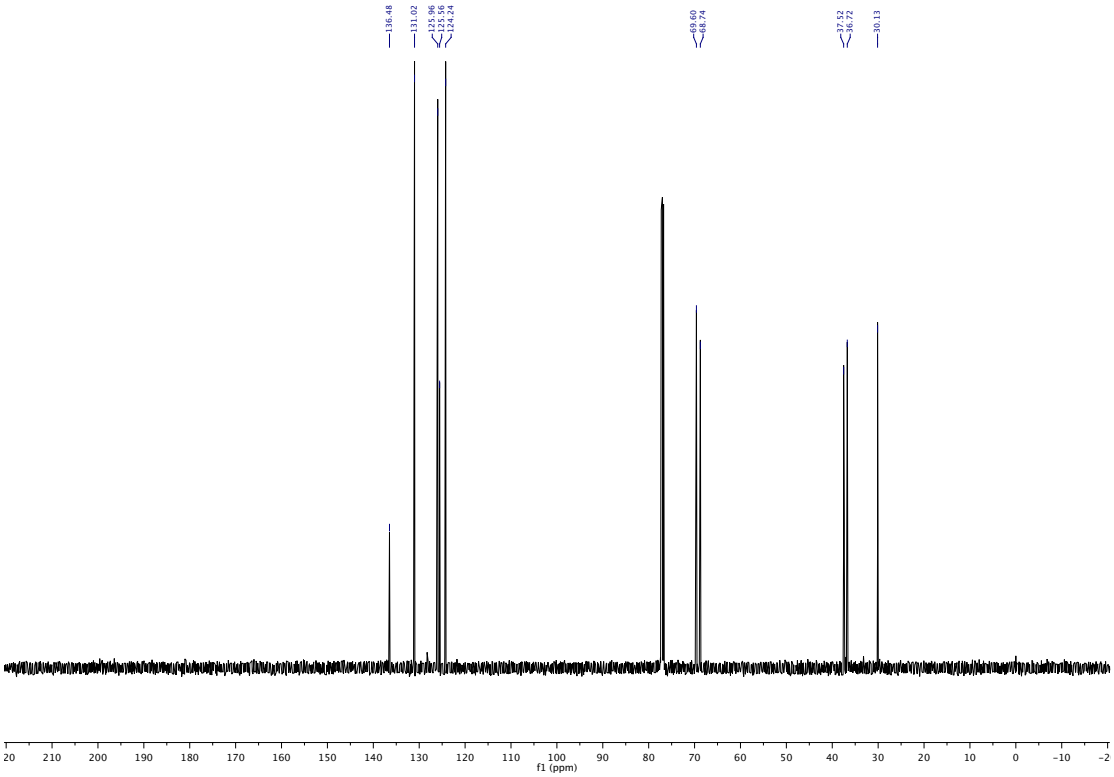

6.71
6.70
6.69
6.21
6.20
6.19
6.19
6.18
5.58
5.58
5.58
5.57
5.56
5.56
5.18
5.17
5.16
5.15
2.36
2.35
2.34
2.34
2.33
1.80
1.58
2.00
2.02
1.01
2.01
1.00
3.13
3.06
f1 (ppm)

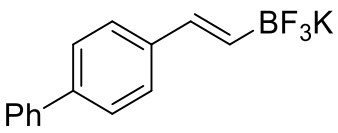

133.67
130.92
126.81
126.31
124.07
38.58
25.67
18.04
f1 (ppm)



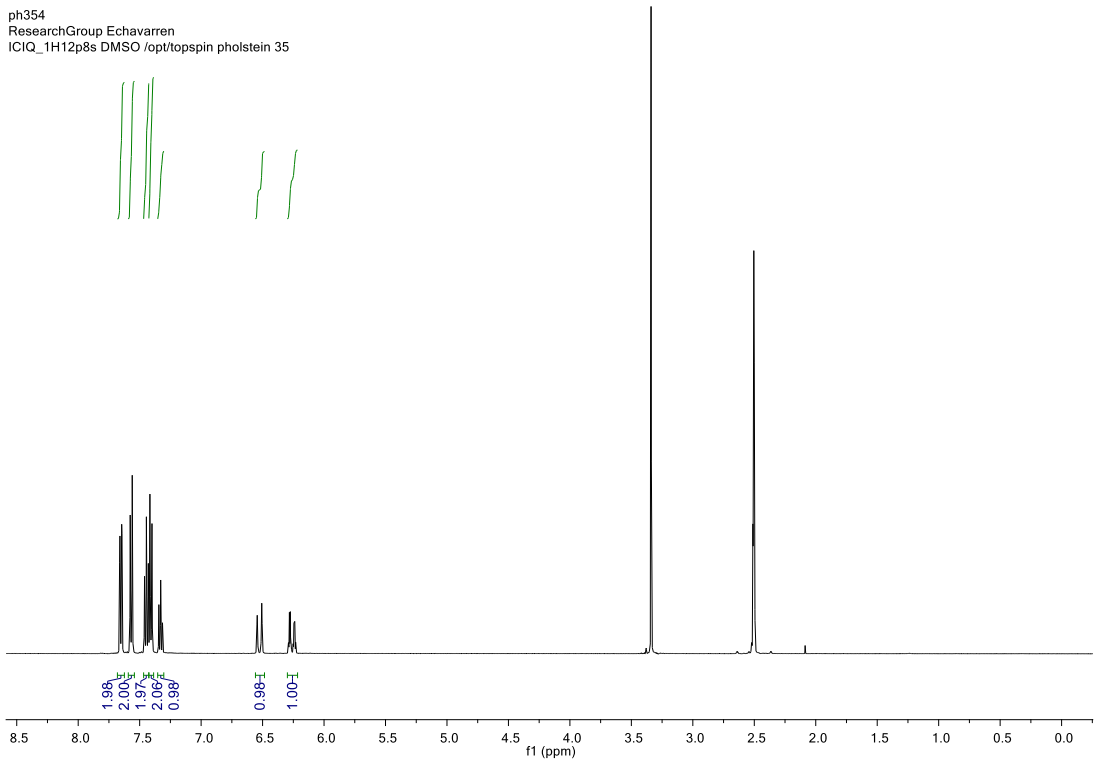
1h

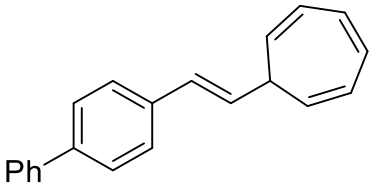

6.71
6.70
6.70
6.22
6.22
6.21
6.21
6.21
6.21
6.20
6.20
6.20
6.19
5.66
5.64
3.76
3.74
3.73
3.67
3.66
3.64
2.39
2.38
2.37
2.37
2.36
2.33
2.32
2.31
2.30
2.30
2.21
2.21
2.20
2.19
2.19
1.90
1.93
1.00
1.94
2.19
2.03
1.01
2.16
2.10
f1 (ppm)


136.48
131.02
125.96
125.56
124.24
69.60
68.74
37.52
36.72
30.13
f1 (ppm)

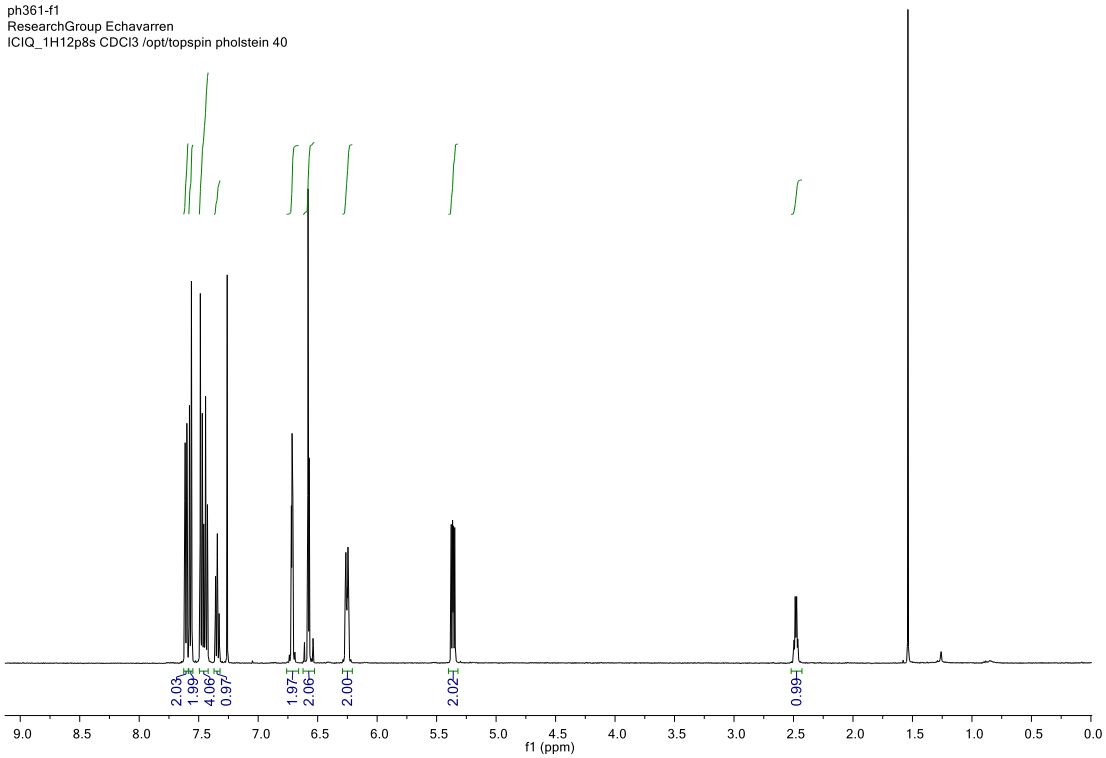

BF3K
Ph

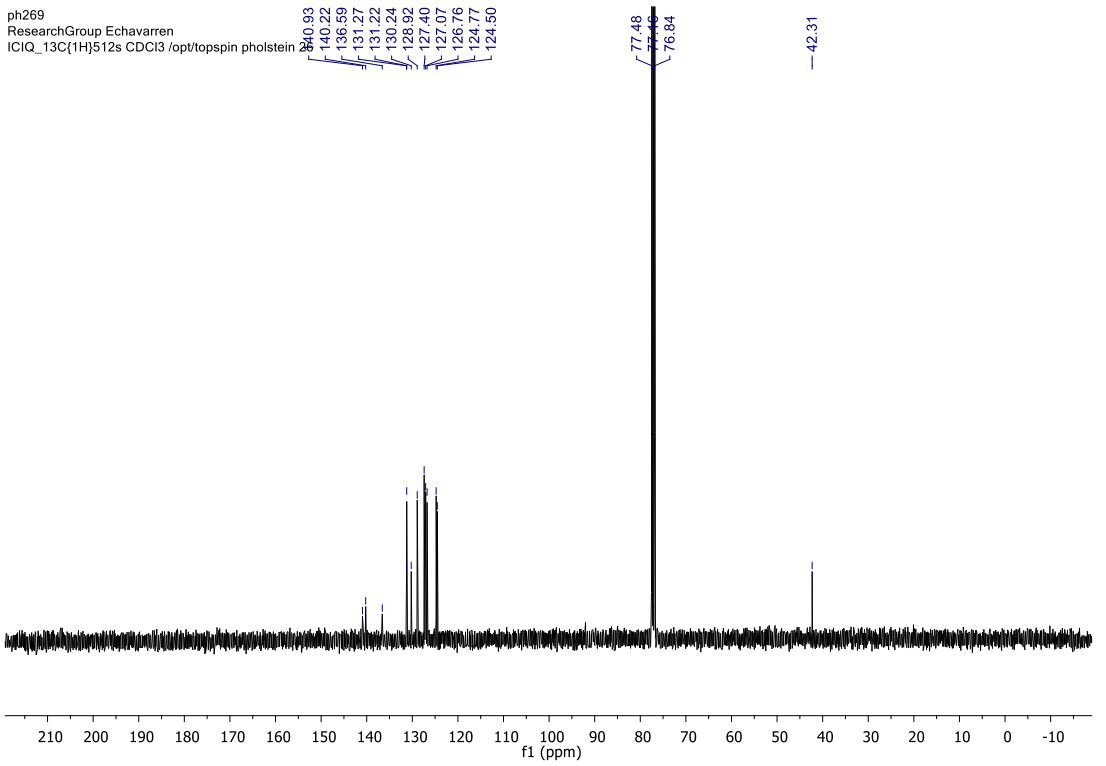
1i

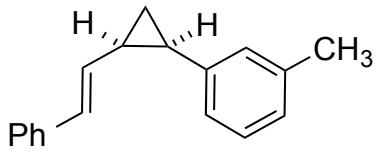

ph354
ResearchGroup Echavarren
ICIQ_1H12p8s DMSO /opt/topspin pholstein 35
1.98
2.00
1.97
2.06
0.98
0.98
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Ph

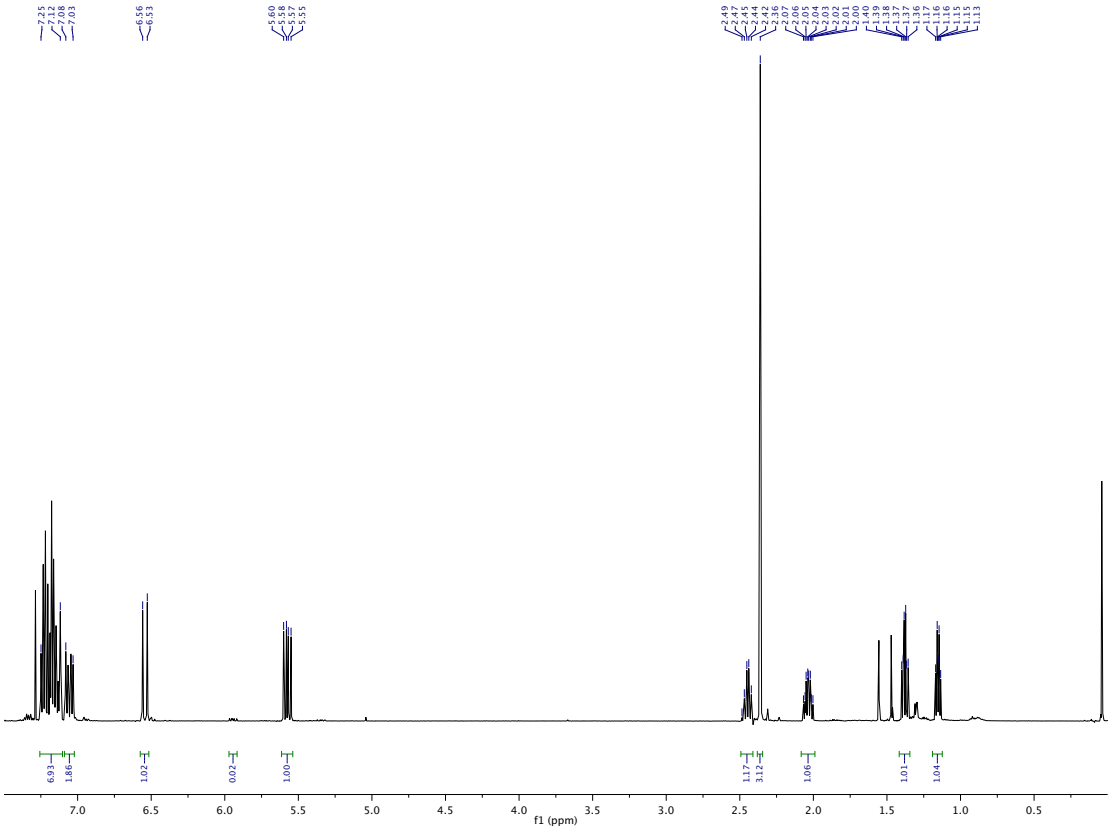
1i

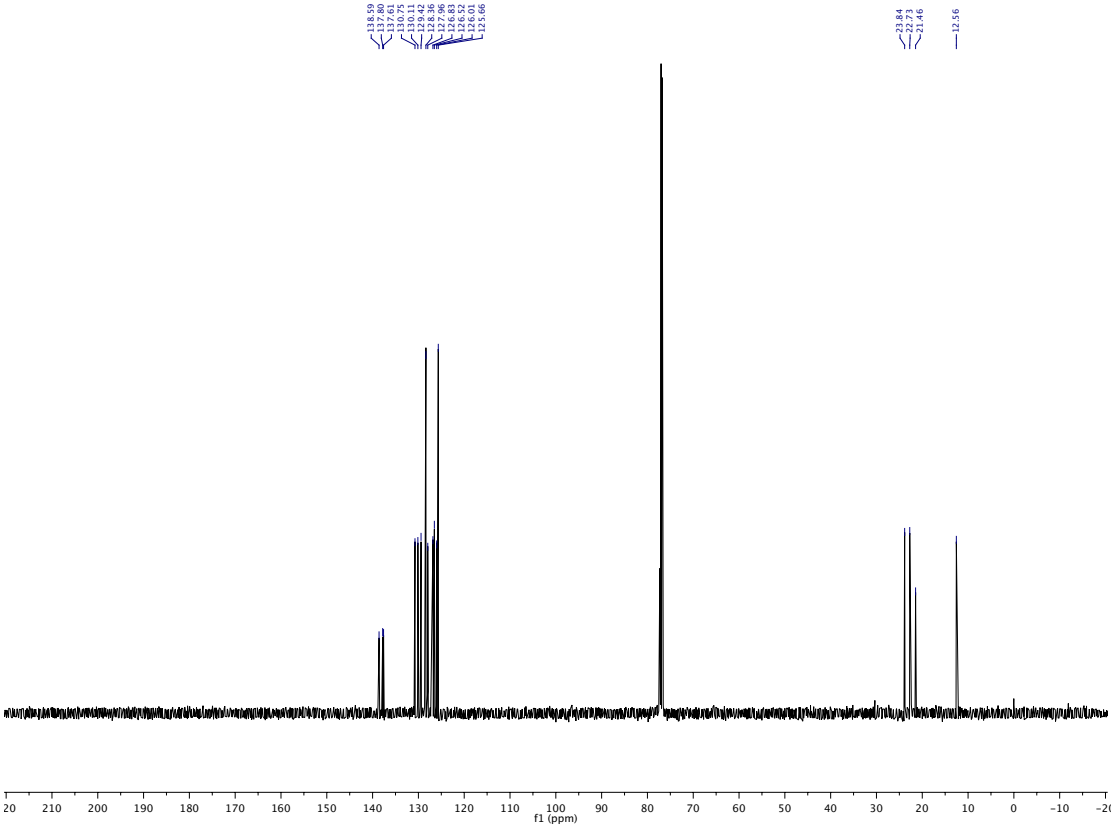

ph361-f1
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 40
2.03
1.99
4.06
0.97
1.97
2.06
2.00
2.02
0.99
f1 (ppm)

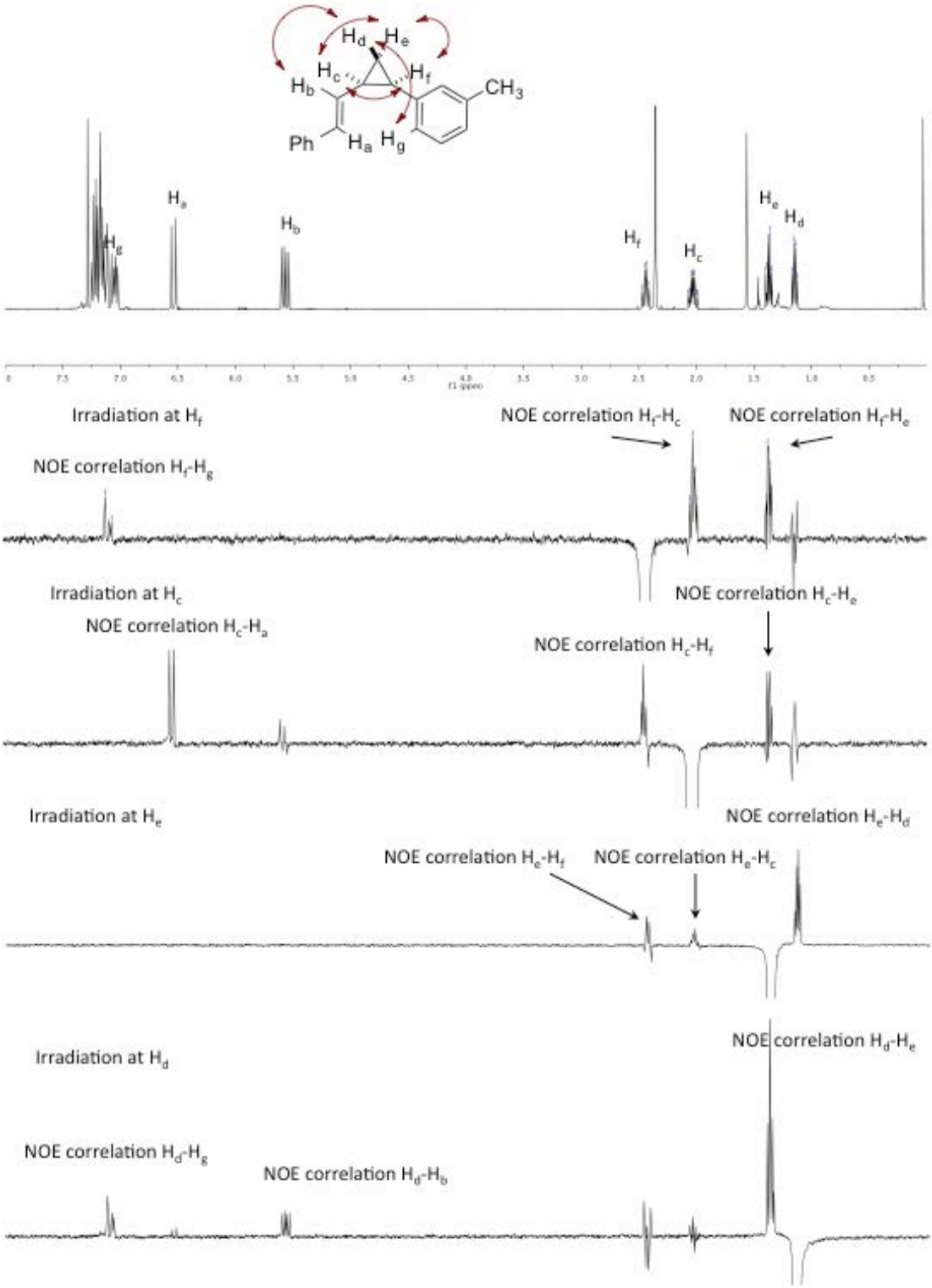

ph269
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 26
140.93
140.22
136.59
131.27
131.22
130.24
128.92
127.40
127.07
126.76
124.77
124.50
77.48
77.16
76.84
42.31
f1 (ppm)

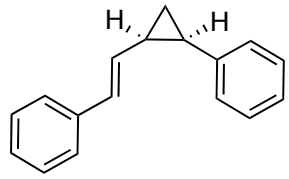


3a



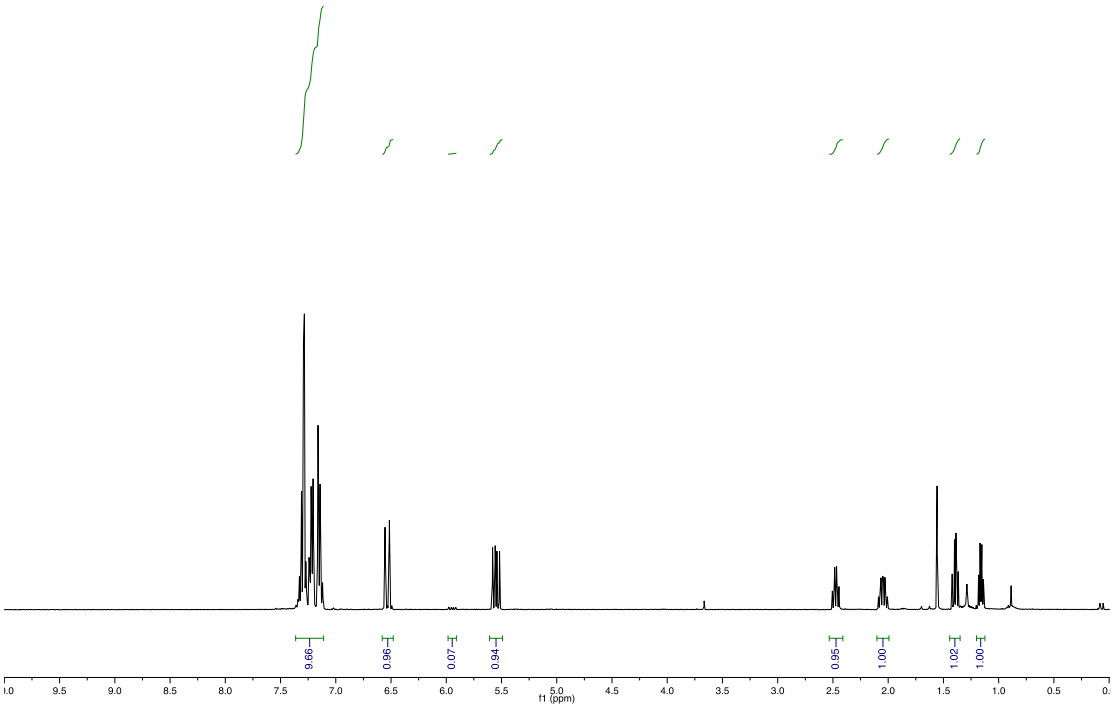



Hd
He
Hc
Hf
Hb
CH3
Ph
Ha
Hg
Ha
Hb
Hg
Hf
Hc
He
Hd
Irradiation at Hf
NOE correlation Hf-Hc
NOE correlation Hf-He
NOE correlation Hf-Hg
Irradiation at Hc
NOE correlation Hc-He
NOE correlation Hc-Ha
NOE correlation Hc-Hf
Irradiation at He
NOE correlation He-Hd
NOE correlation He-Hf
NOE correlation He-Hc
Irradiation at Hd
NOE correlation Hd-He
NOE correlation Hd-Hg
NOE correlation Hd-Hb

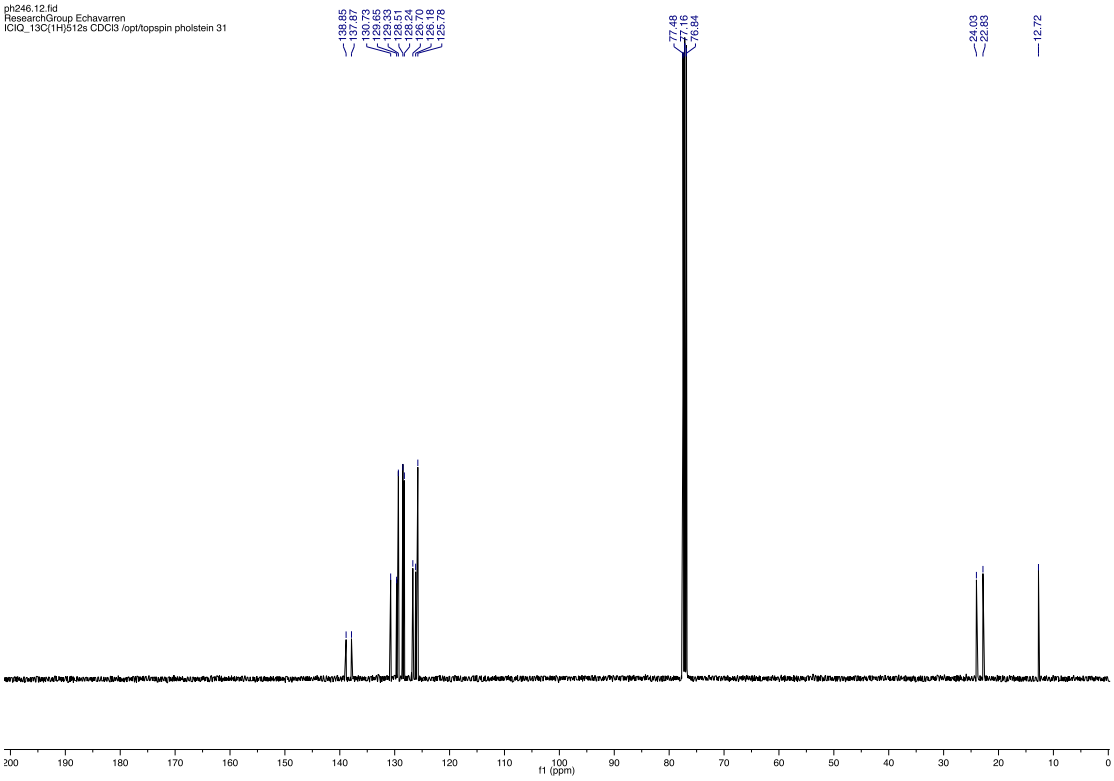


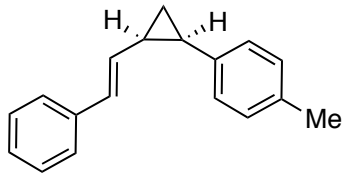
3b

ph246.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 31

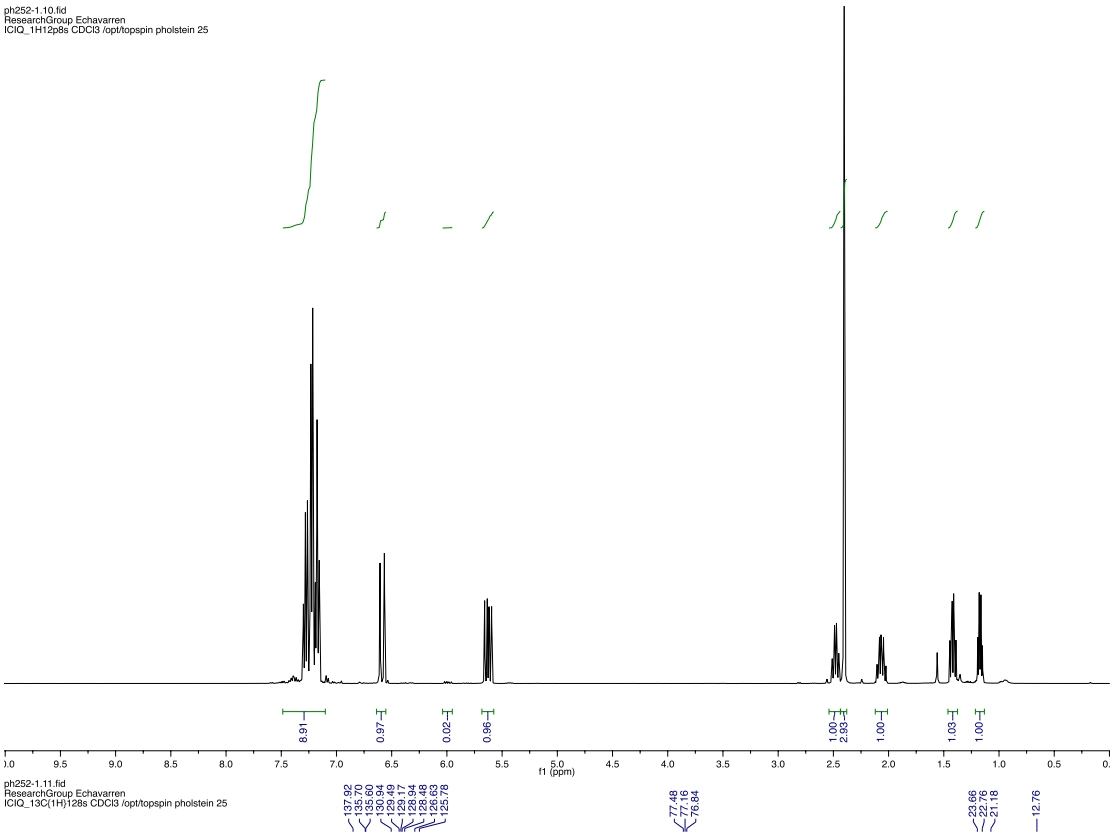


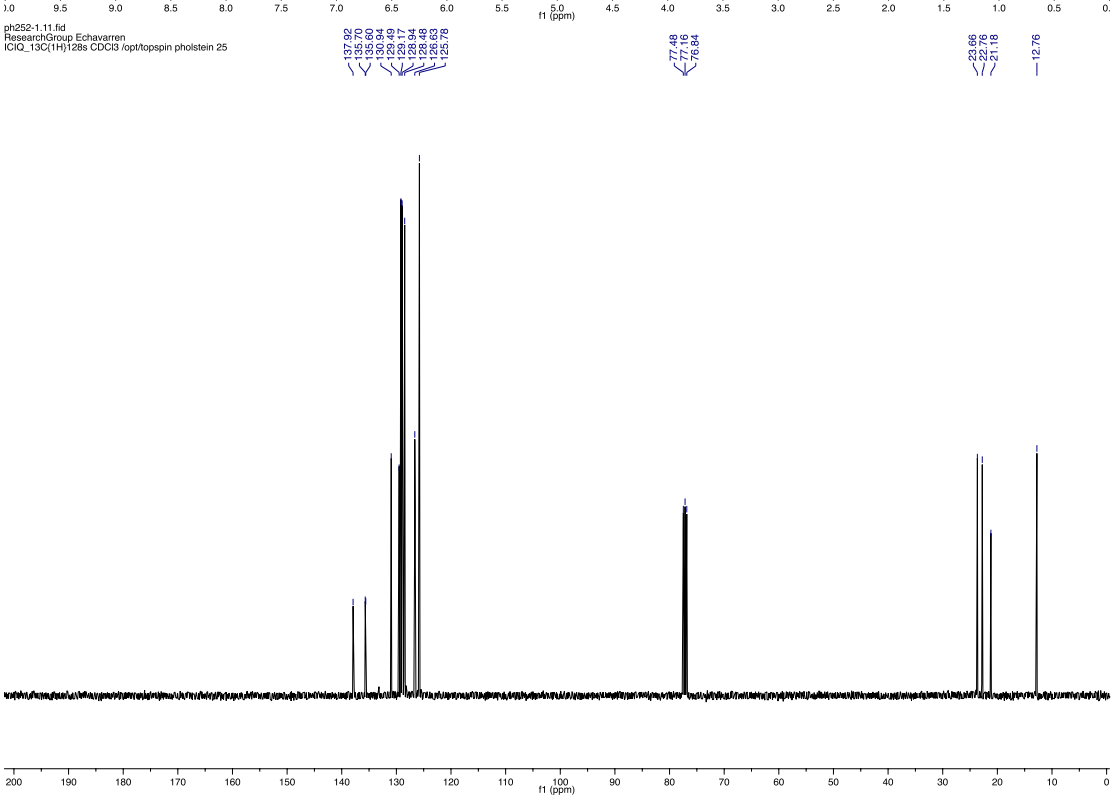
ph246.12.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 31

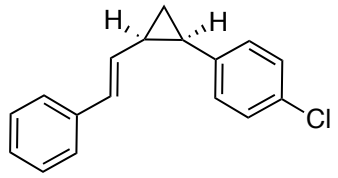



H
H
Me

3c

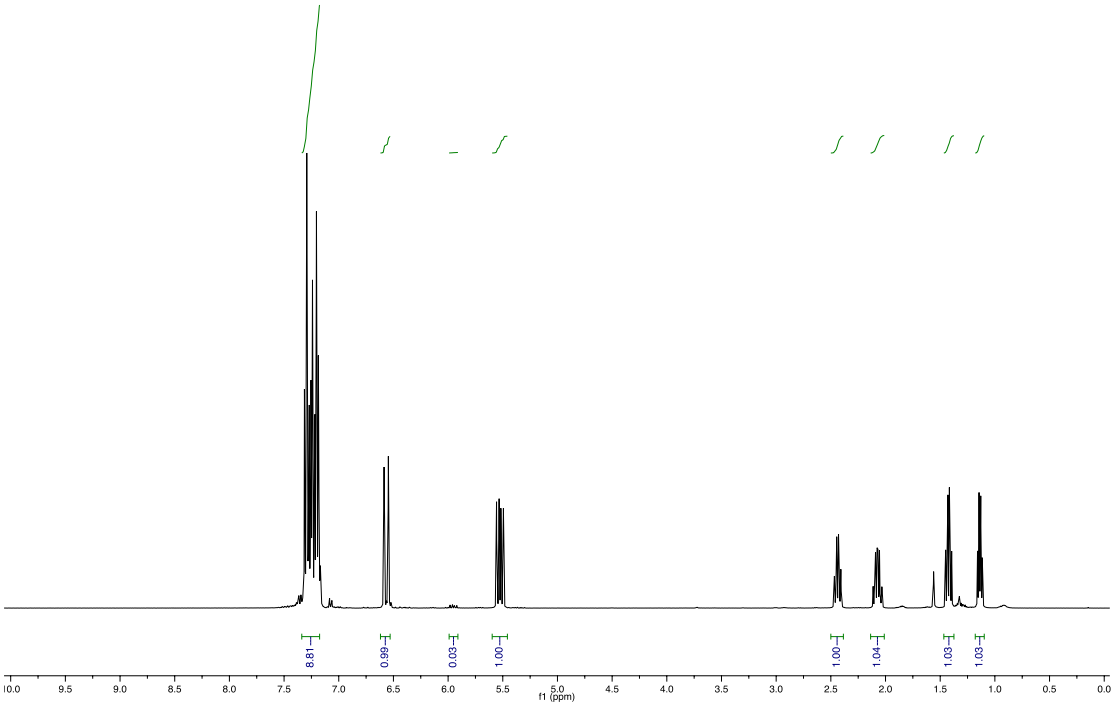

ph252-1.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 25
8.91
0.97
0.02
0.96
1.00
2.93
1.00
1.03
1.00
f1 (ppm)


ph252-1.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin pholstein 25
137.92
135.70
135.60
130.44
129.49
129.17
128.94
128.48
126.63
125.78
77.48
77.16
76.84
23.66
22.78
21.18
12.76
f1 (ppm)

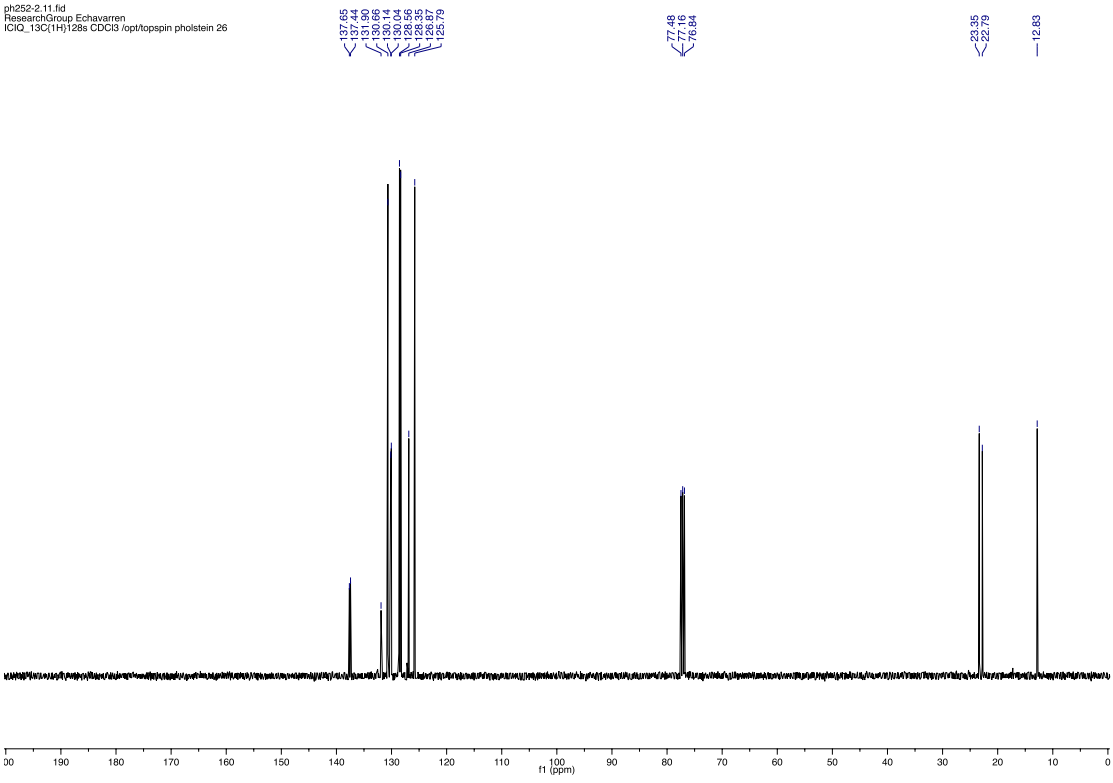


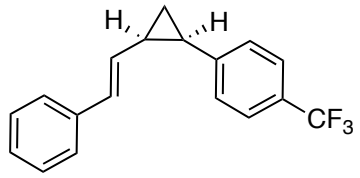
3d

ph252-2.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 26



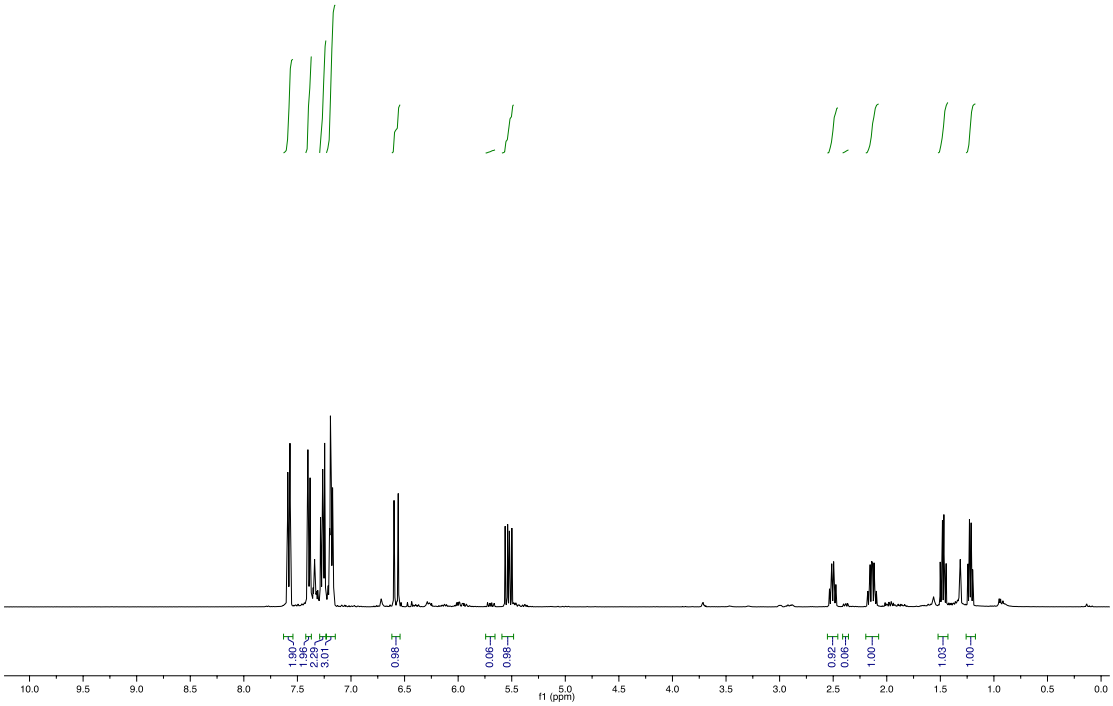
ph252-2.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin pholstein 26



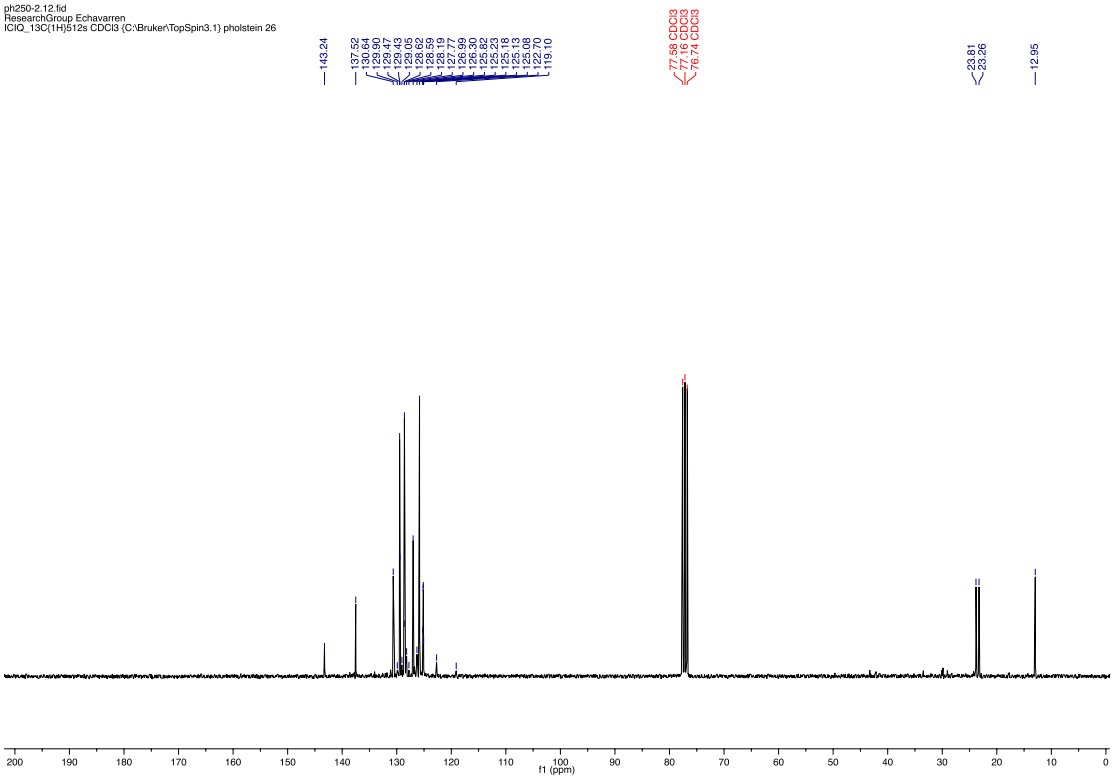


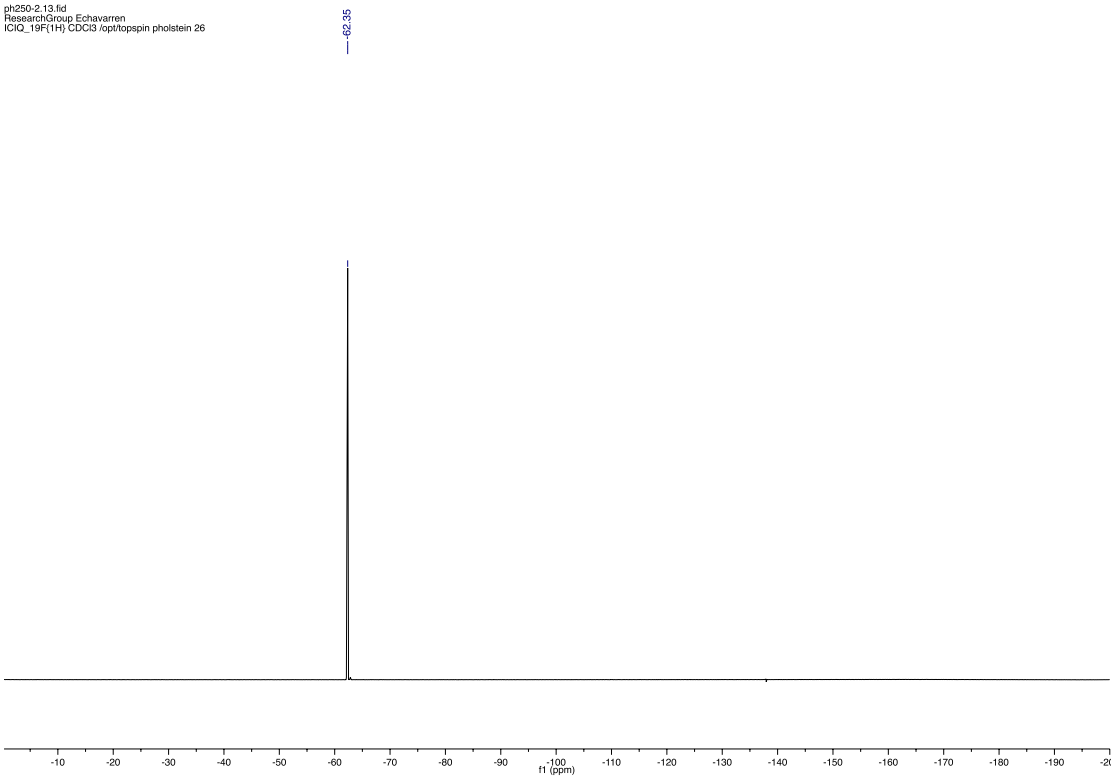
3e

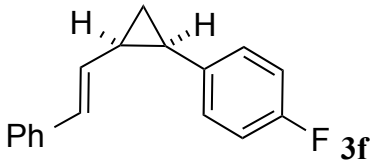
ph250-2.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 26



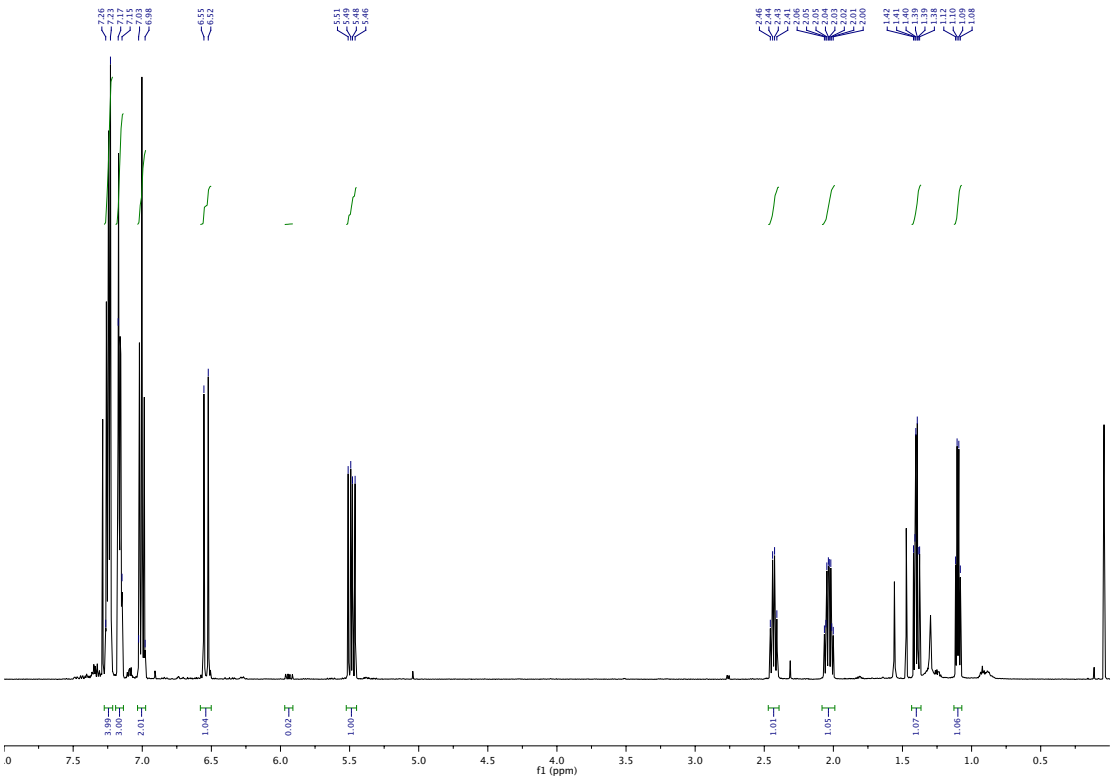
ph250-2.12.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1} pholstein 26

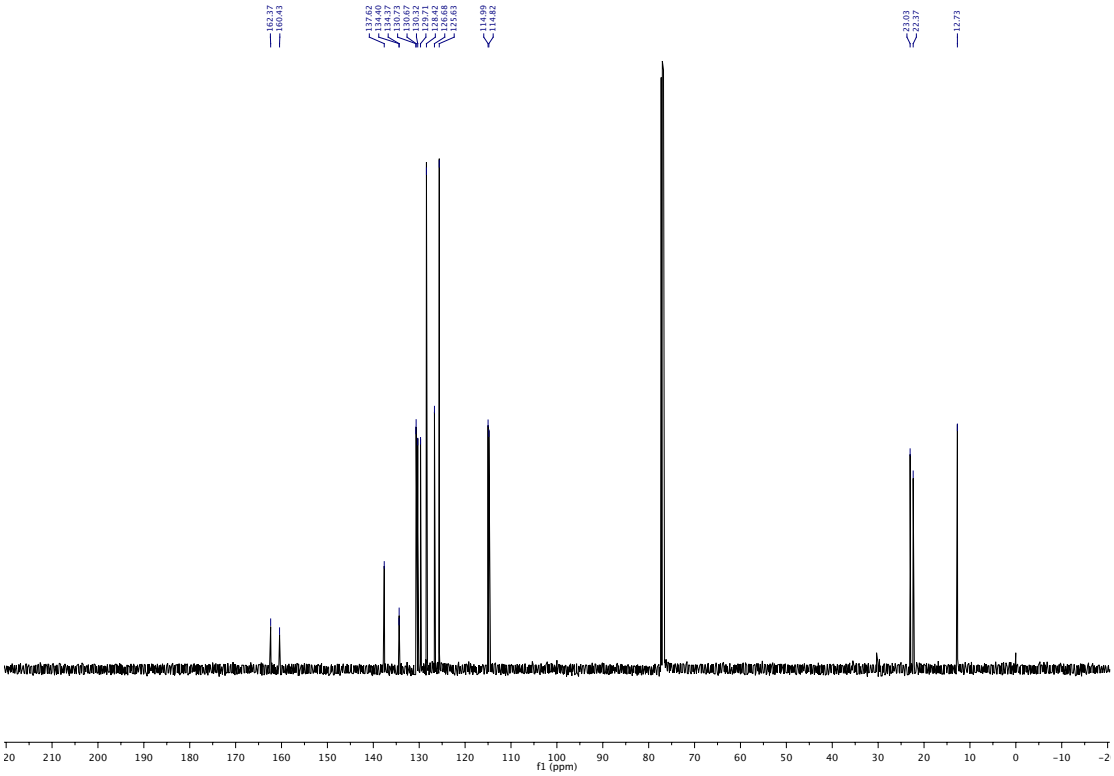


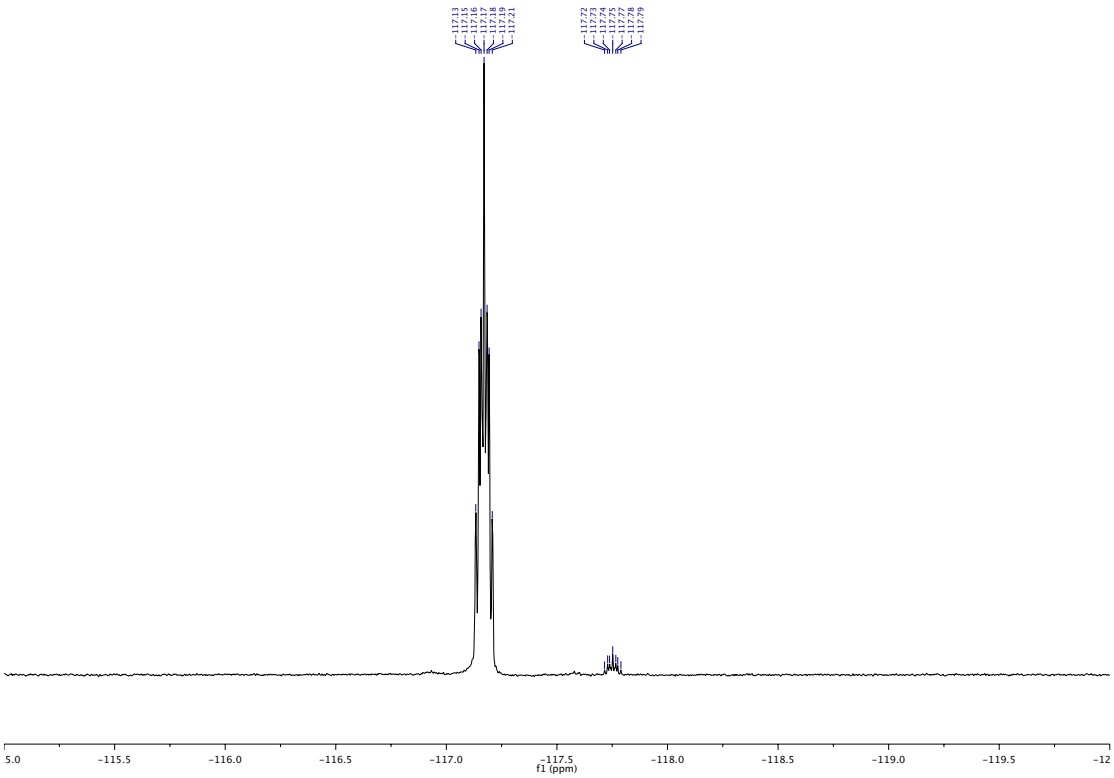

ph250-2.13.fid
ResearchGroup Echavarren
ICIQ_19F{1H} CDCl3 /opt/topspin pholstein 26
-62.35
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

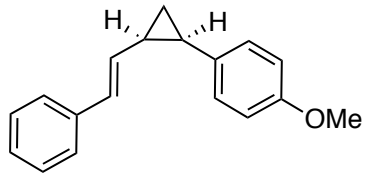

H
H
Ph
F

3f

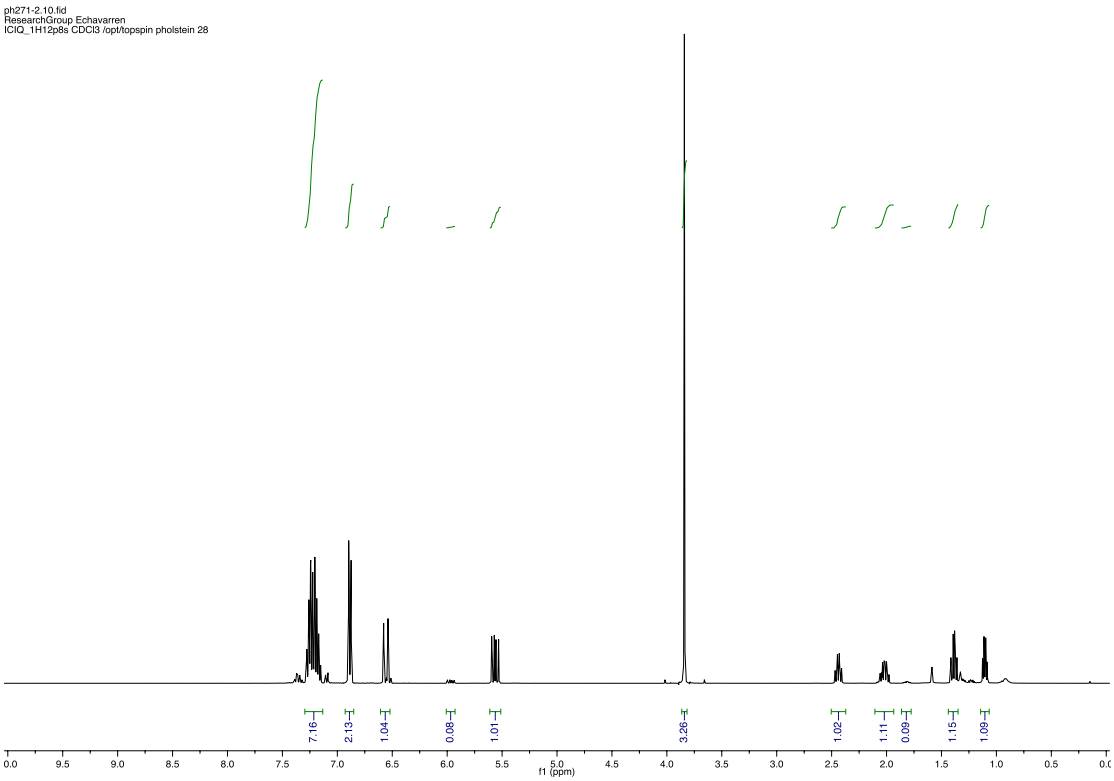

7.26
7.23
7.17
7.15
7.03
6.98
6.55
6.52
5.51
5.49
5.48
5.46
2.46
2.44
2.43
2.41
2.06
2.05
2.04
2.03
2.02
2.01
2.00
1.42
1.41
1.40
1.39
1.39
1.38
1.12
1.10
1.09
1.08
3.99
3.00
2.01
1.04
0.02
1.00
1.01
1.05
1.07
1.06
f1 (ppm)

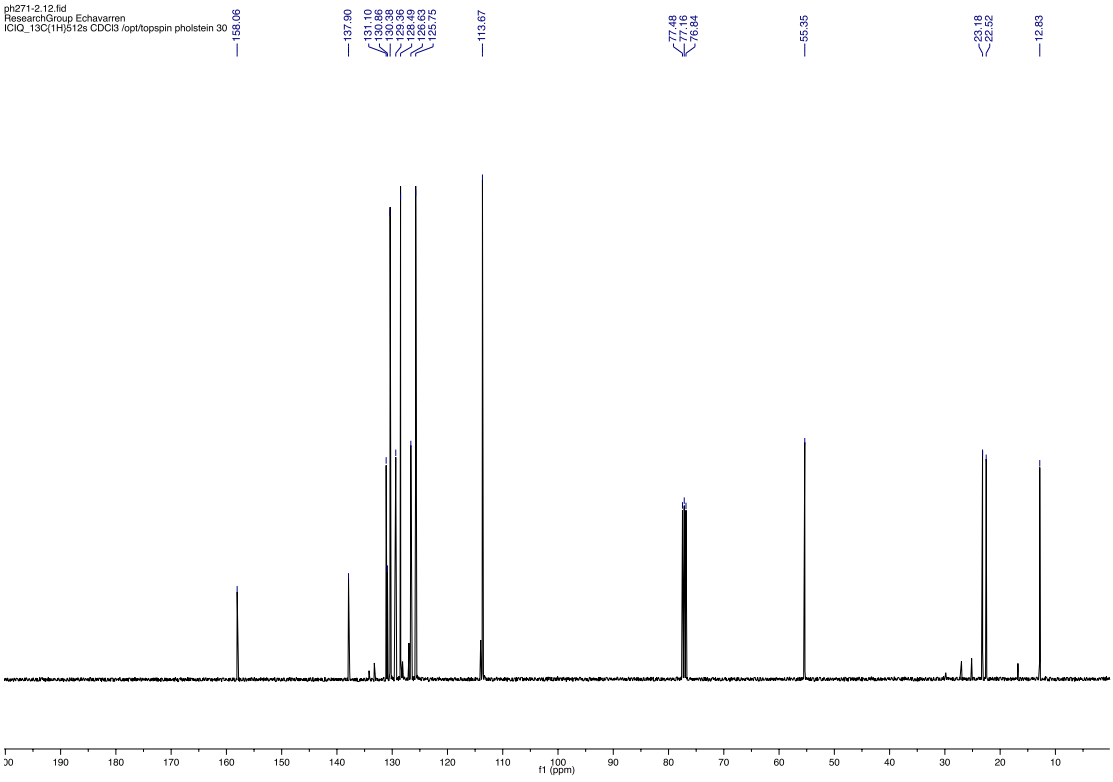

162.37
160.43
137.62
134.60
134.37
130.73
130.67
130.32
129.71
128.42
126.68
125.63
114.99
114.82
23.03
22.37
12.73
f1 (ppm)

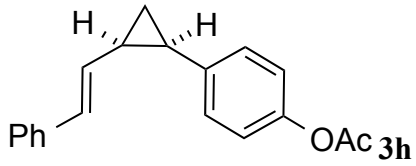

-117.13
-117.15
-117.16
-117.17
-117.18
-117.19
-117.21
-117.72
-117.73
-117.74
-117.75
-117.77
-117.78
-117.79
5.0
-115.5
-116.0
-116.5
-117.0
-117.5
f1 (ppm)
-118.0
-118.5
-119.0
-119.5
-12


H
H
OMe

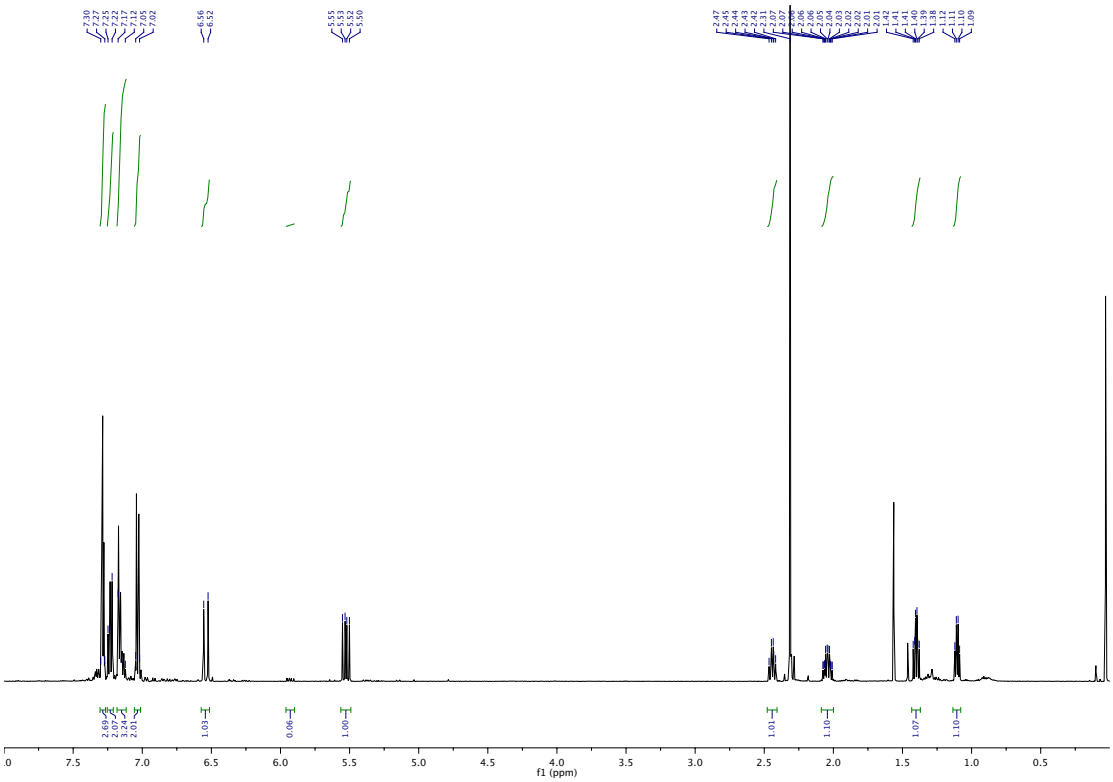
3g

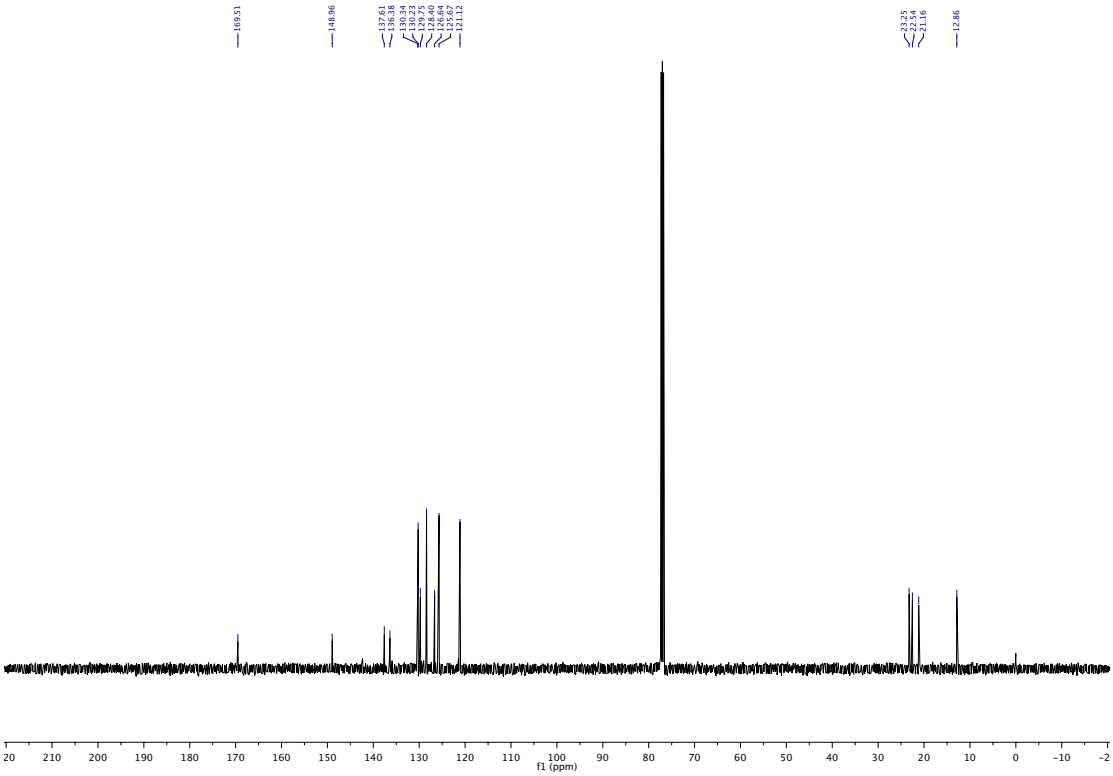

ph271-2.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 28
7.16
2.13
1.04
0.08
1.01
3.26
1.02
1.11
0.09
1.15
1.09
f1 (ppm)

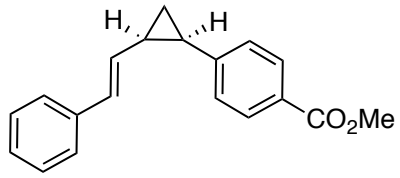

ph271-2.12.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 30
158.06
137.90
131.10
130.88
130.38
129.36
128.49
126.63
125.75
113.67
77.48
77.16
76.84
55.35
23.18
22.52
12.83
f1 (ppm)



3h

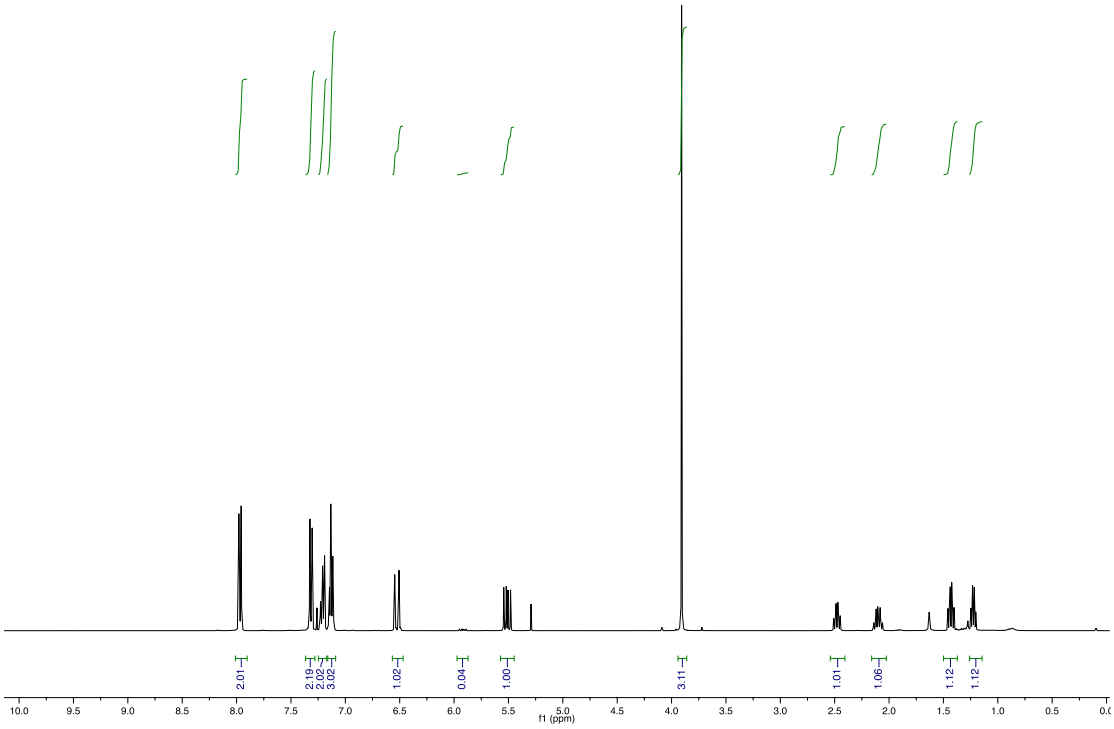




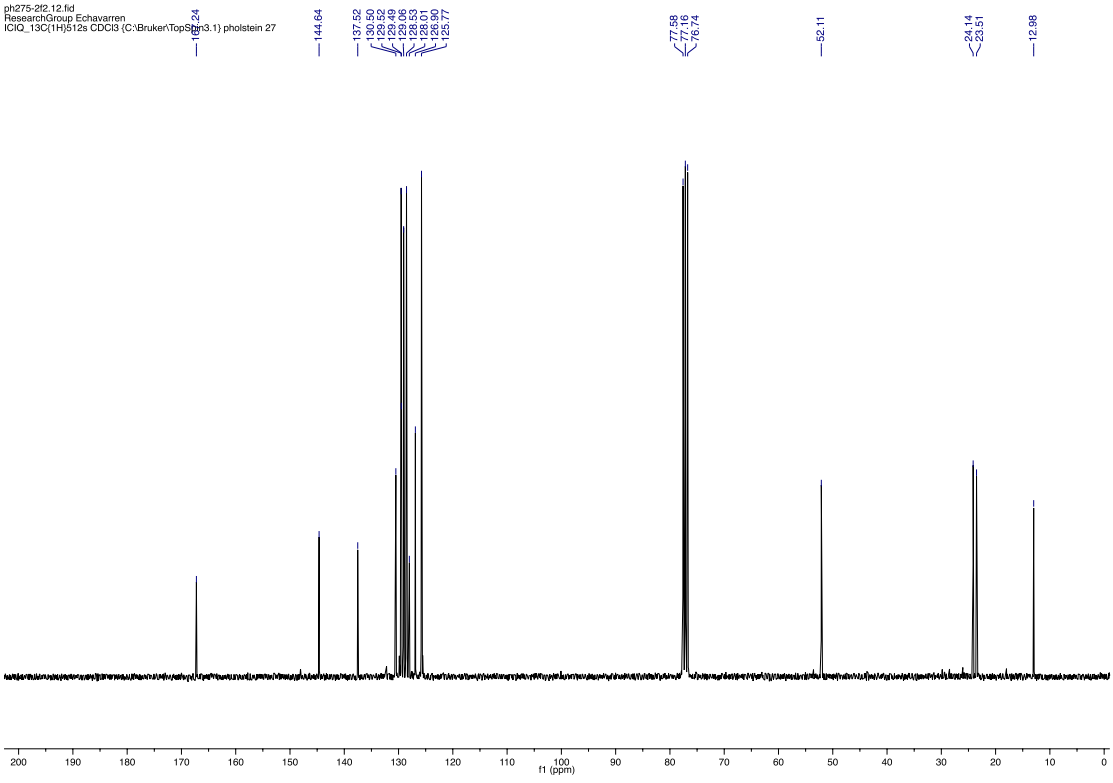


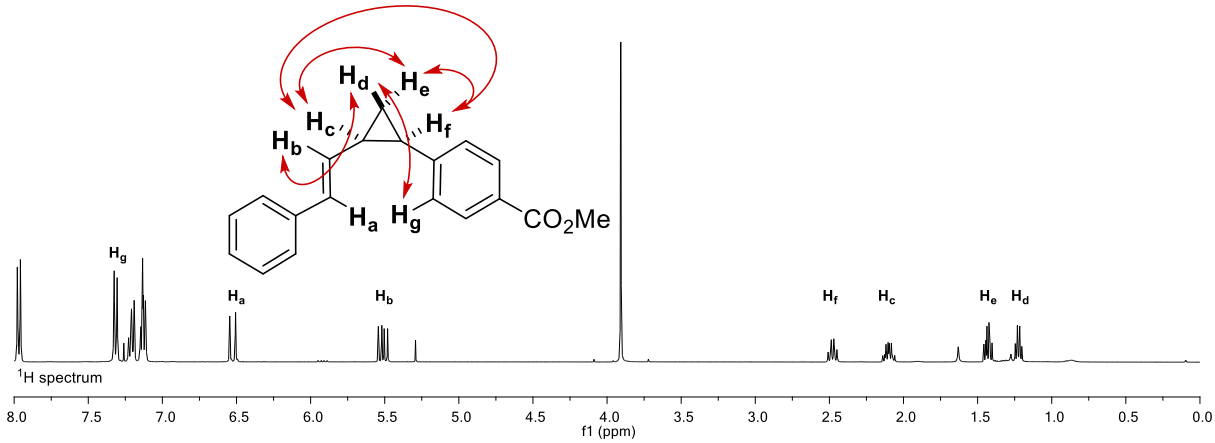
3i

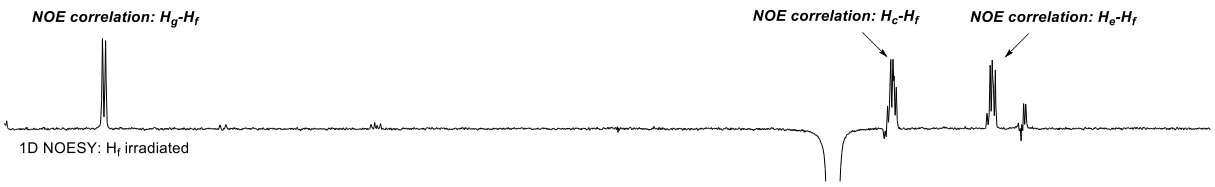
ph275-2f2.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 27

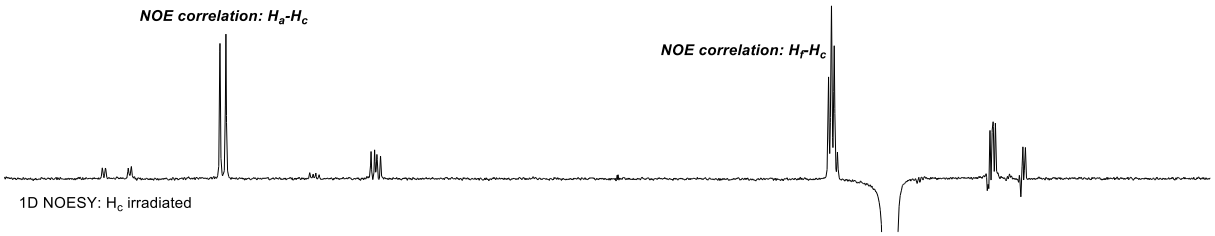


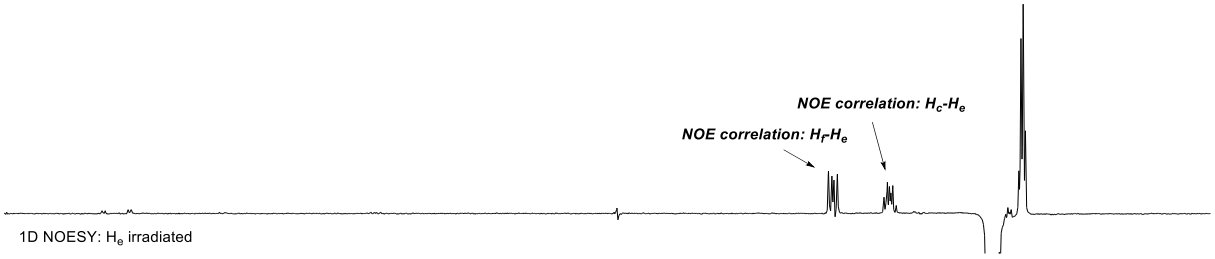
ph275-2f2.12.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1} pholstein 27



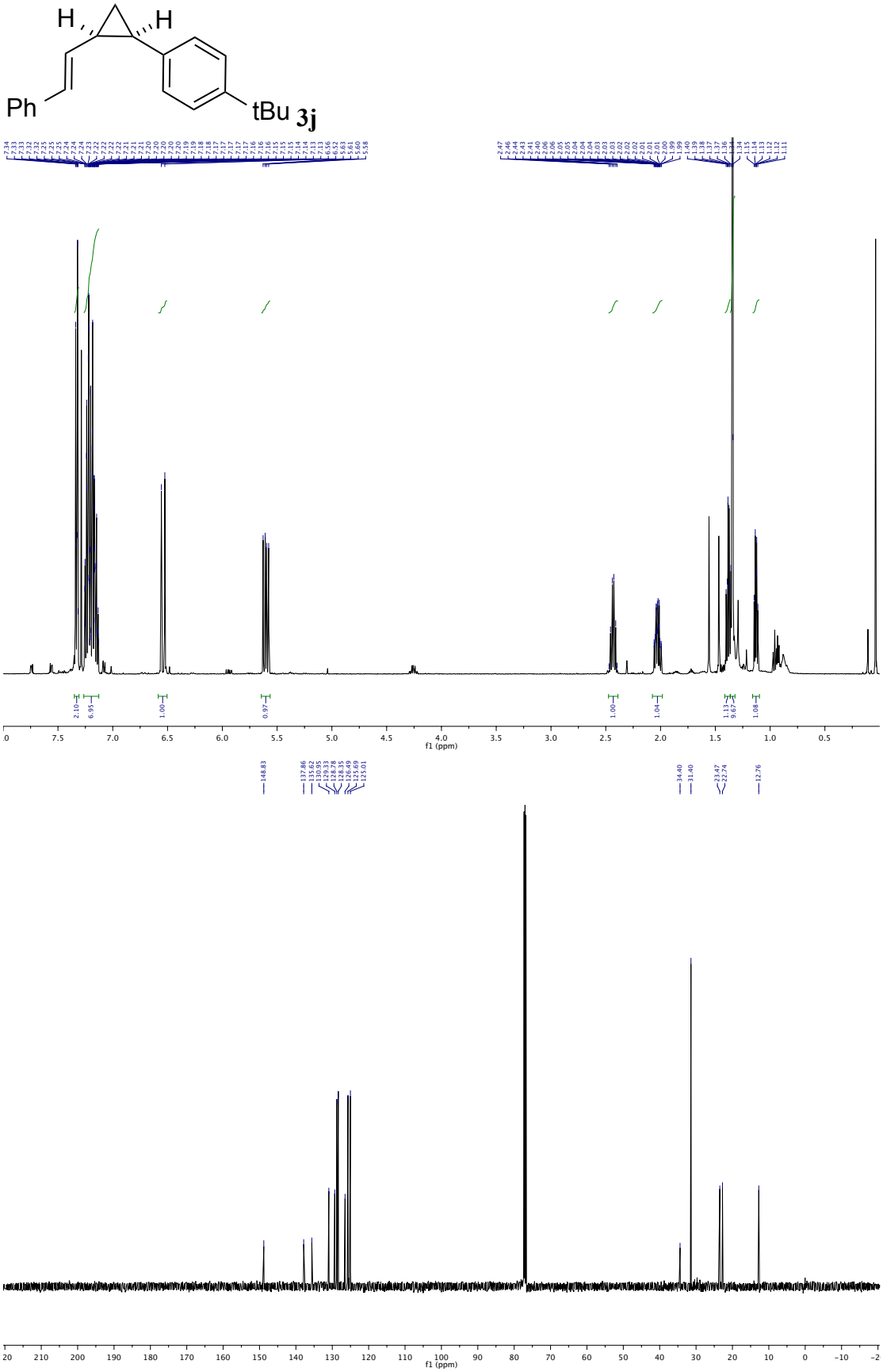

Hd
He
Hc
Hf
Hb
Ha
Hg
CO2Me
Hg
Ha
Hb
Hf
Hc
He
Hd
1H spectrum
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

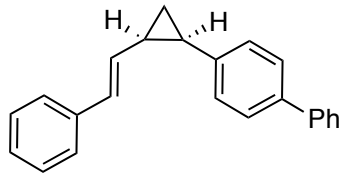

NOE correlation: Hg-Hf
NOE correlation: Hc-Hf
NOE correlation: He-Hf
1D NOESY: Hf irradiated


NOE correlation: Ha-Hc
NOE correlation: Hf-Hc
1D NOESY: Hc irradiated


NOE correlation: Hc-He
NOE correlation: Hf-He
1D NOESY: He irradiated

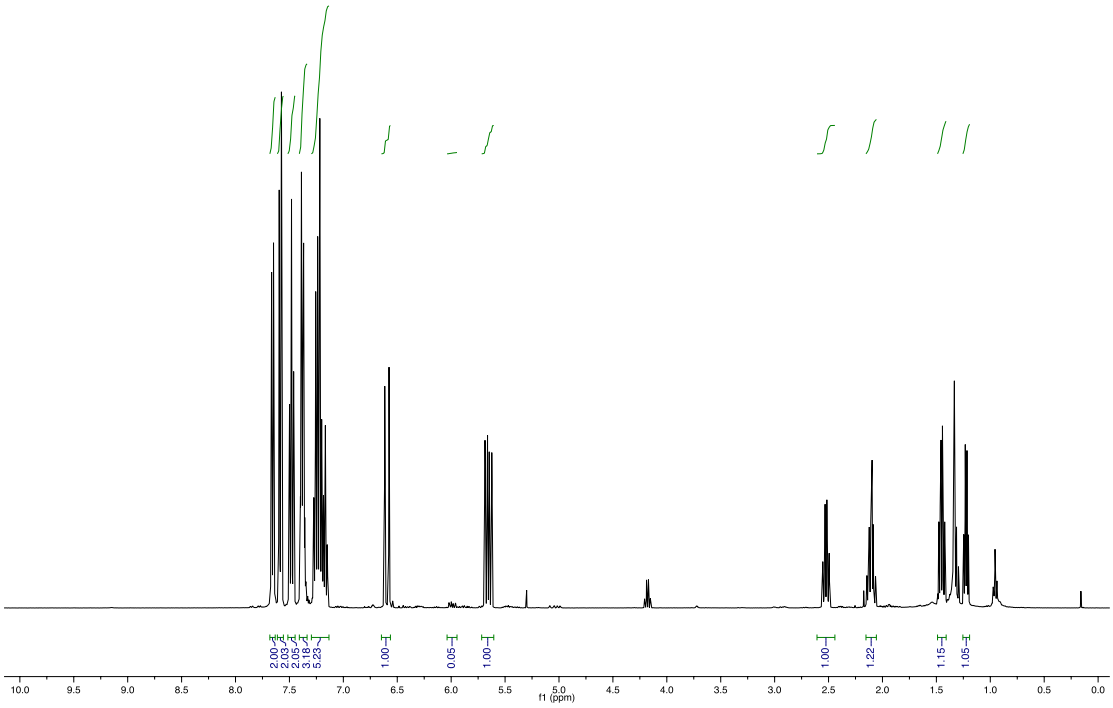

NOE correlation: Hg-Hd
NOE correlation: Hb-Hd
1D NOESY: Hd irradiated


H
H
Ph
tBu
3j
f1 (ppm)
f1 (ppm)

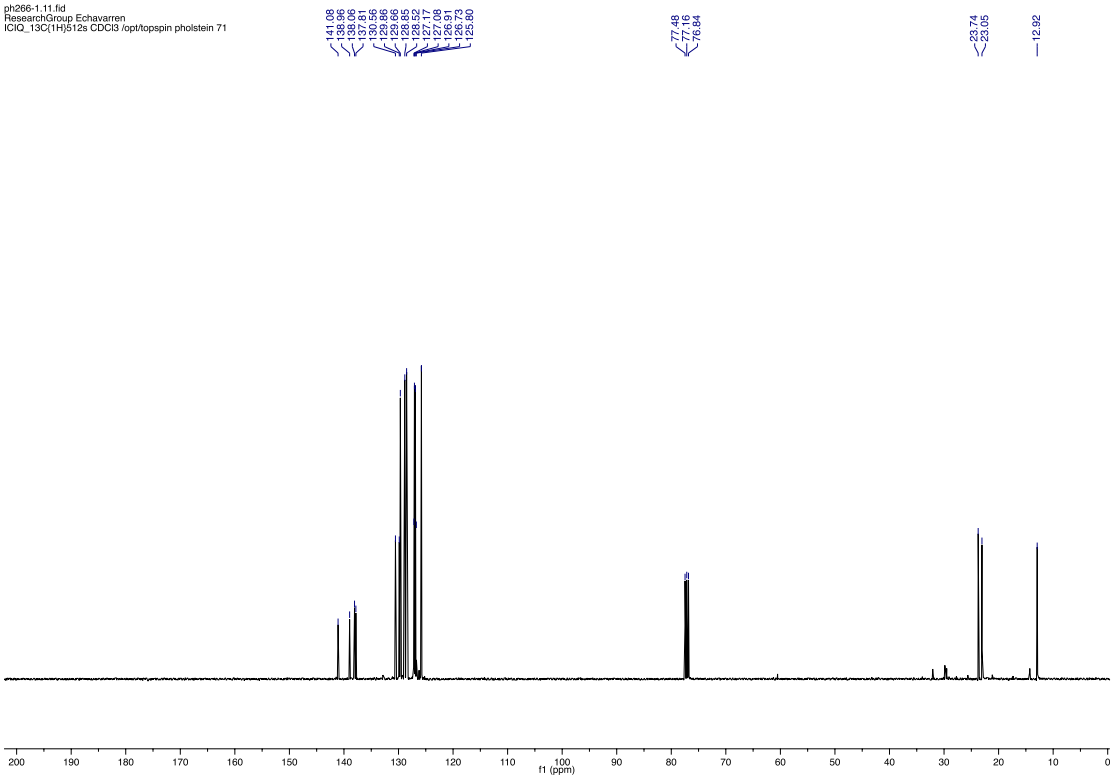


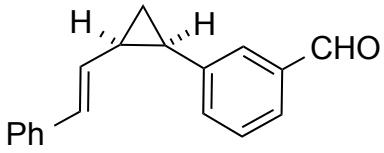
3k

ph266-1.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 71

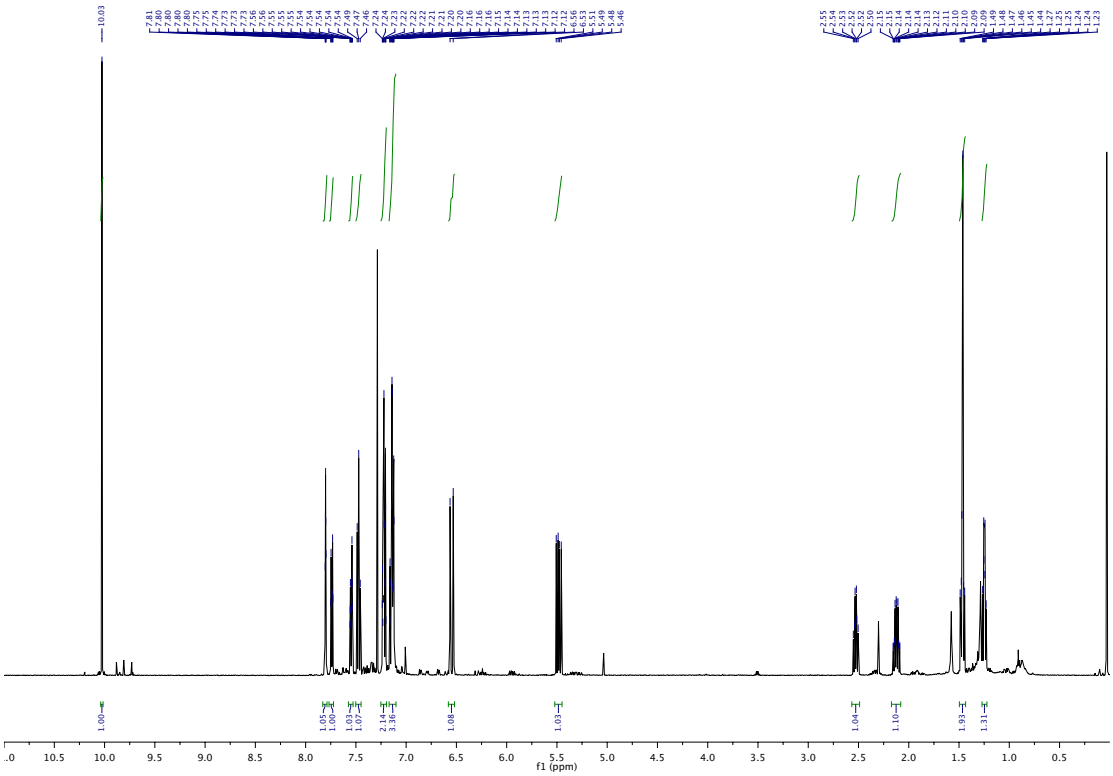


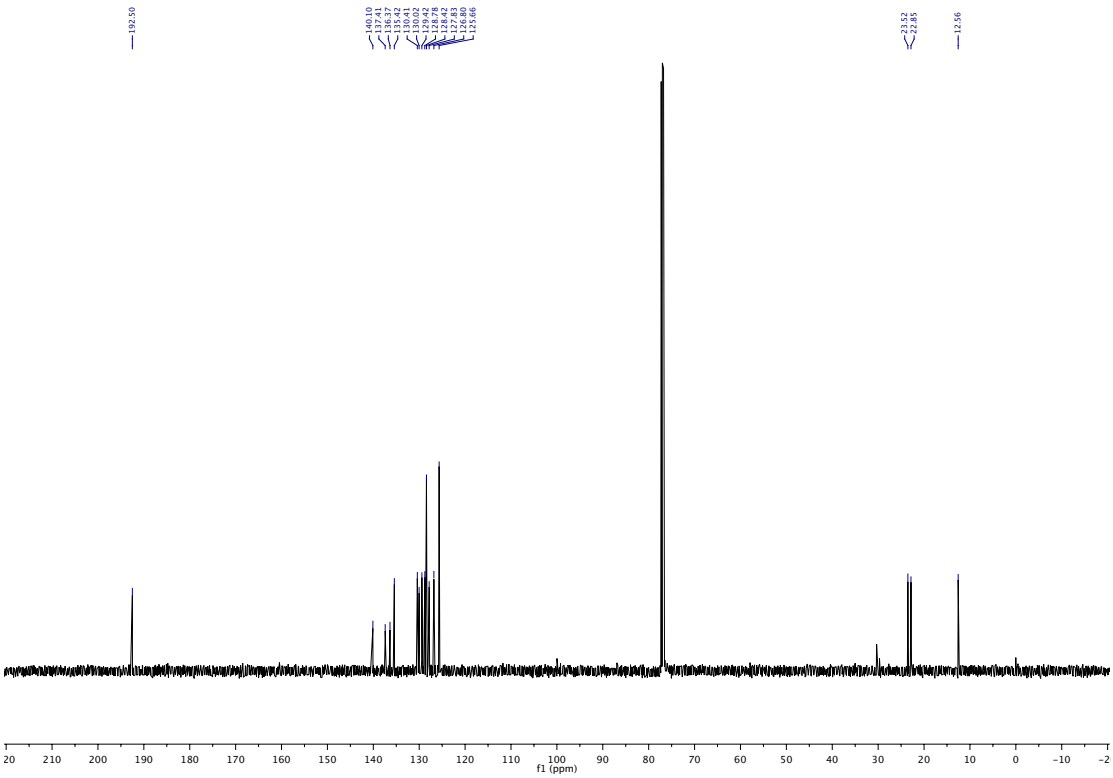
ph266-1.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 71

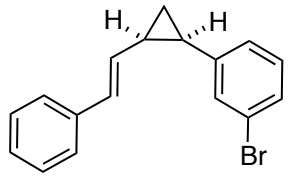




3l

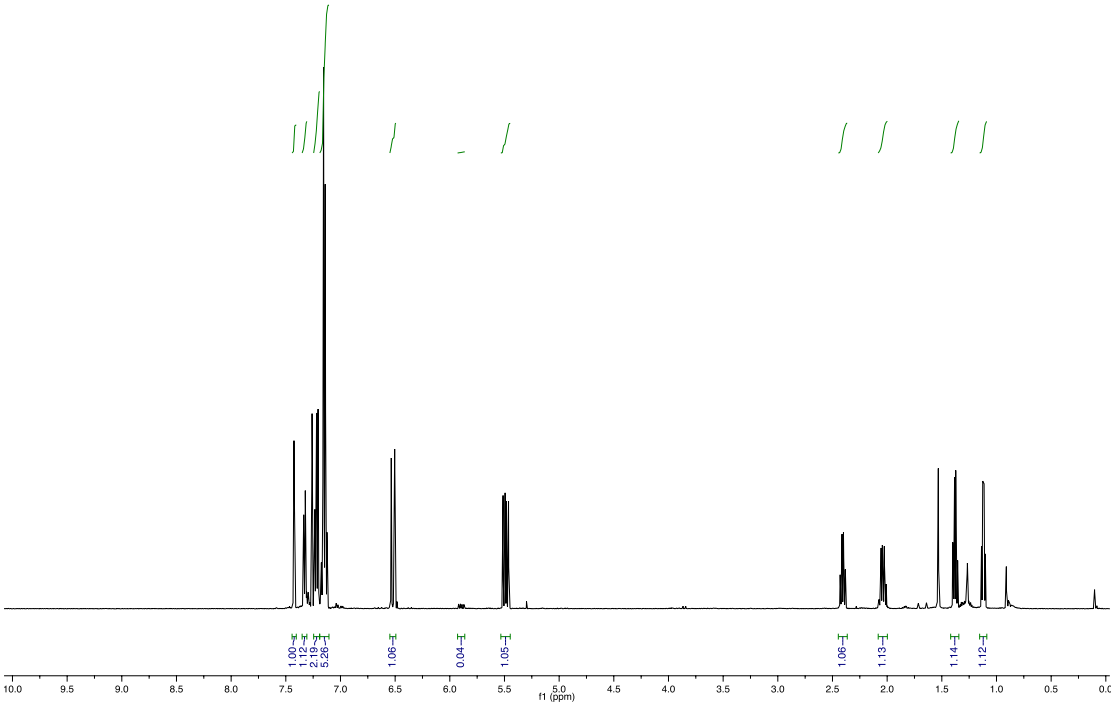




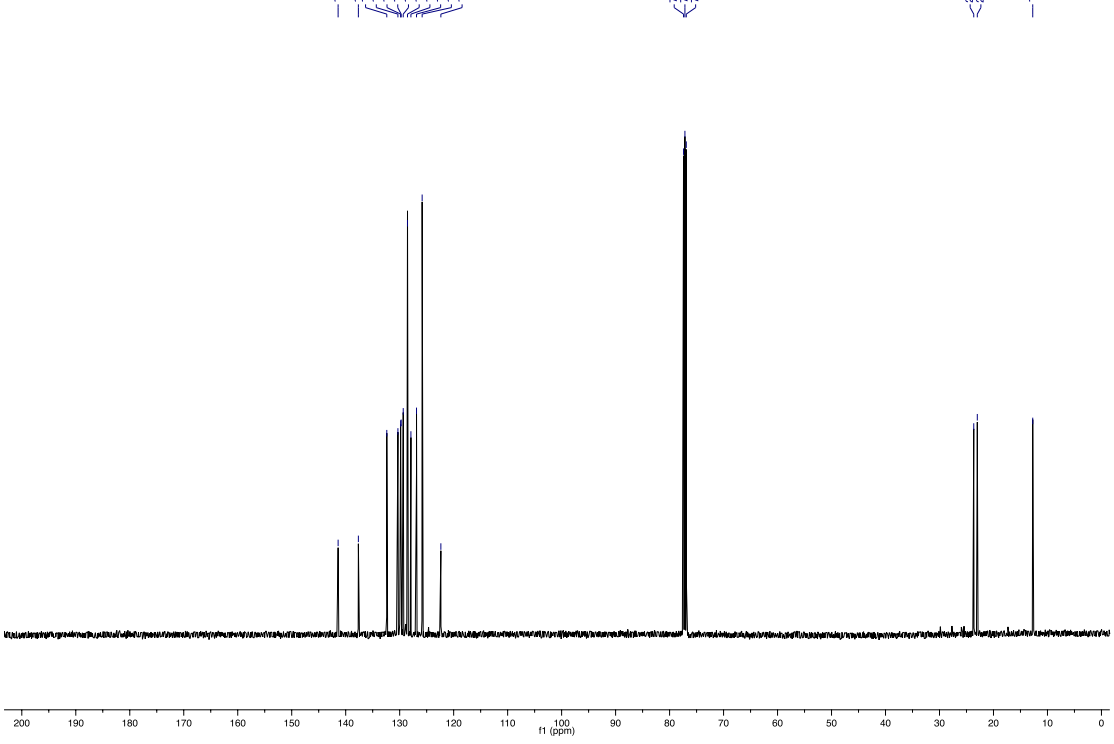


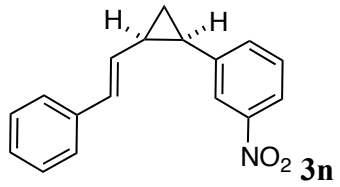
3m

ph250-1.9.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 25



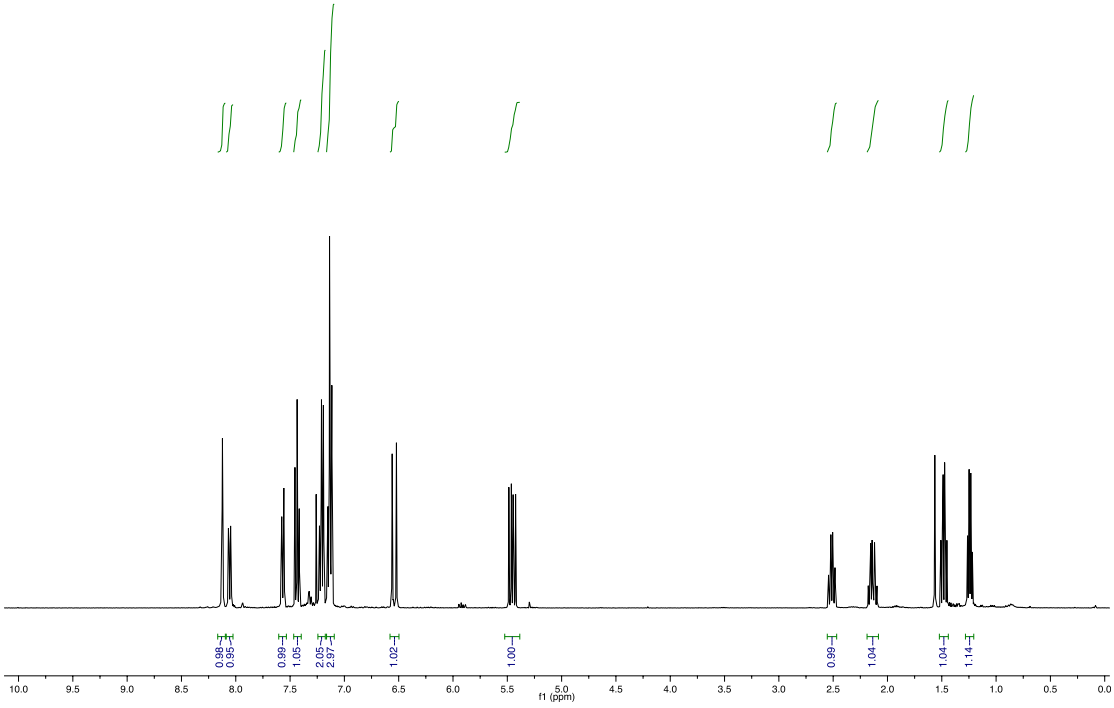
ph250-1.2.fid
13C{1H} Experiment



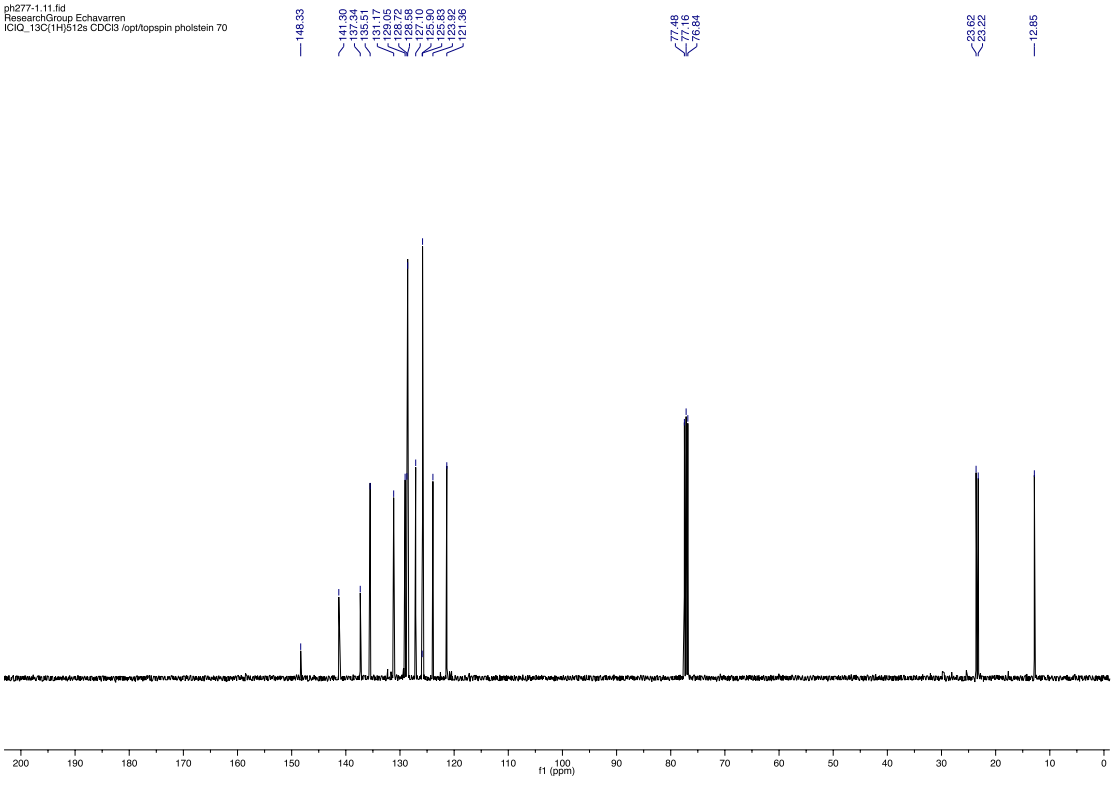


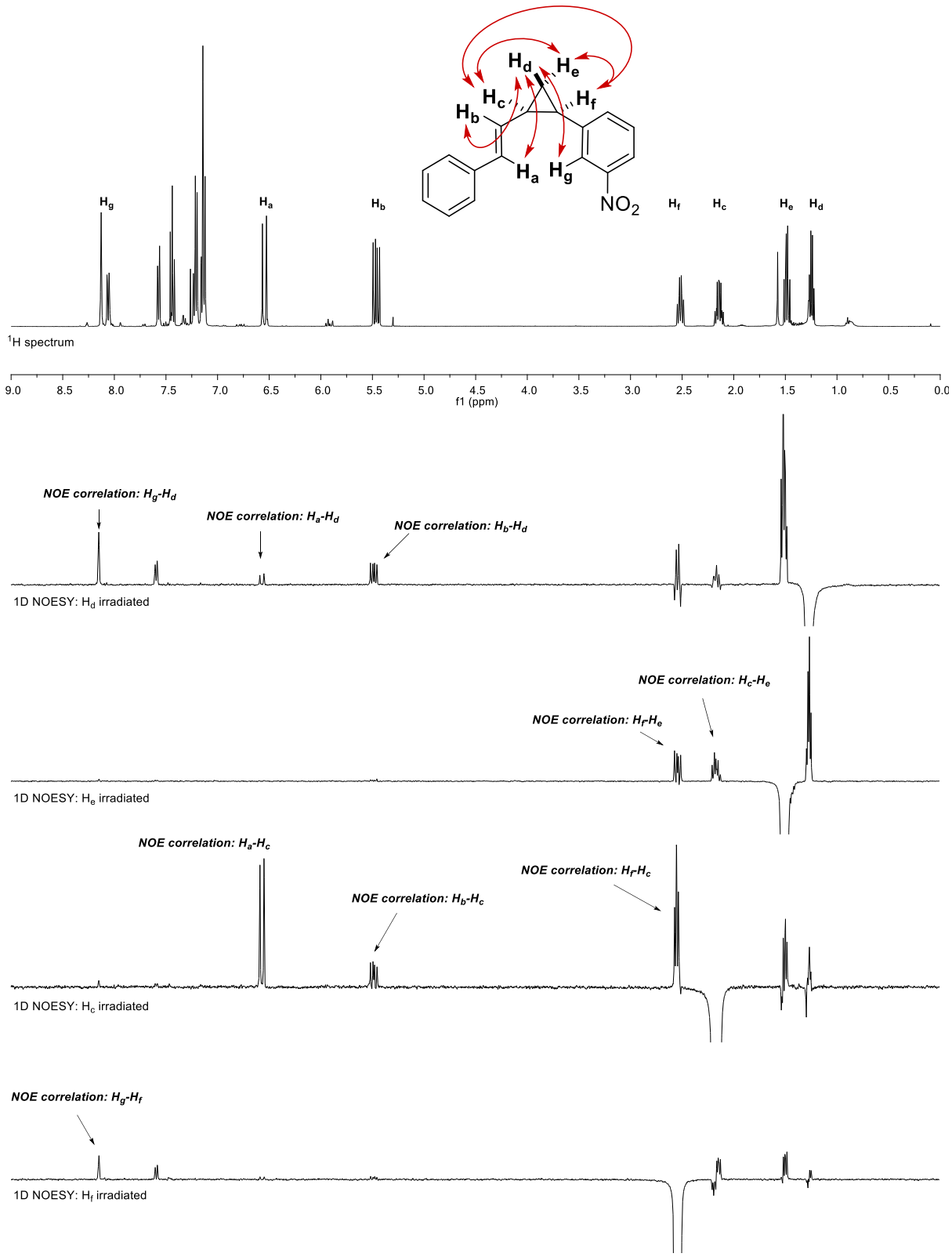
3n

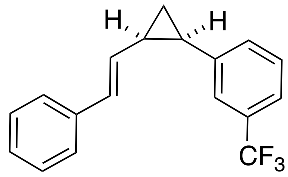
ph370-f1.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 32



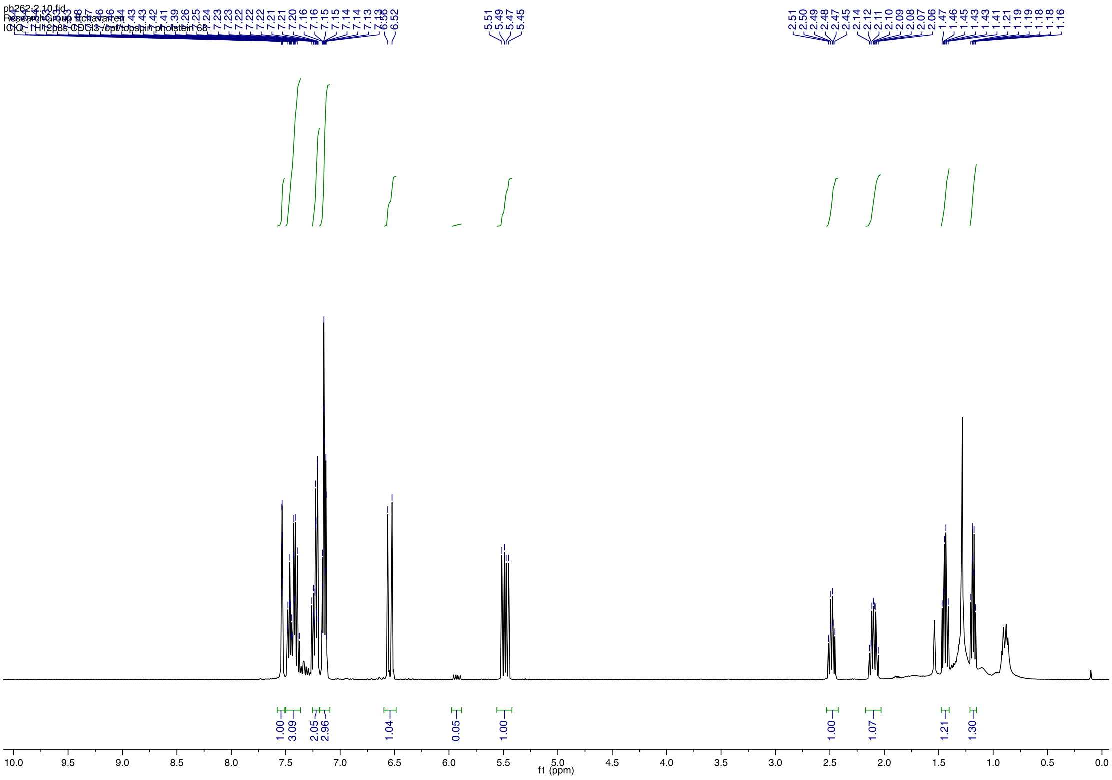
ph277-1.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 70

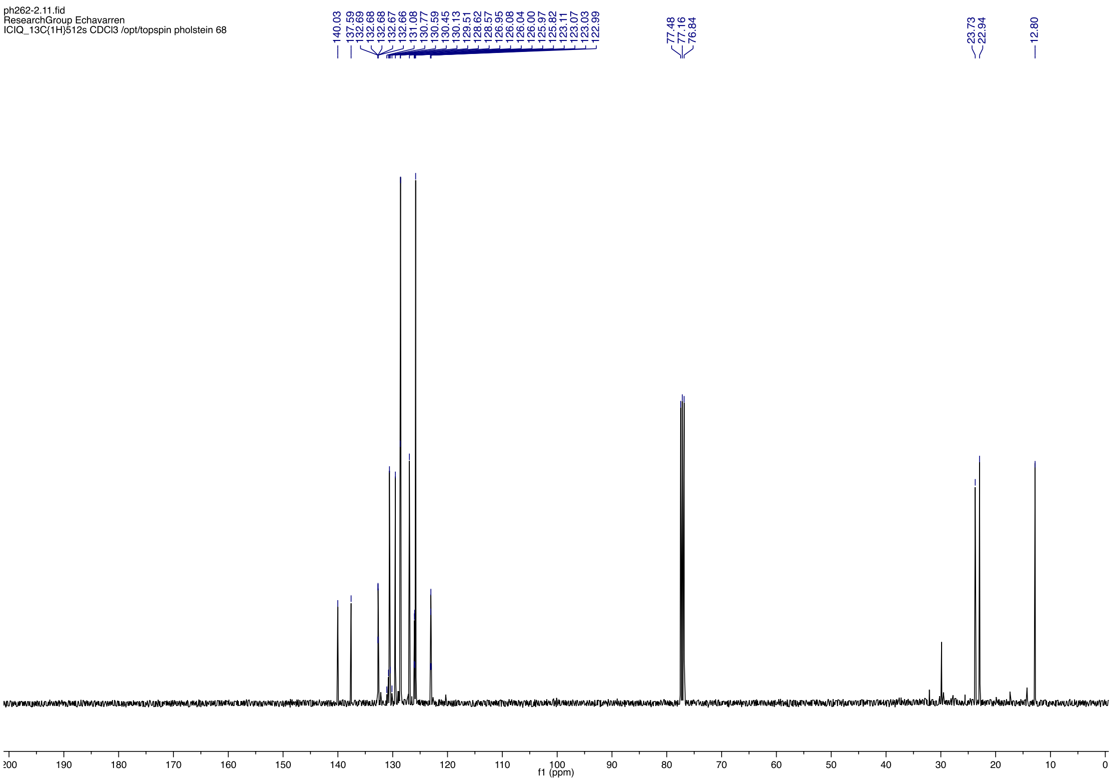


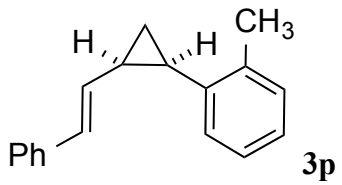

Hd
He
Hc
Hf
Hb
Ha
Hg
NO2
Hg
Ha
Hb
Hf
Hc
He
Hd
1H spectrum
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
NOE correlation: Hg-Hd
NOE correlation: Ha-Hd
NOE correlation: Hb-Hd
1D NOESY: Hd irradiated
NOE correlation: Hc-He
NOE correlation: Hf-He
1D NOESY: He irradiated
NOE correlation: Ha-Hc
NOE correlation: Hb-Hc
NOE correlation: Hf-Hc
1D NOESY: Hc irradiated
NOE correlation: Hg-Hf
1D NOESY: Hf irradiated


H
H
CF3

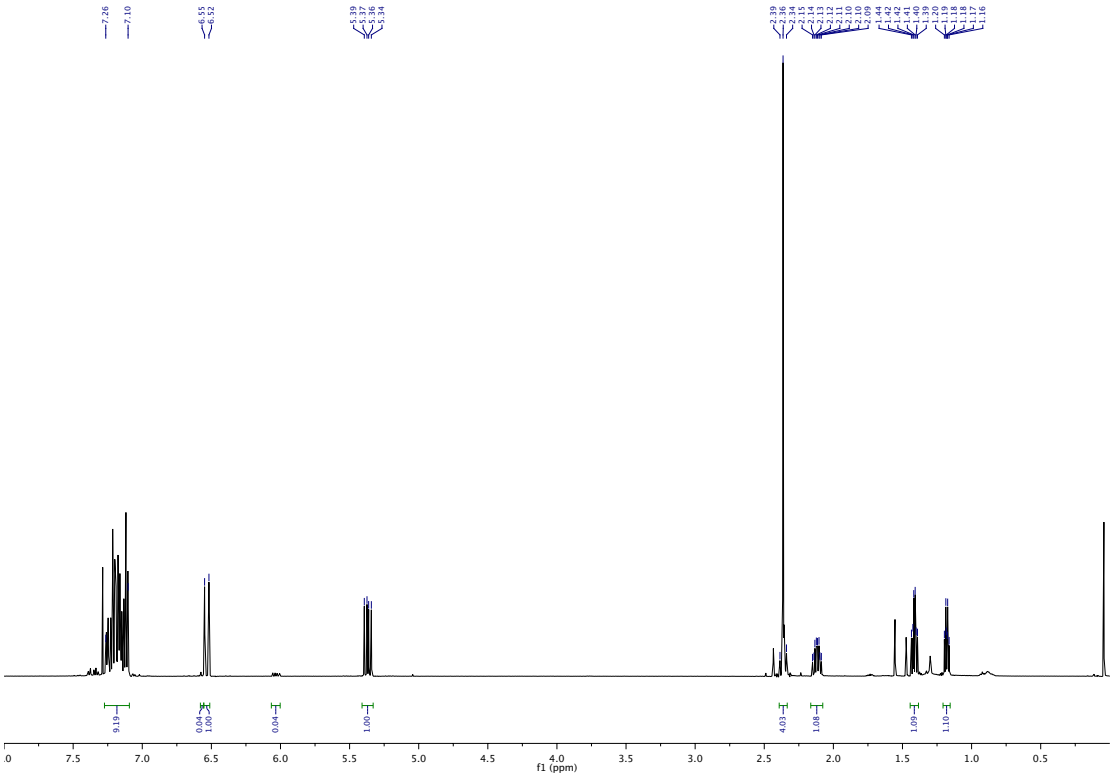
3o

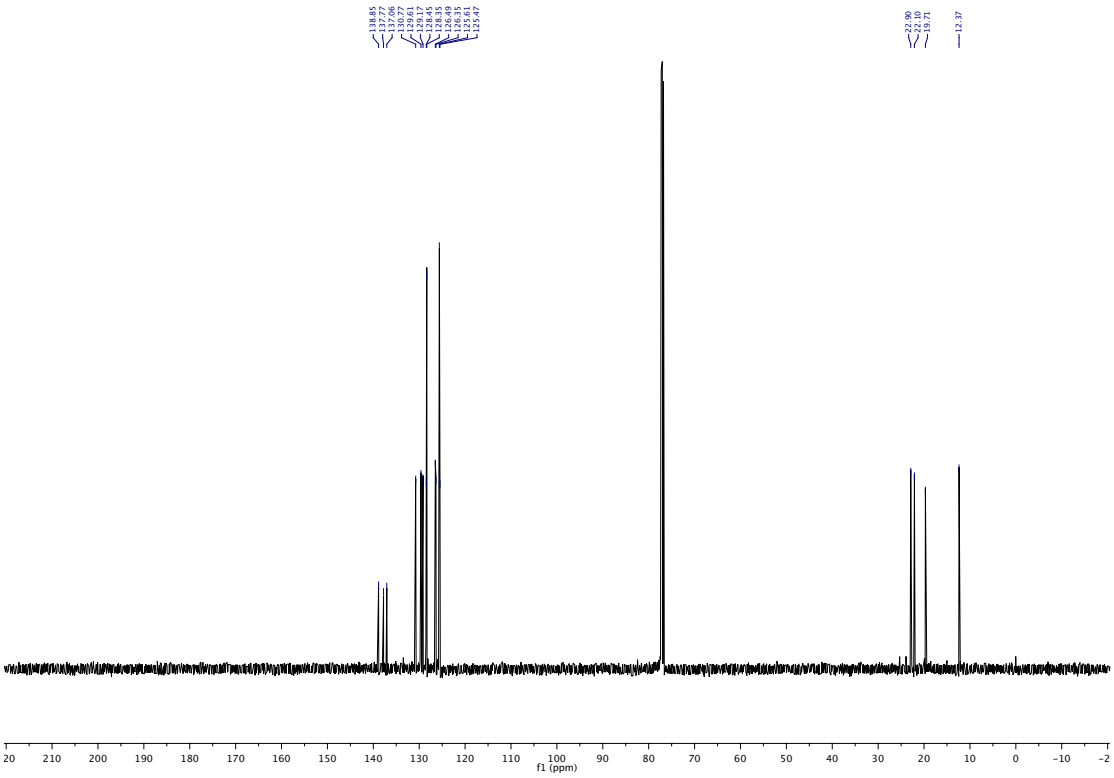

ph262-2.10.fid
ResearchGroup Echavarren
5.51
5.49
5.47
5.45
2.51
2.50
2.49
2.48
2.47
2.45
2.14
2.12
2.11
2.10
2.09
2.08
2.07
2.06
1.47
1.46
1.45
1.43
1.43
1.41
1.21
1.19
1.18
1.16
1.00
3.09
2.05
2.96
1.04
0.05
1.00
1.00
1.07
1.21
1.30
f1 (ppm)

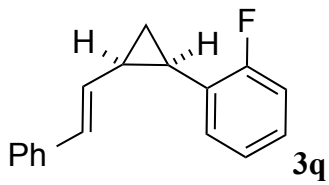

ph262-2.11.fid
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin pholstein 68
140.03
137.59
132.69
132.68
132.67
132.66
131.08
130.77
130.59
130.45
130.13
129.51
128.62
128.57
126.95
126.08
126.04
126.00
125.97
125.82
123.11
123.07
123.03
122.99
77.48
77.16
76.84
23.73
22.94
12.80
f1 (ppm)



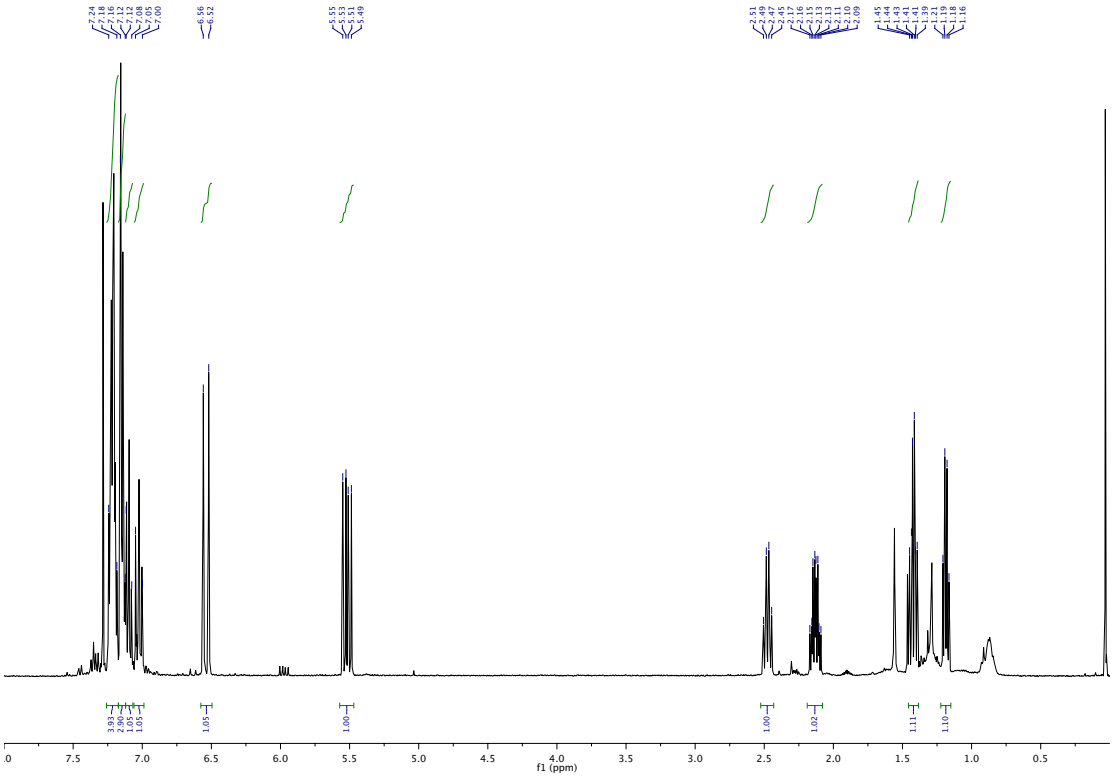
3p

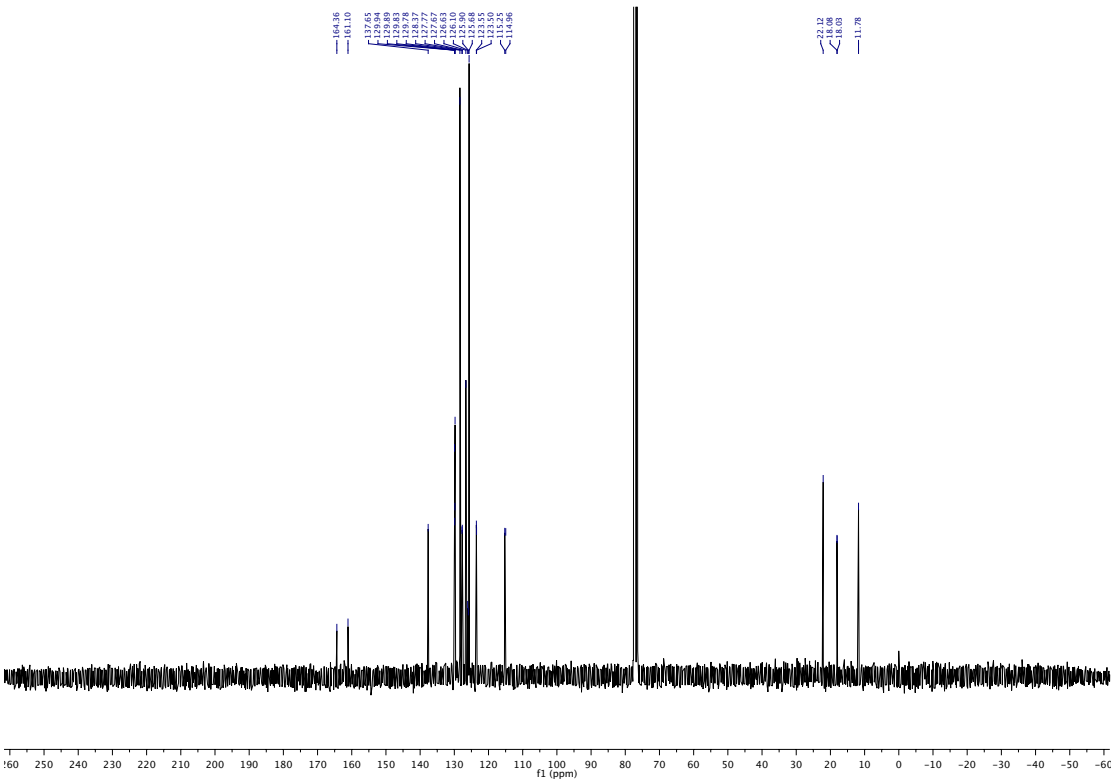


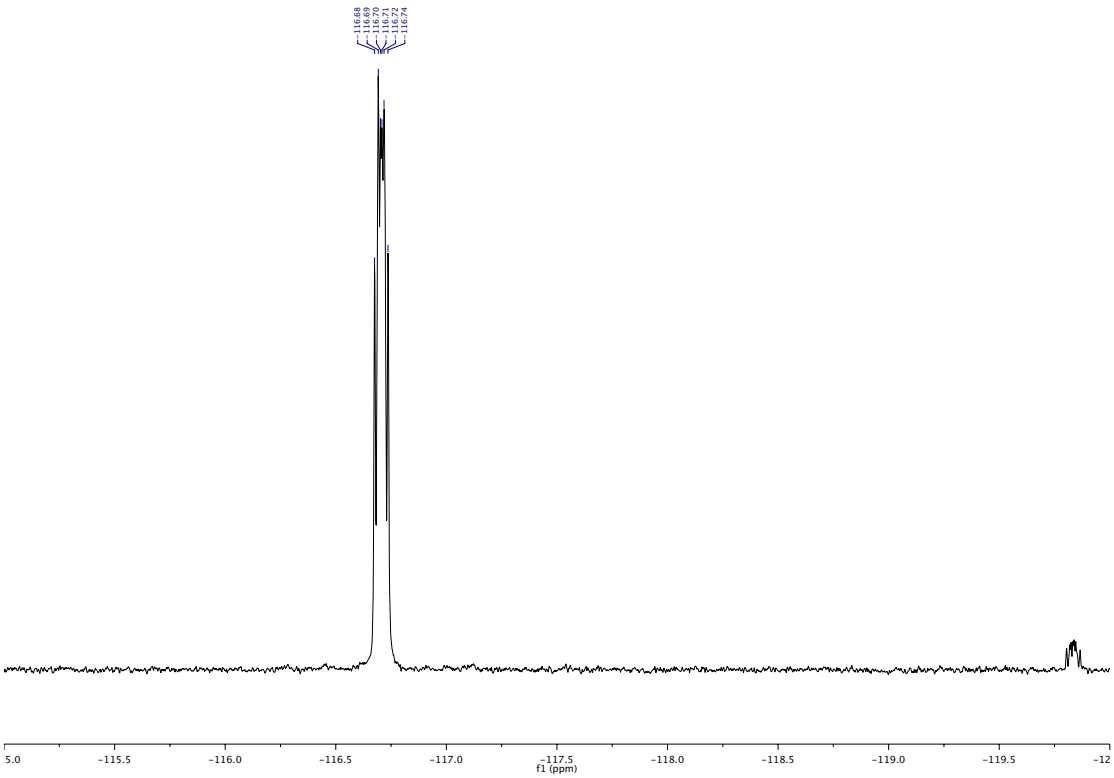


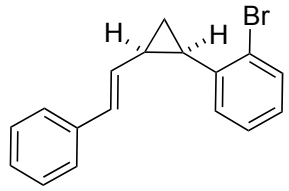


3q



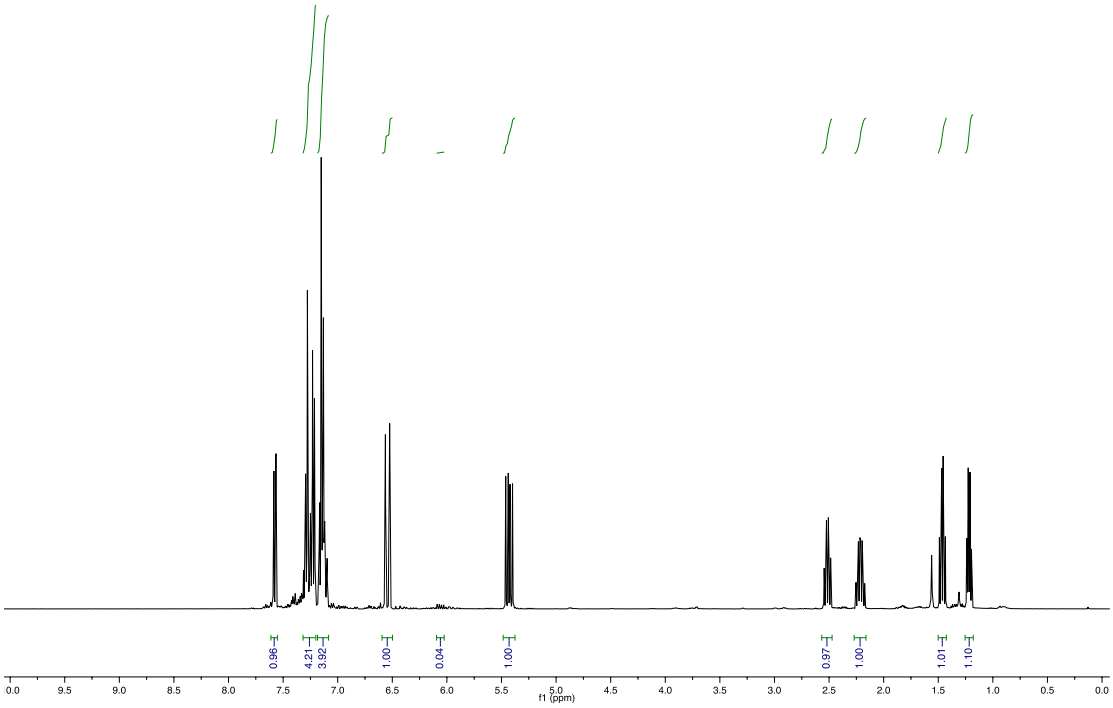



-116.68
-116.69
-116.70
-116.71
-116.72
-116.74
-115.5
-116.0
-116.5
-117.0
-117.5
f1 (ppm)
-118.0
-118.5
-119.0
-119.5

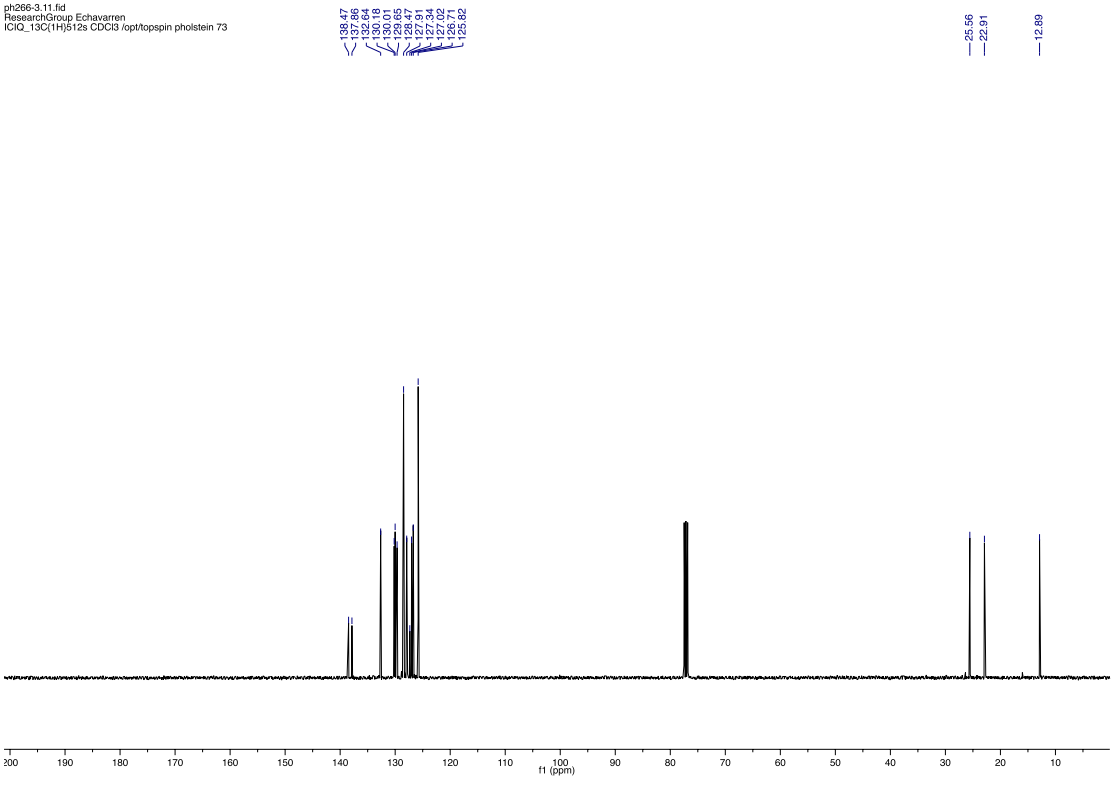


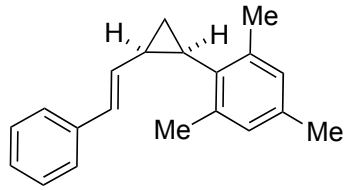
3r

ph266-3.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 73

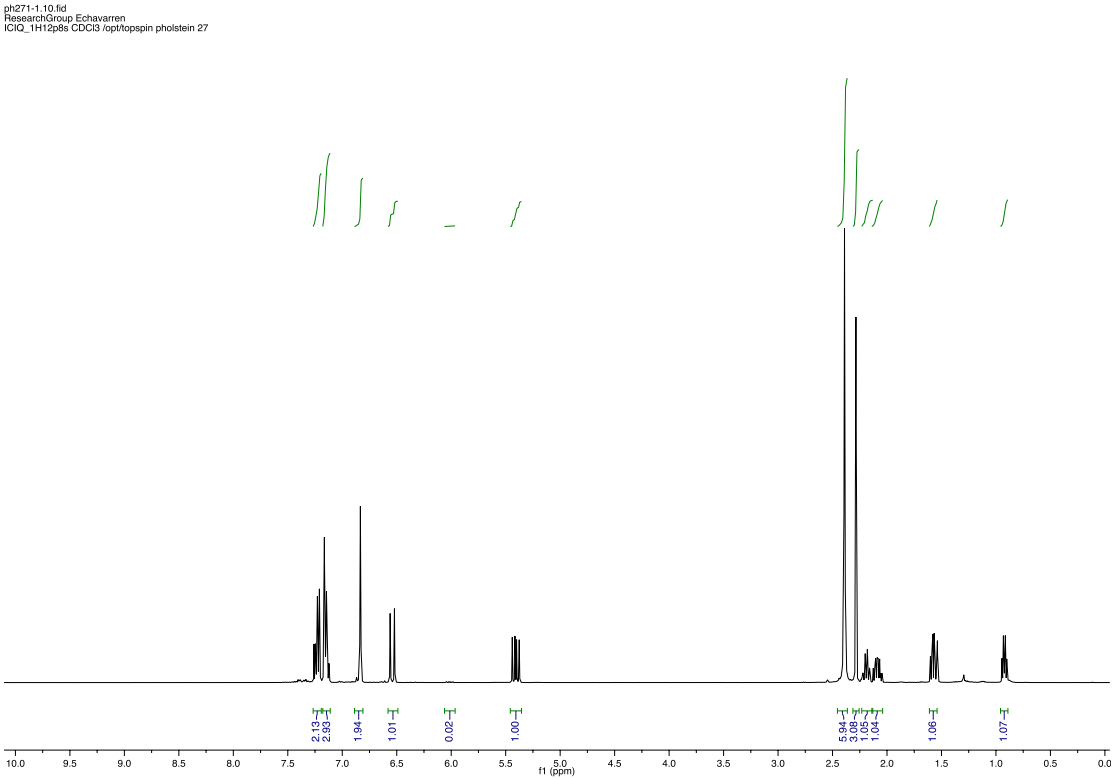


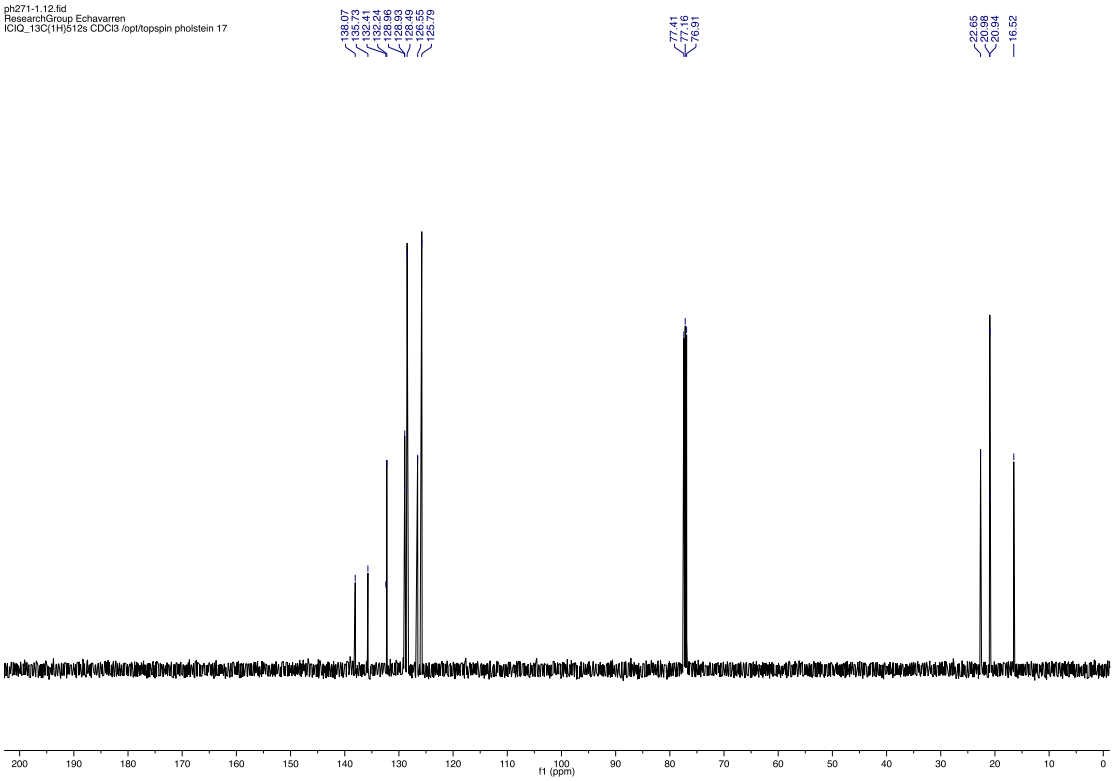
ph266-3.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 73

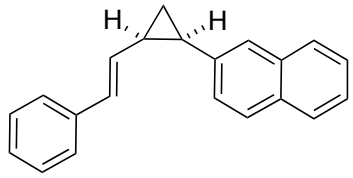



H
H
Me
Me
Me

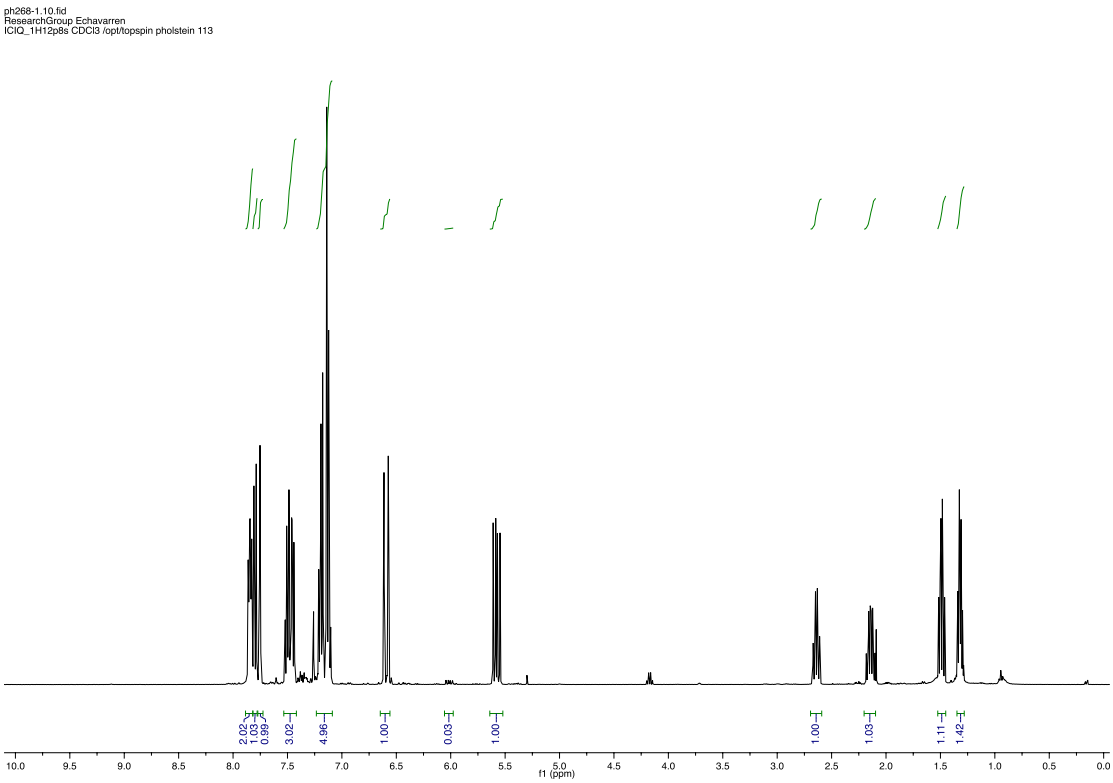
3s

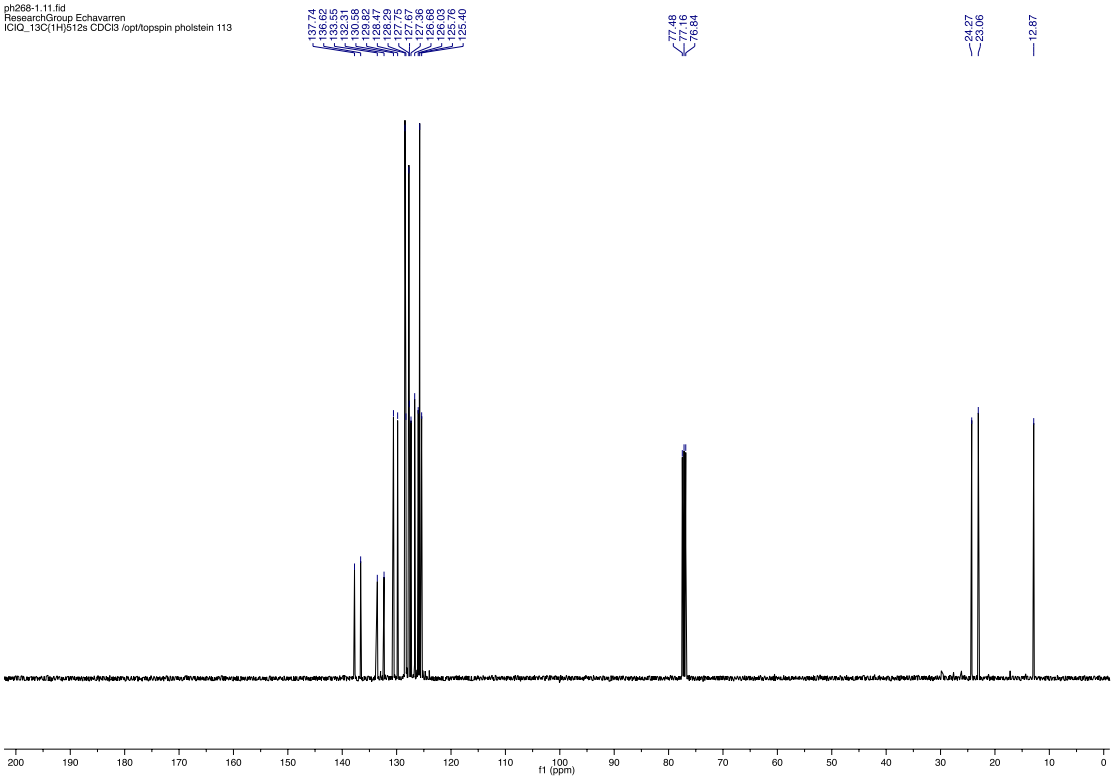

ph271-1.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 27
2.13
2.93
1.94
1.01
0.02
1.00
5.04
3.08
1.05
1.04
1.06
1.07
f1 (ppm)

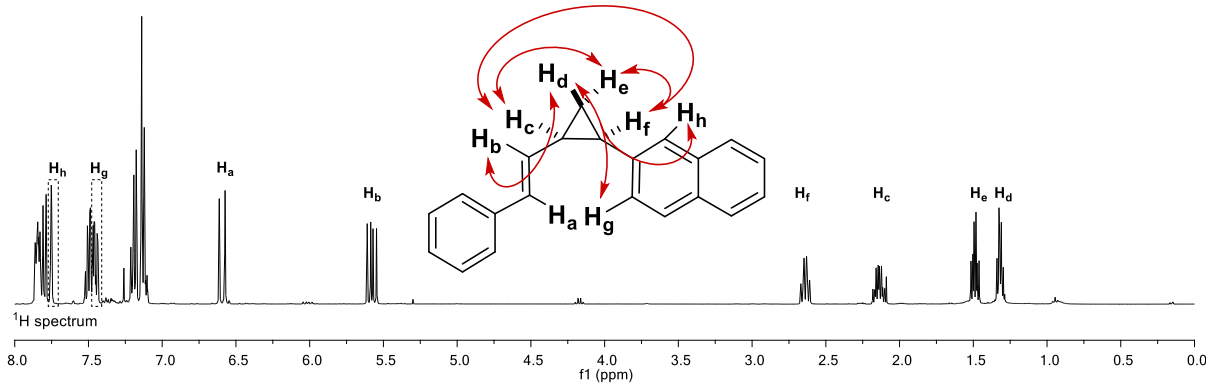

ph271-1.12.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 17
138.07
135.73
132.41
132.24
128.96
128.93
128.49
126.55
125.79
77.41
77.16
76.91
22.65
20.98
20.94
16.52
f1 (ppm)



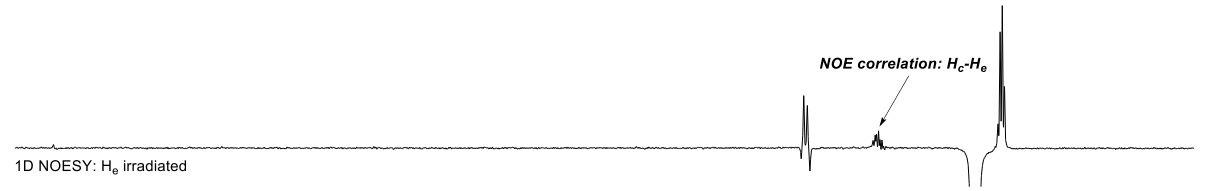
3t


ph268-1.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 113
2.02
1.97
0.99
3.02
4.96
1.00
0.03
1.00
1.00
1.03
1.11
1.42
f1 (ppm)

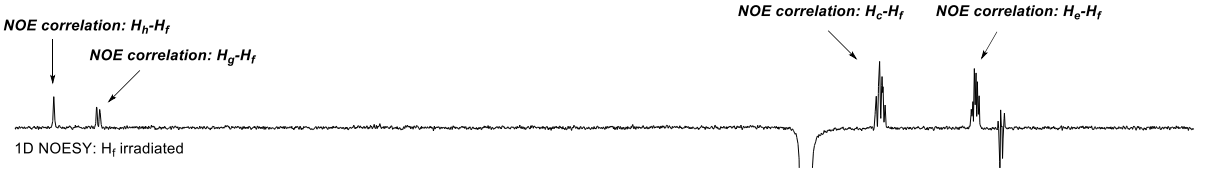

ph268-1.11.fid
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin pholstein 113
137.74
136.62
133.55
132.31
130.58
129.82
128.47
128.29
127.75
127.67
127.36
126.68
126.03
125.76
125.40
77.48
77.16
76.84
24.27
23.06
12.87
f1 (ppm)

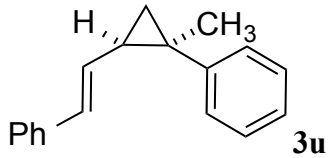

Hd
He
Hc
Hf
Hh
Hb
Ha Hg
Hh
Hg
Ha
Hb
Hf
Hc
He Hd
1H spectrum
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


NOE correlation: Hh-Hd
NOE correlation: Hg-Hd
NOE correlation: Hb-Hd
1D NOESY: Hd irradiated

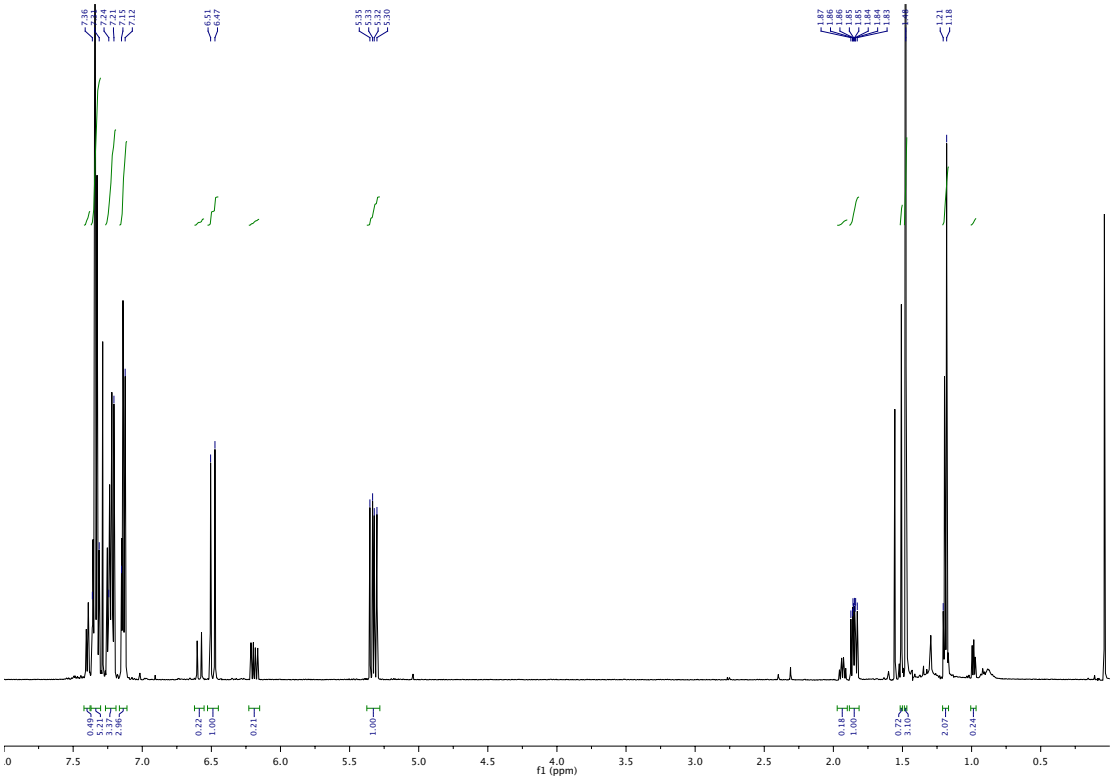

NOE correlation: Hc-He
1D NOESY: He irradiated

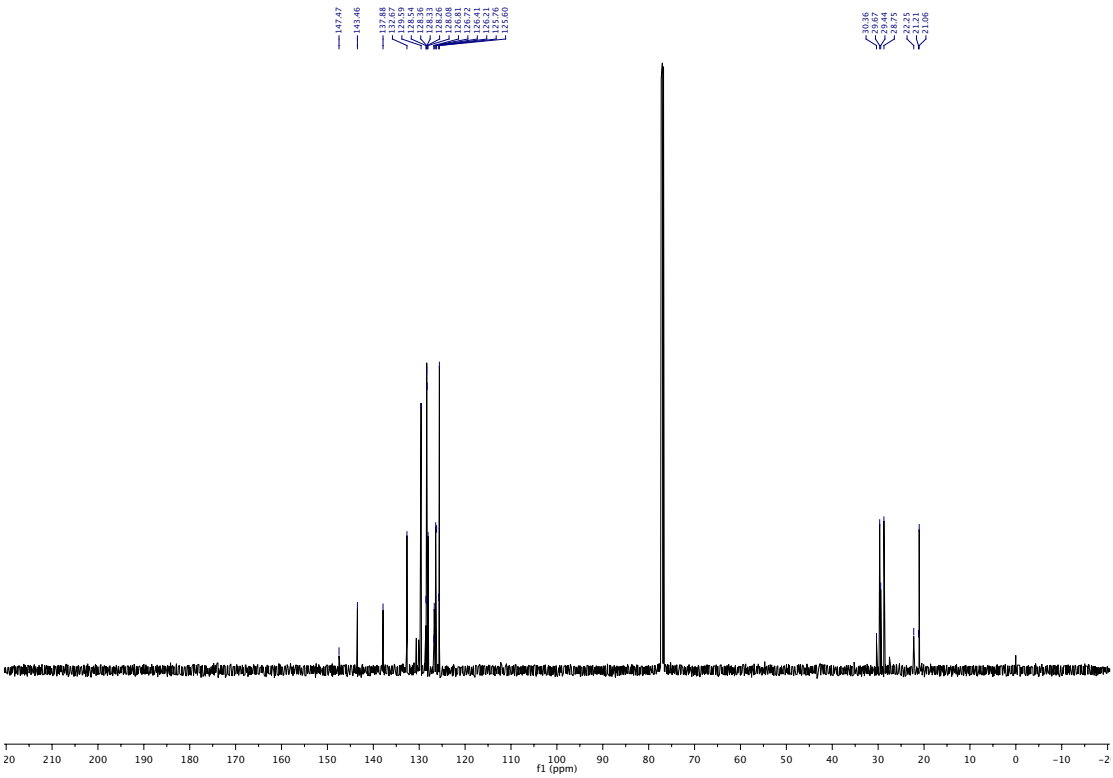

NOE correlation: Ha-Hc
NOE correlation: Hf-Hc
1D NOESY: Hc irradiated

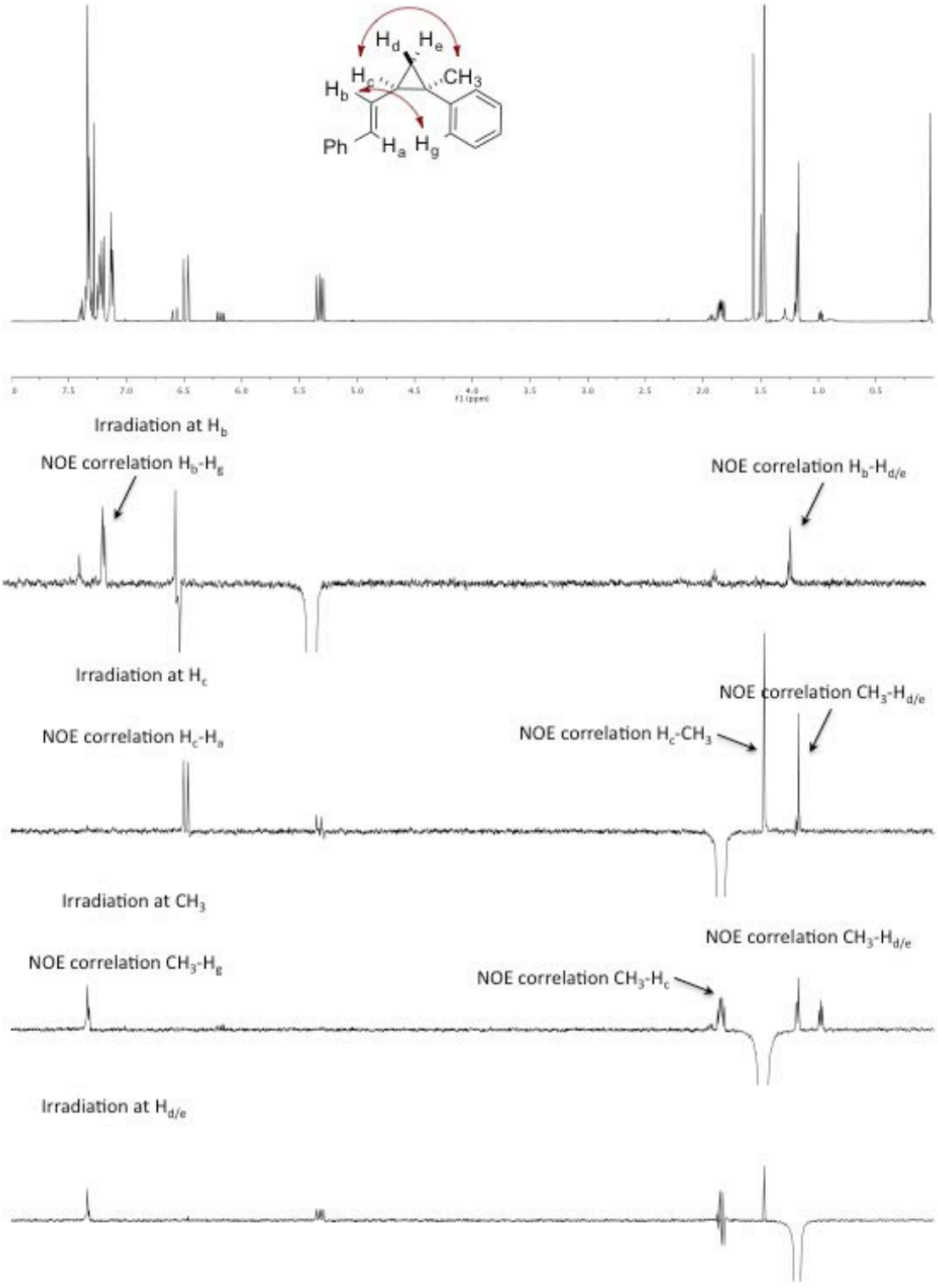

NOE correlation: Hh-Hf
NOE correlation: Hg-Hf
NOE correlation: Hc-Hf
NOE correlation: He-Hf
1D NOESY: Hf irradiated

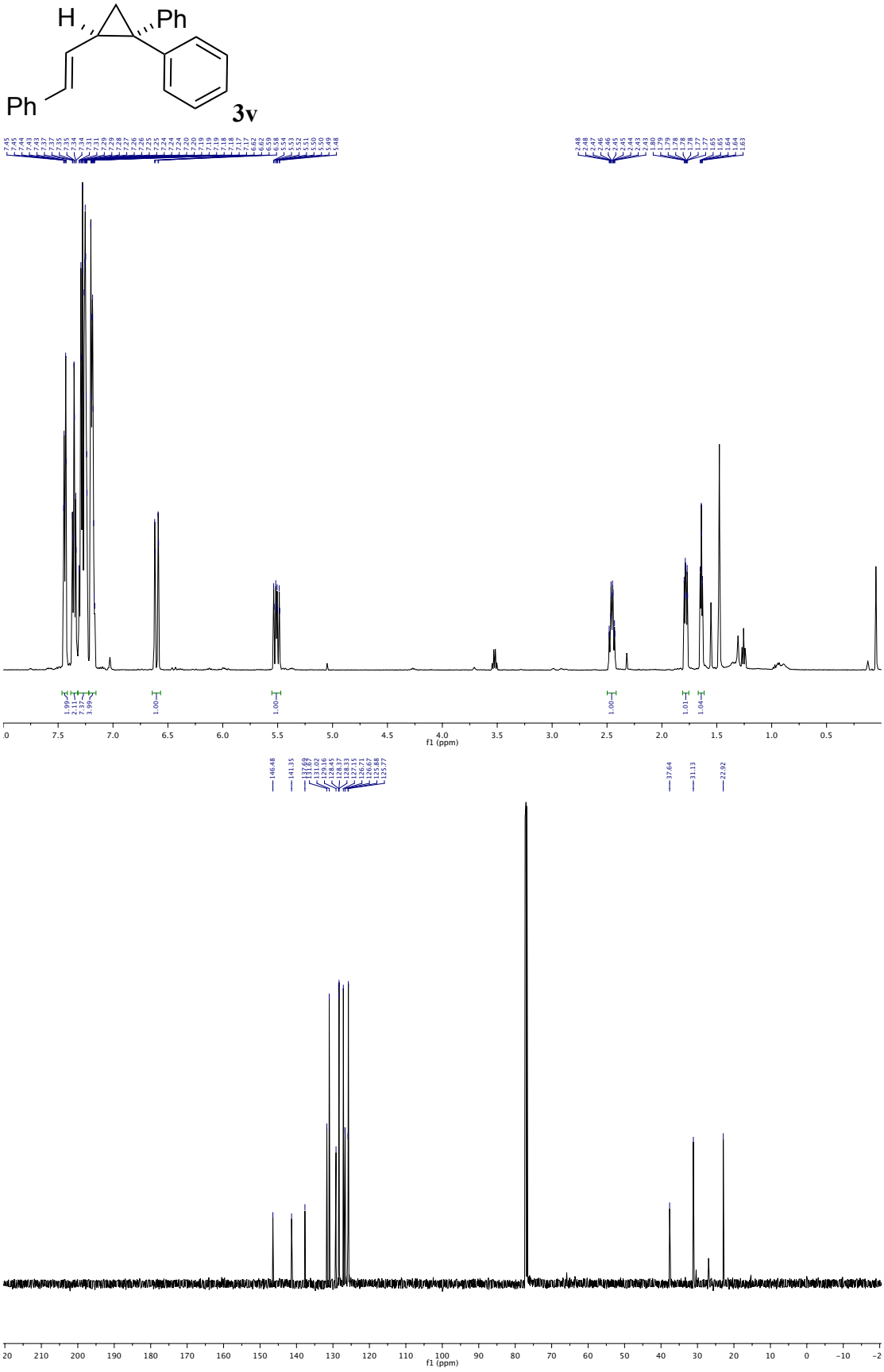


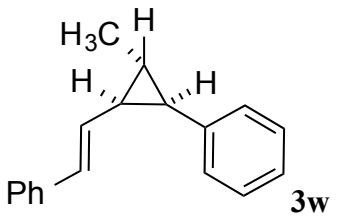
3u



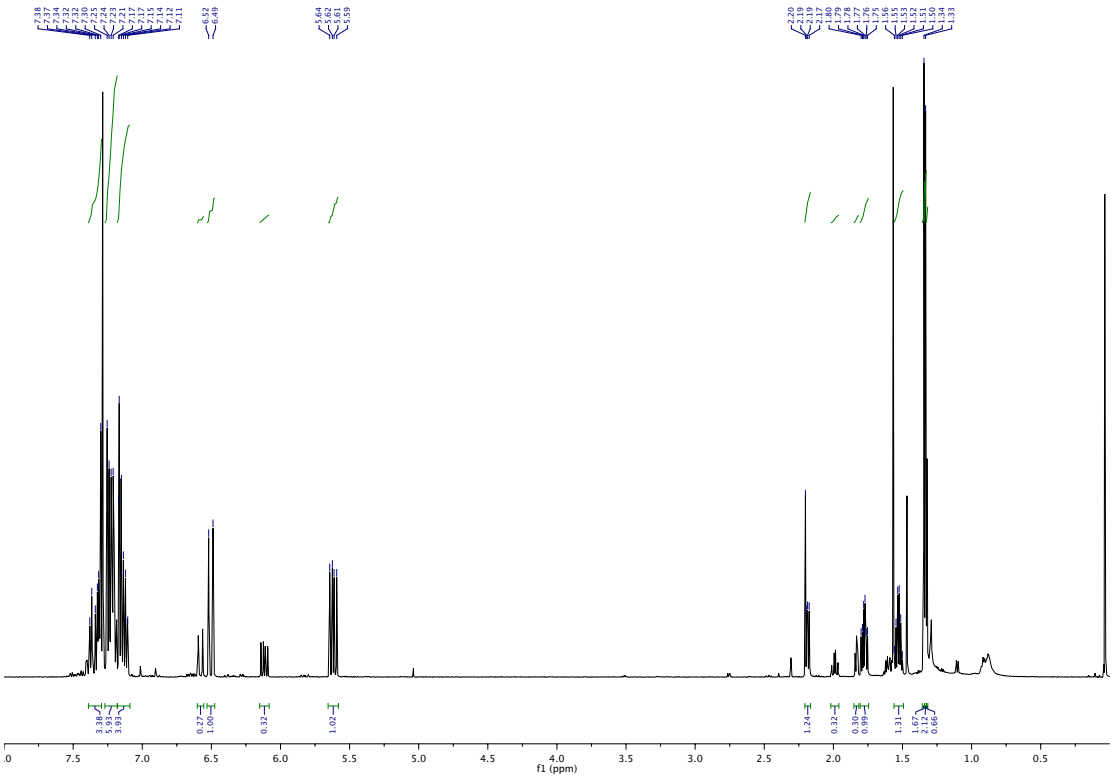


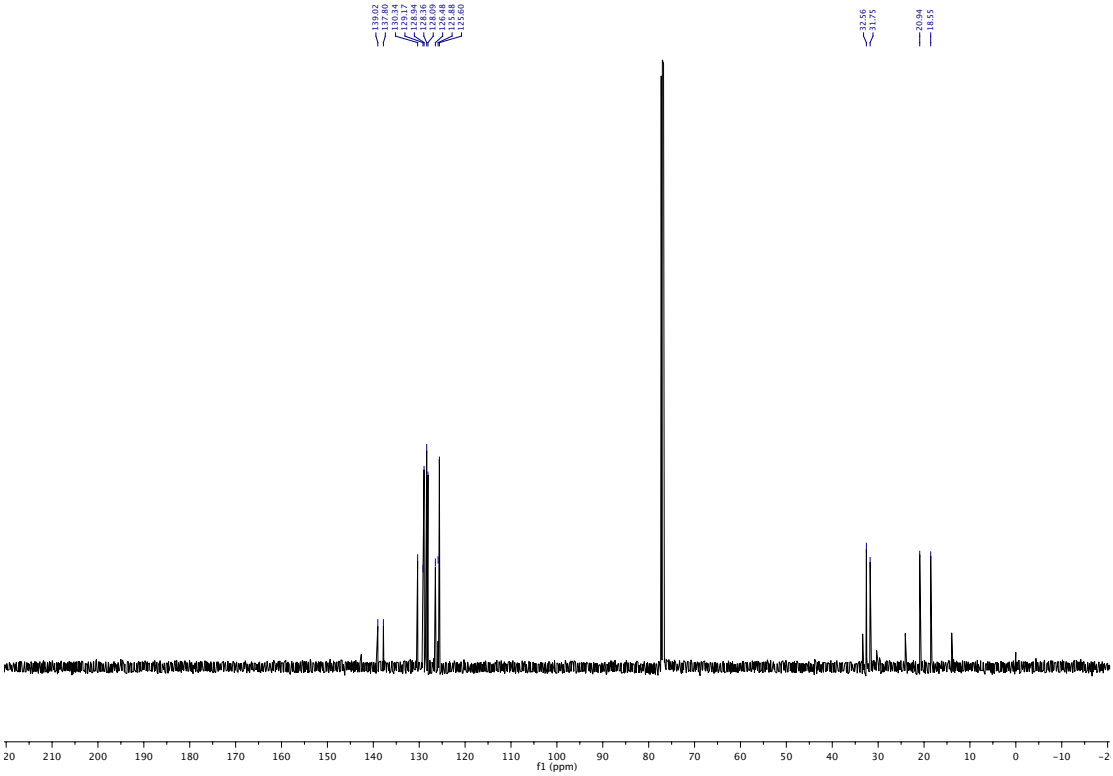

Hd He
Hc
CH3
Hb
Ph
Ha Hg
Irradiation at Hb
NOE correlation Hb-Hg
NOE correlation Hb-Hd/e
Irradiation at Hc
NOE correlation CH3-Hd/e
NOE correlation Hc-Ha
NOE correlation Hc-CH3
Irradiation at CH3
NOE correlation CH3-Hd/e
NOE correlation CH3-Hg
NOE correlation CH3-Hc
Irradiation at Hd/e

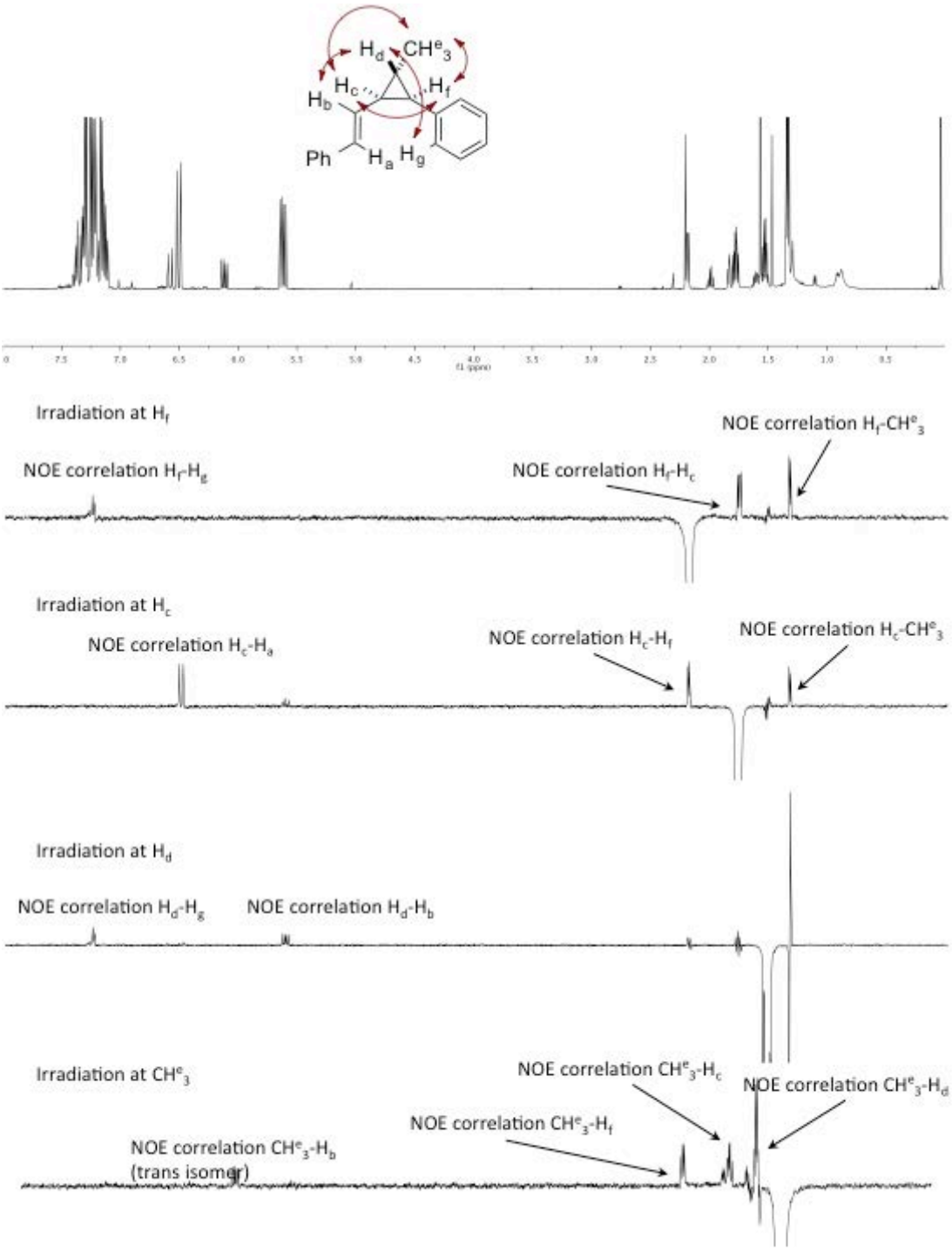

H
Ph
Ph
3v
f1 (ppm)
f1 (ppm)

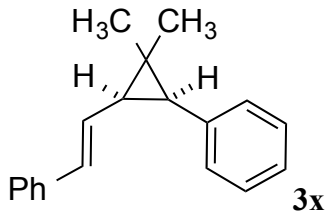


3w

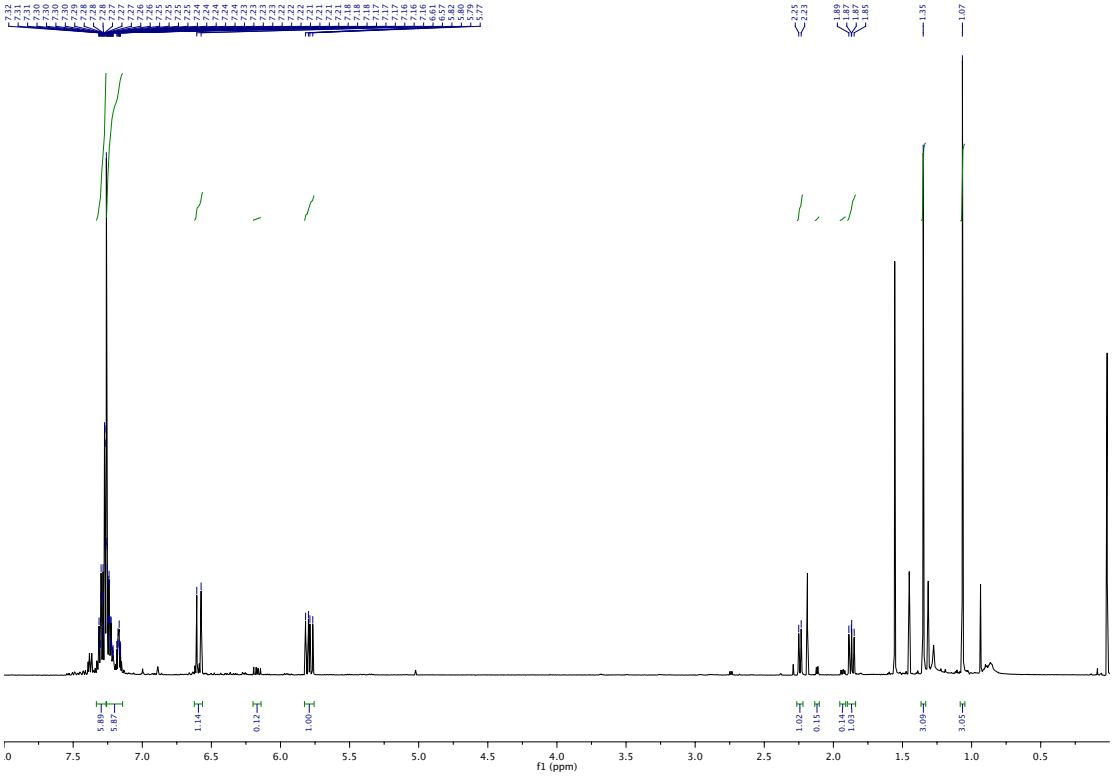


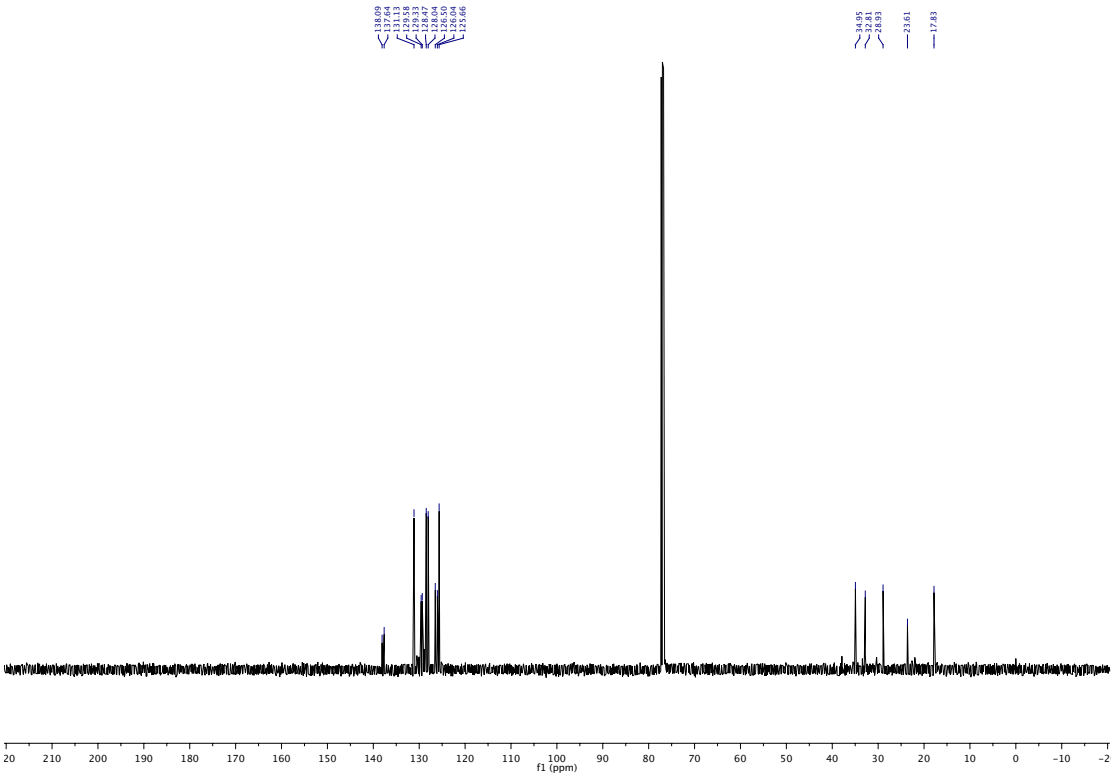


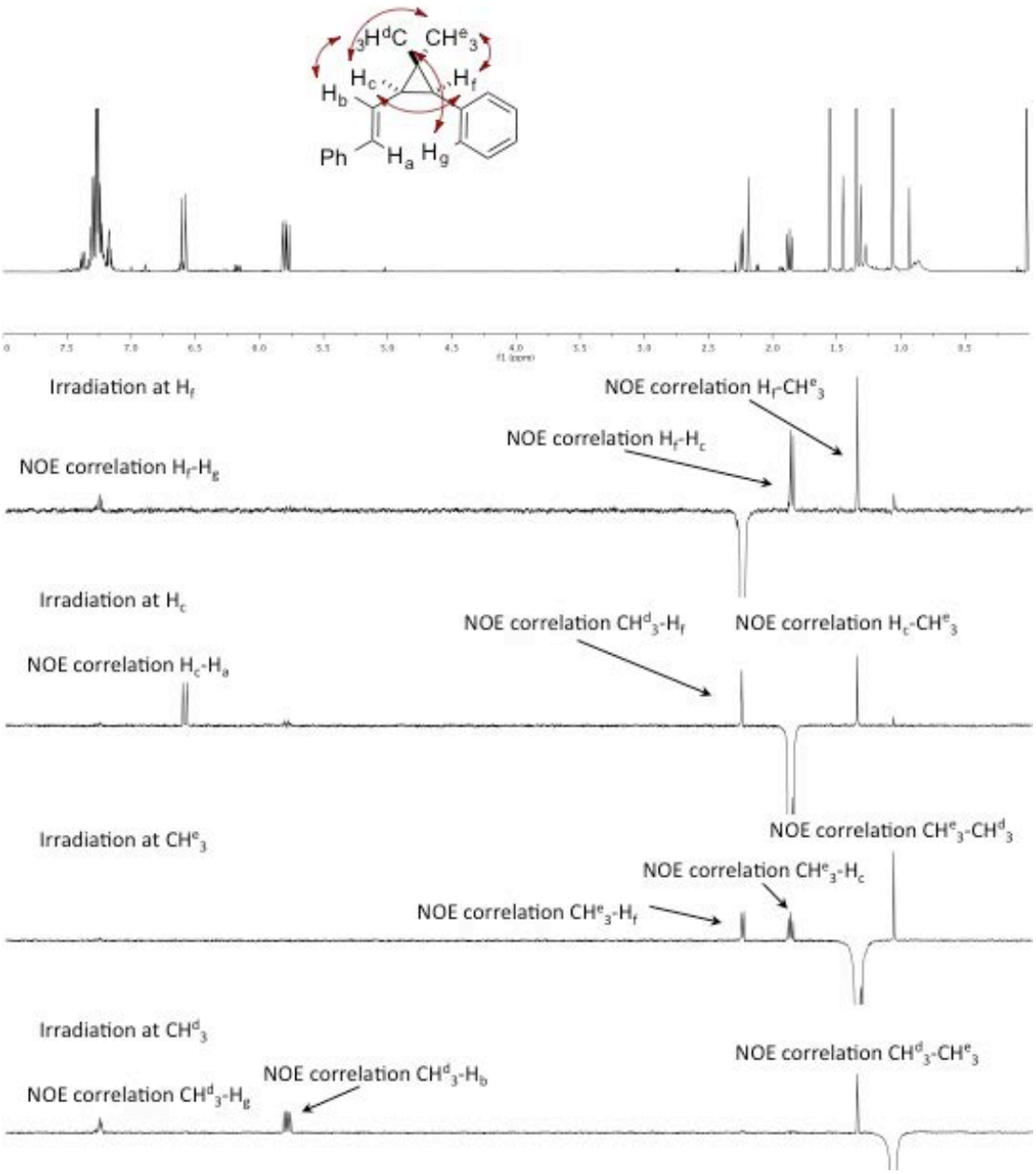

Hd
CHe3
Hc
Hf
Hb
Ph
Ha
Hg
Irradiation at Hf
NOE correlation Hf-Hg
NOE correlation Hf-Hc
NOE correlation Hf-CHe3
Irradiation at Hc
NOE correlation Hc-Ha
NOE correlation Hc-Hf
NOE correlation Hc-CHe3
Irradiation at Hd
NOE correlation Hd-Hg
NOE correlation Hd-Hb
Irradiation at CHe3
NOE correlation CHe3-Hb
(trans isomer)
NOE correlation CHe3-Hf
NOE correlation CHe3-Hc
NOE correlation CHe3-Hd

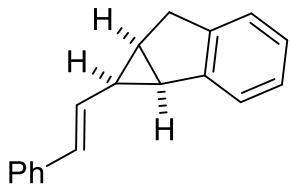


3x



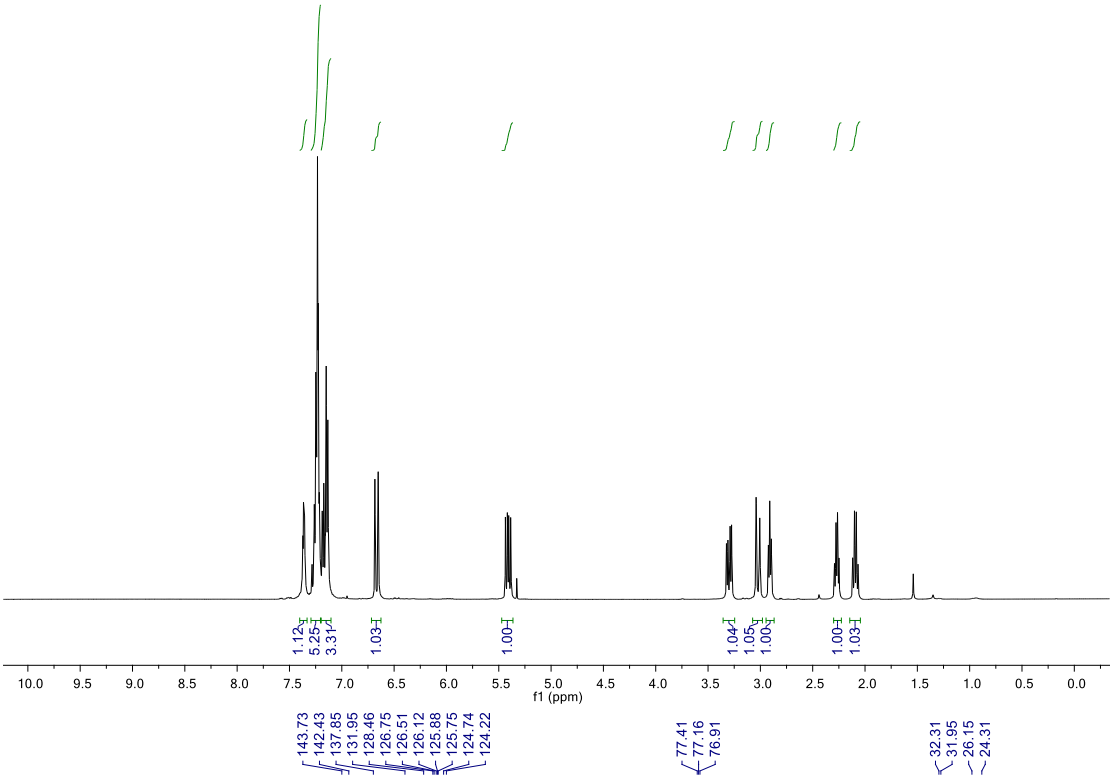


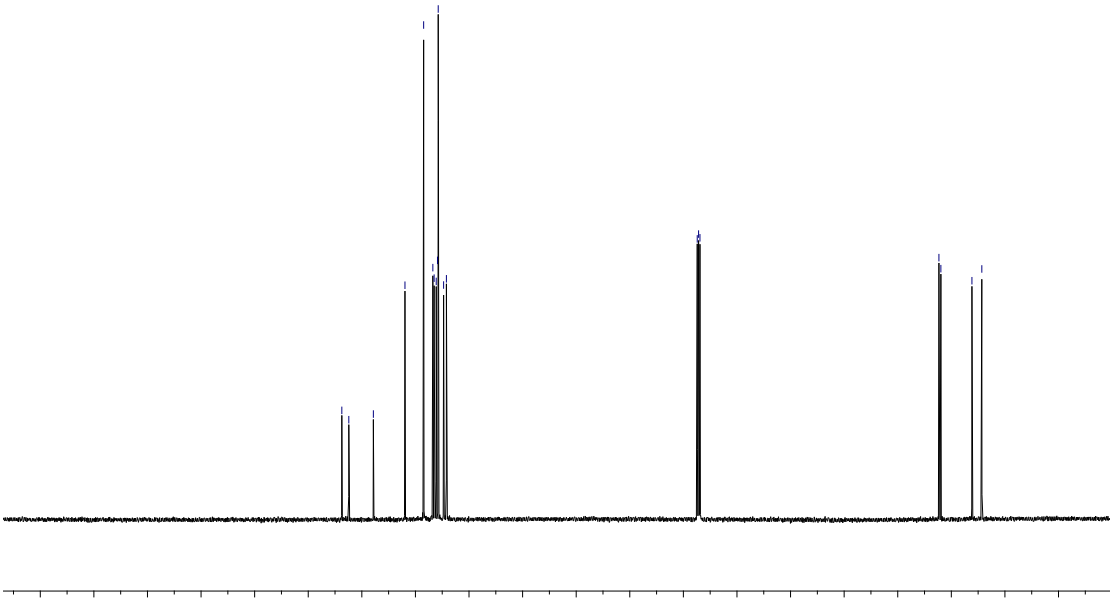

Irradiation at H_f
NOE correlation H_f-CH^e_3
NOE correlation H_f-H_c
NOE correlation H_f-H_g
Irradiation at H_c
NOE correlation CH^d_3-H_f
NOE correlation H_c-CH^e_3
NOE correlation H_c-H_a
Irradiation at CH^e_3
NOE correlation CH^e_3-CH^d_3
NOE correlation CH^e_3-H_c
NOE correlation CH^e_3-H_f
Irradiation at CH^d_3
NOE correlation CH^d_3-CH^e_3
NOE correlation CH^d_3-H_b
NOE correlation CH^d_3-H_g

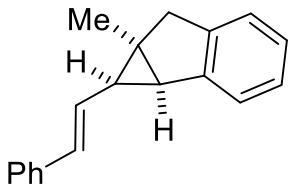


3y

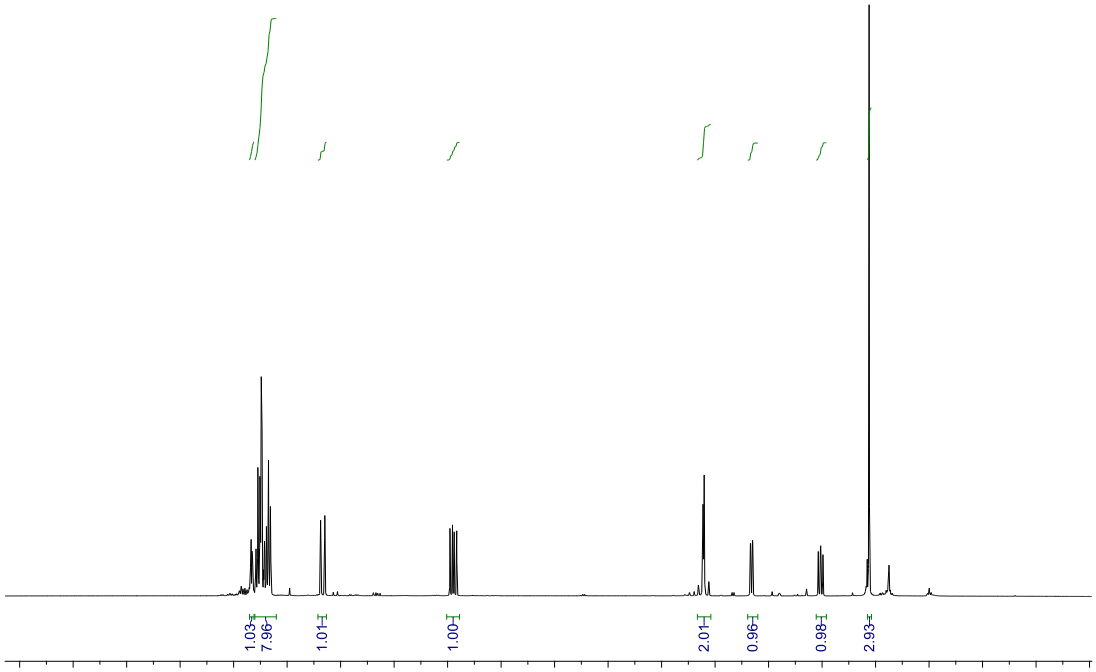
ph250-3.1.fid
1H Experiment

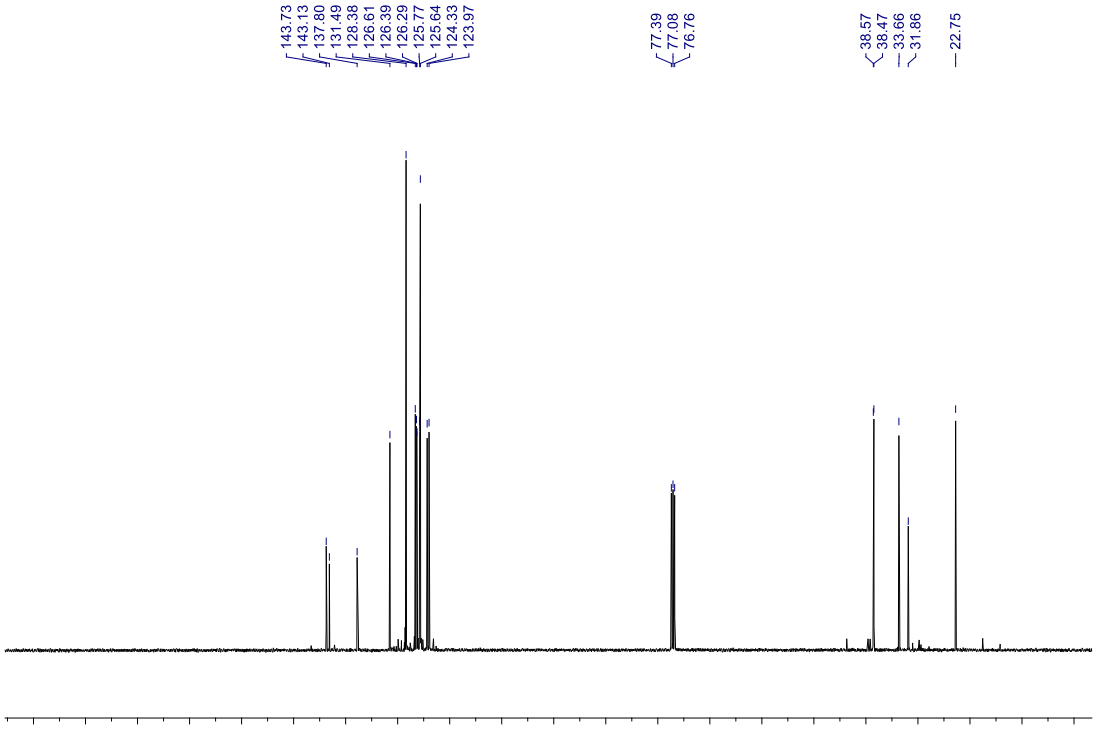


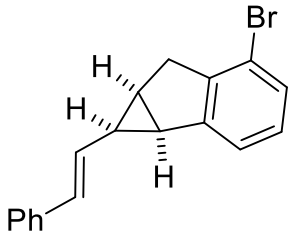



Me
H
H
Ph

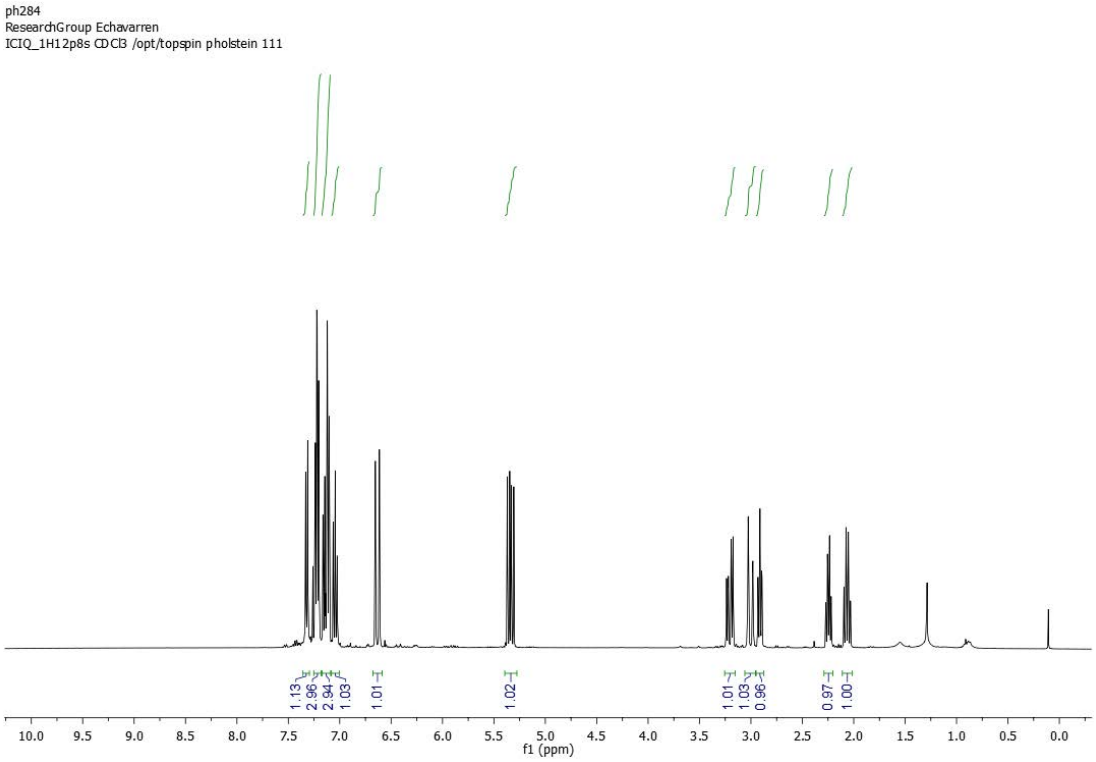
3z

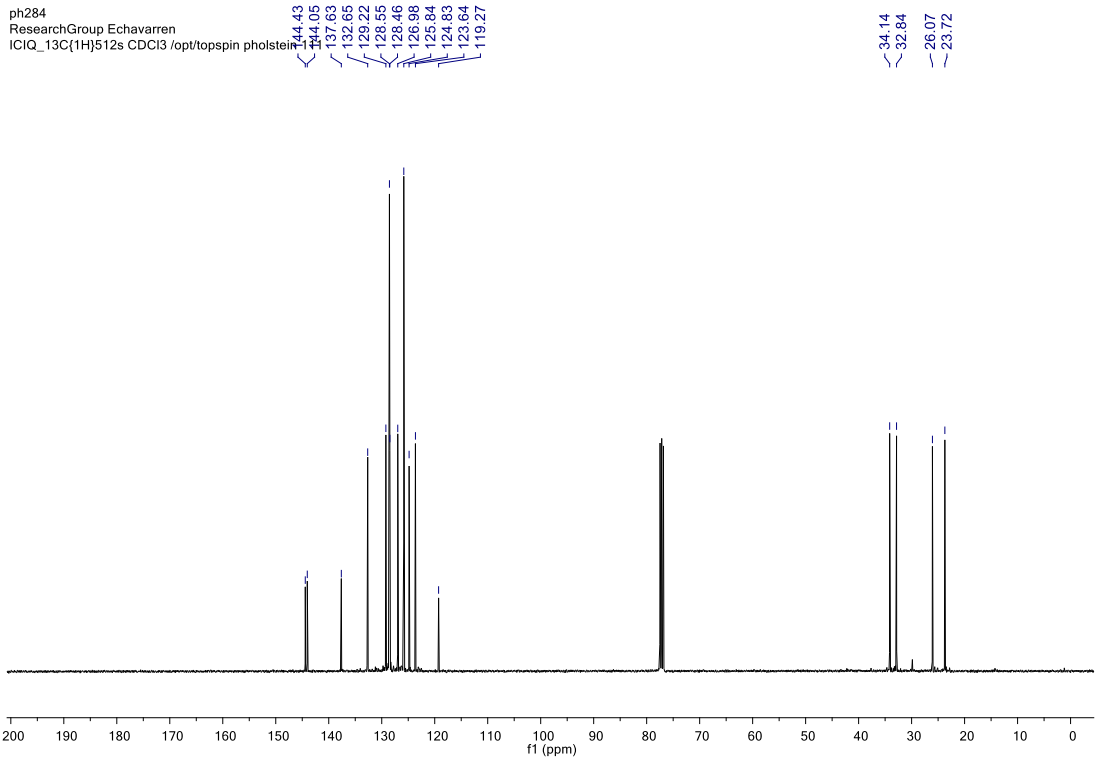

1.03
7.96
1.01
1.00
2.01
0.96
0.98
2.93

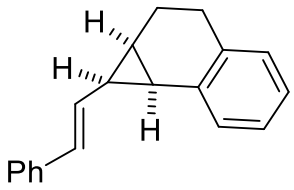

143.73
143.13
137.80
131.49
128.38
126.61
126.39
126.29
125.77
125.64
124.33
123.97
77.39
77.08
76.76
38.57
38.47
33.66
31.86
22.75


Br
H
H
H
Ph

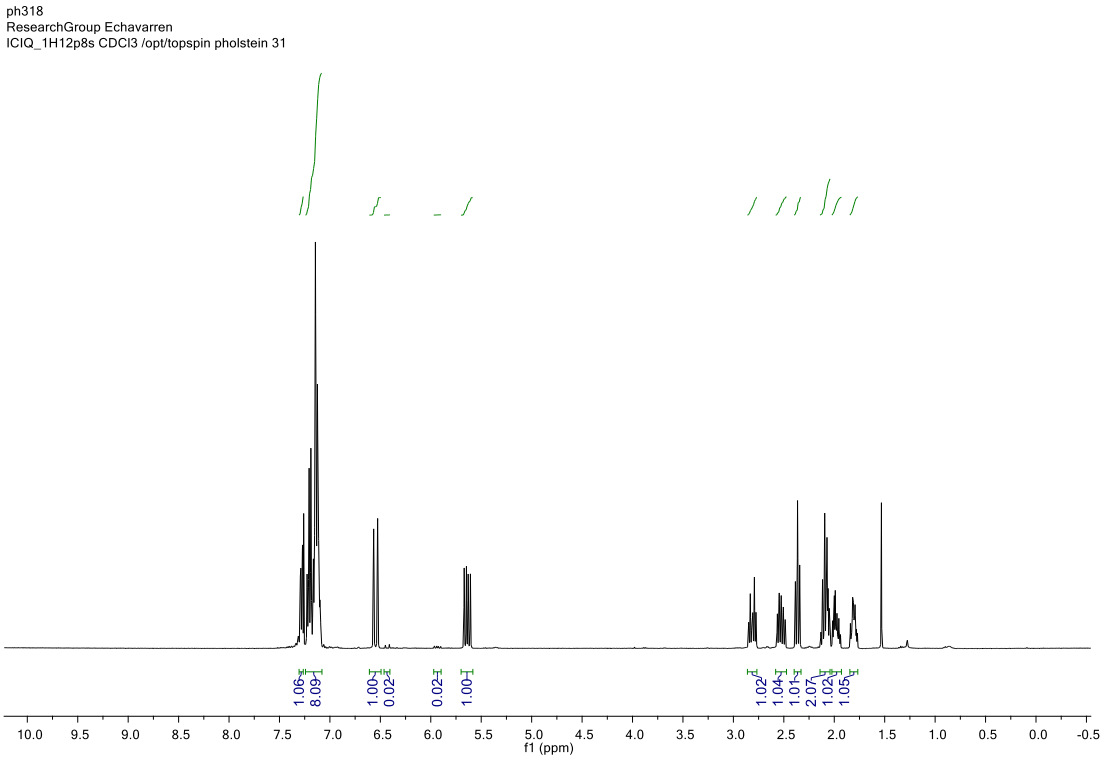
3aa

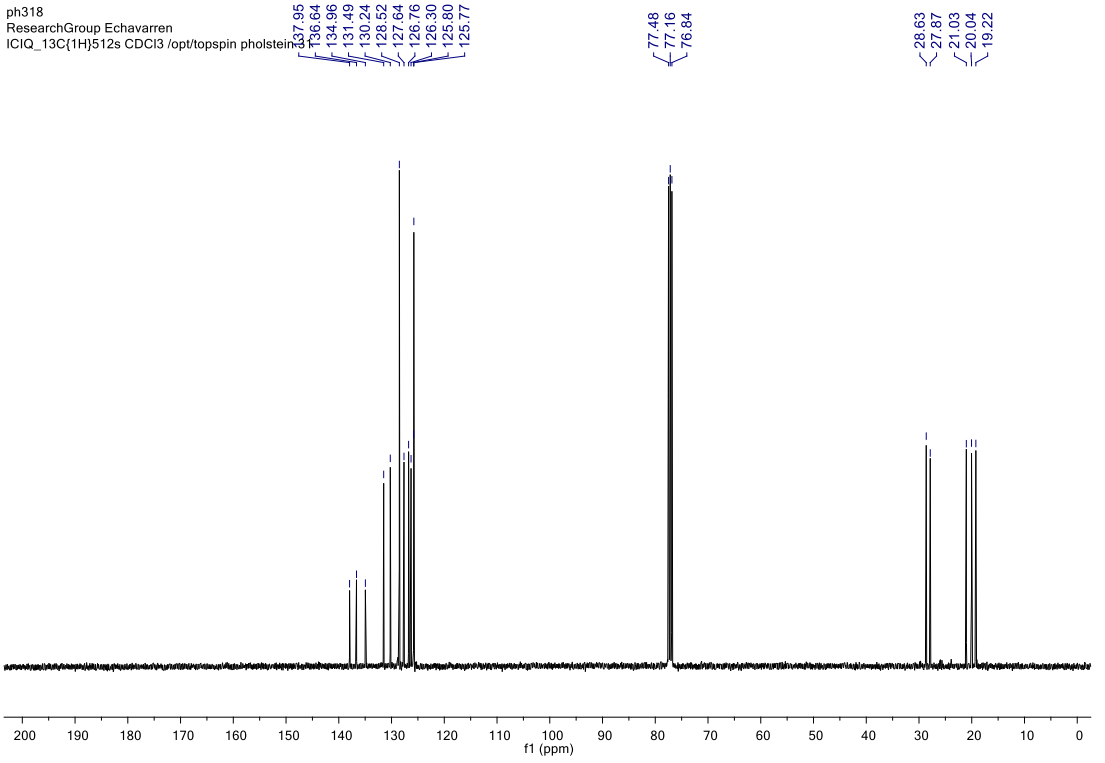

ph284
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 111
1.13
2.96
2.94
1.03
1.01
1.02
1.01
1.03
0.96
0.97
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

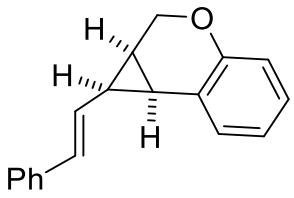

ph284
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein
144.43
144.05
137.63
132.65
129.22
128.55
128.46
126.98
125.84
124.83
123.64
119.27
34.14
32.84
26.07
23.72
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


H
H
H
Ph

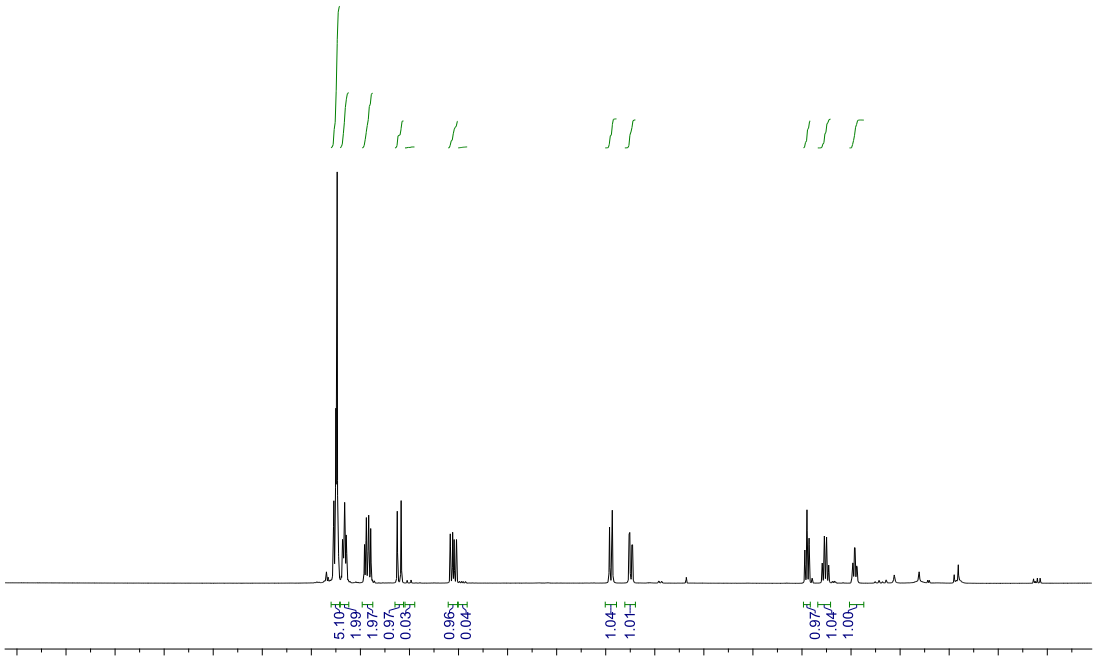
3ab


ph318
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 31
1.06
8.09
1.00
0.02
0.02
1.00
1.02
1.04
1.01
2.07
1.02
1.05
f1 (ppm)

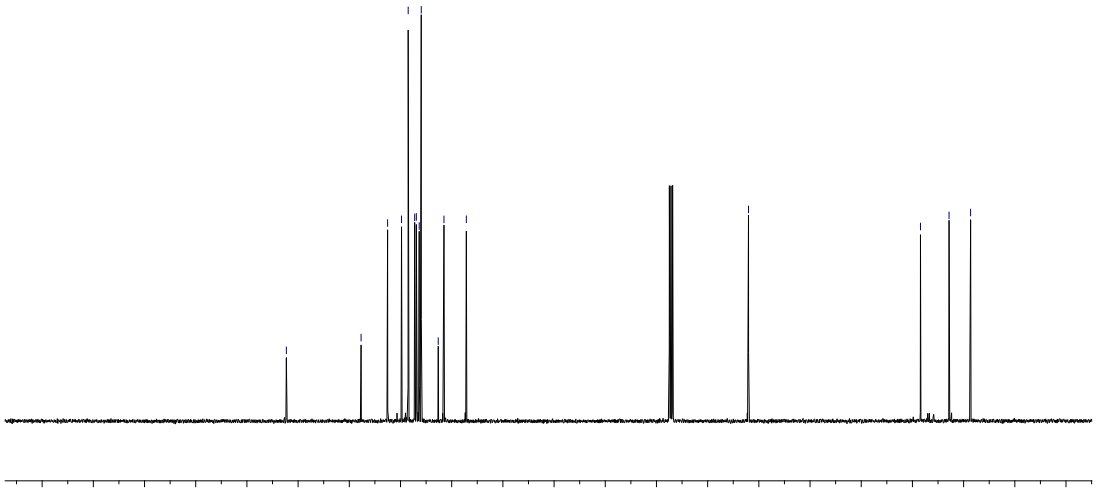

ph318
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin pholstein 31
137.95
136.64
134.96
131.49
130.24
128.52
127.64
126.76
126.30
125.80
125.77
77.48
77.16
76.84
28.63
27.87
21.03
20.04
19.22
f1 (ppm)

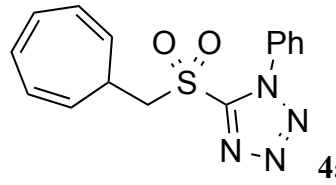

H
O
H
H
Ph

3ac

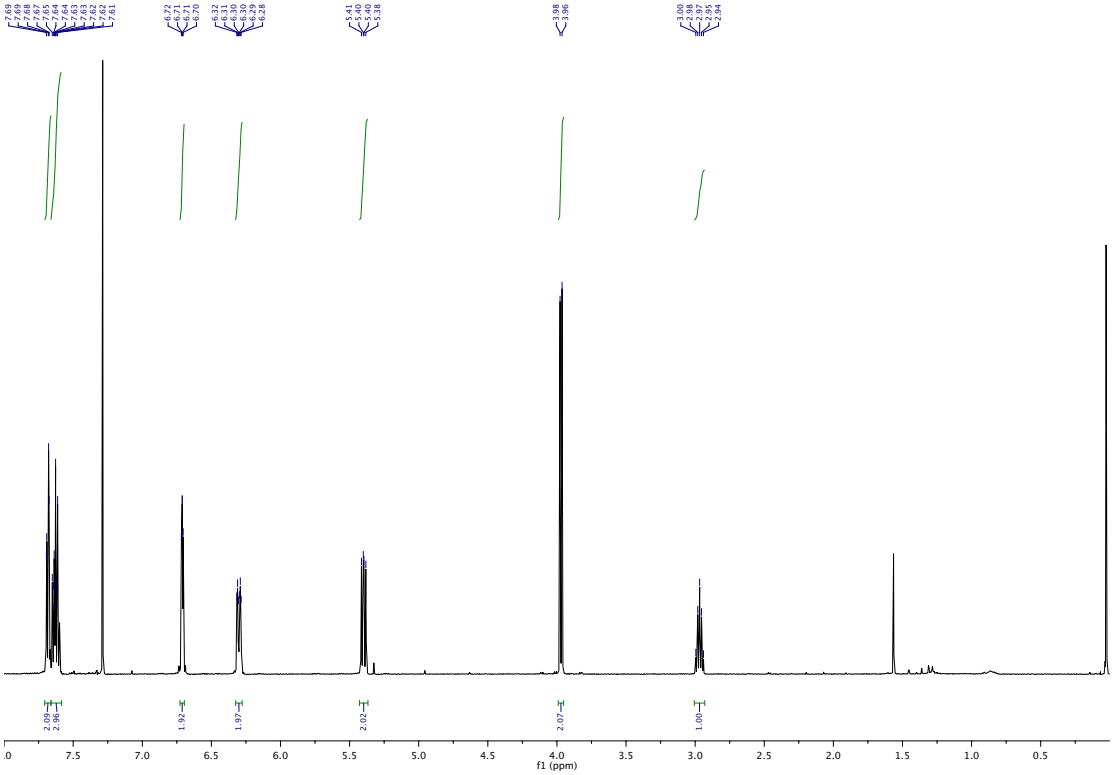

5.10
1.99
1.97
0.97
0.03
0.96
0.04
1.04
1.01
0.97
1.04
1.00

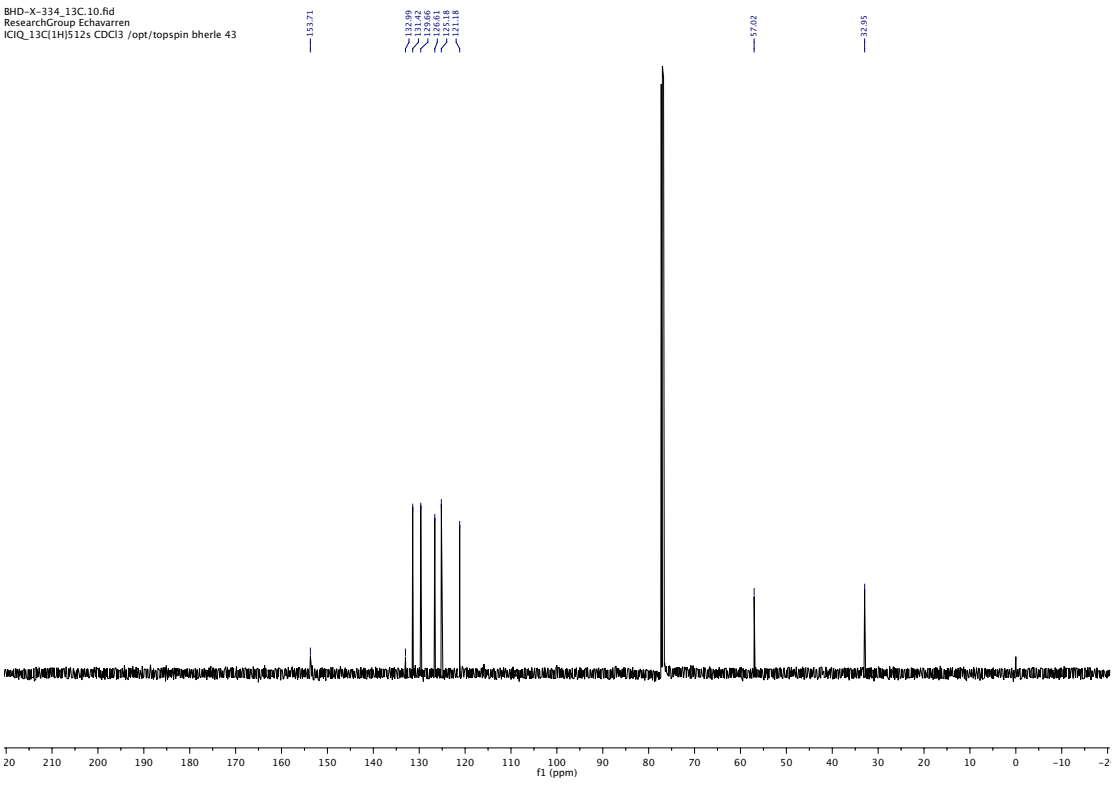

152.30
137.70
132.52
129.80
128.50
127.23
126.90
126.35
125.95
122.63
121.51
117.14
62.02
28.43
22.85
18.64

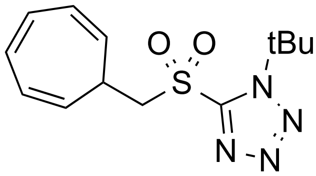



O
O
S
Ph
N
N
N
N

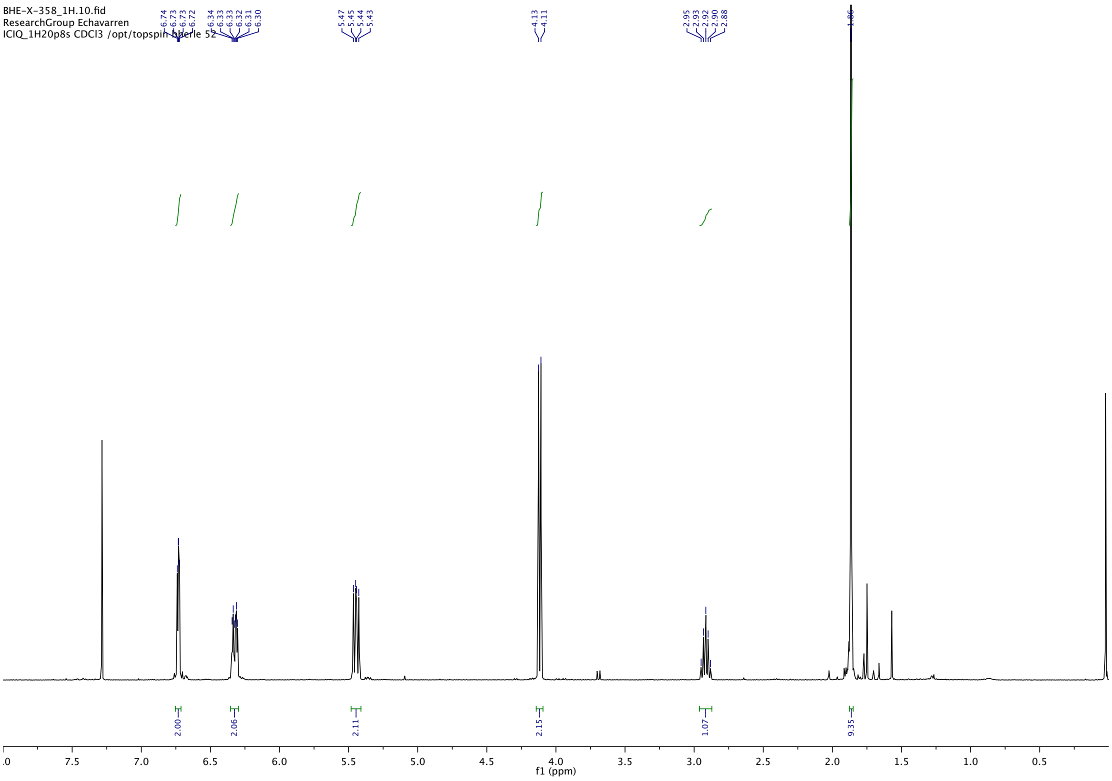
4a

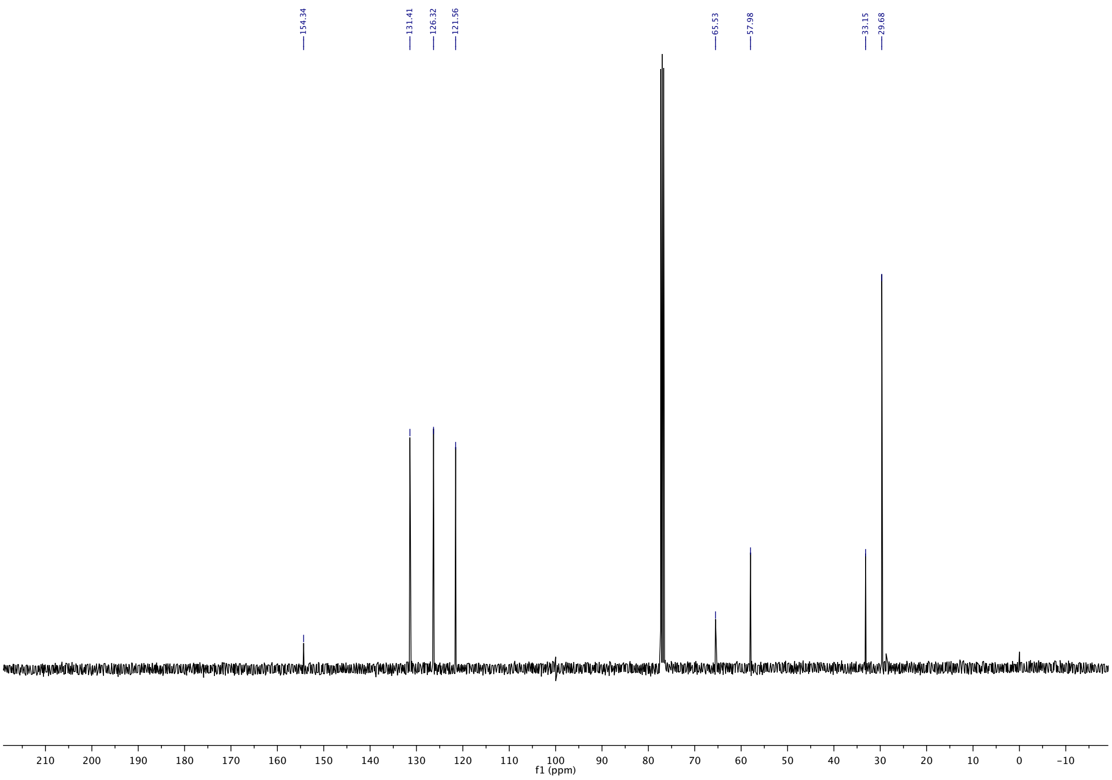

7.69
7.69
7.68
7.68
7.67
7.65
7.64
7.64
7.63
7.63
7.62
7.62
7.61
6.72
6.71
6.71
6.70
6.32
6.31
6.30
6.30
6.29
6.28
5.41
5.40
5.40
5.38
3.98
3.96
3.00
2.98
2.97
2.95
2.94
2.09
2.08
1.92
1.97
2.02
2.07
1.00
f1 (ppm)

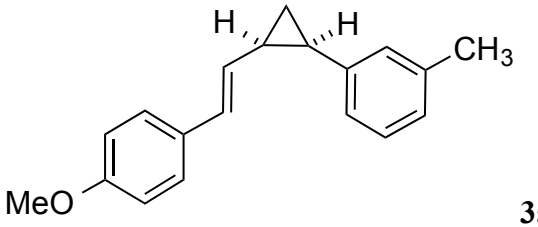

BHD-X-334_13C.10.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin bherle 43
153.71
132.99
131.42
129.66
126.61
125.18
121.18
57.02
32.95
f1 (ppm)



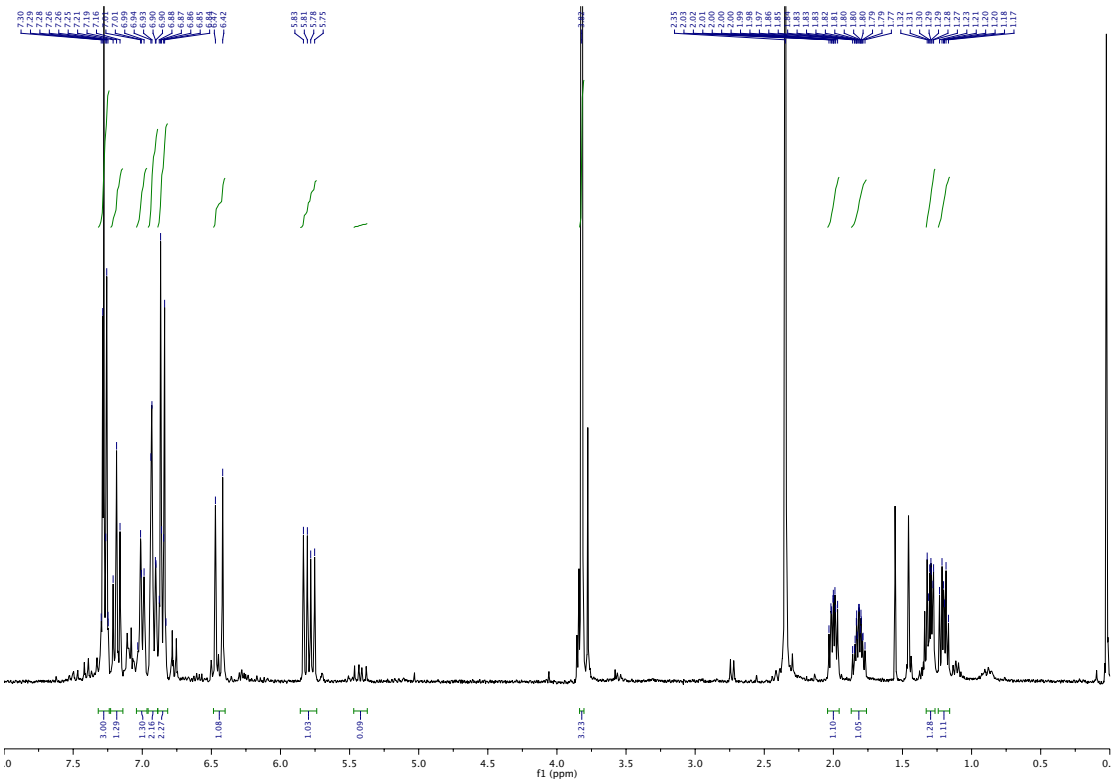
4b

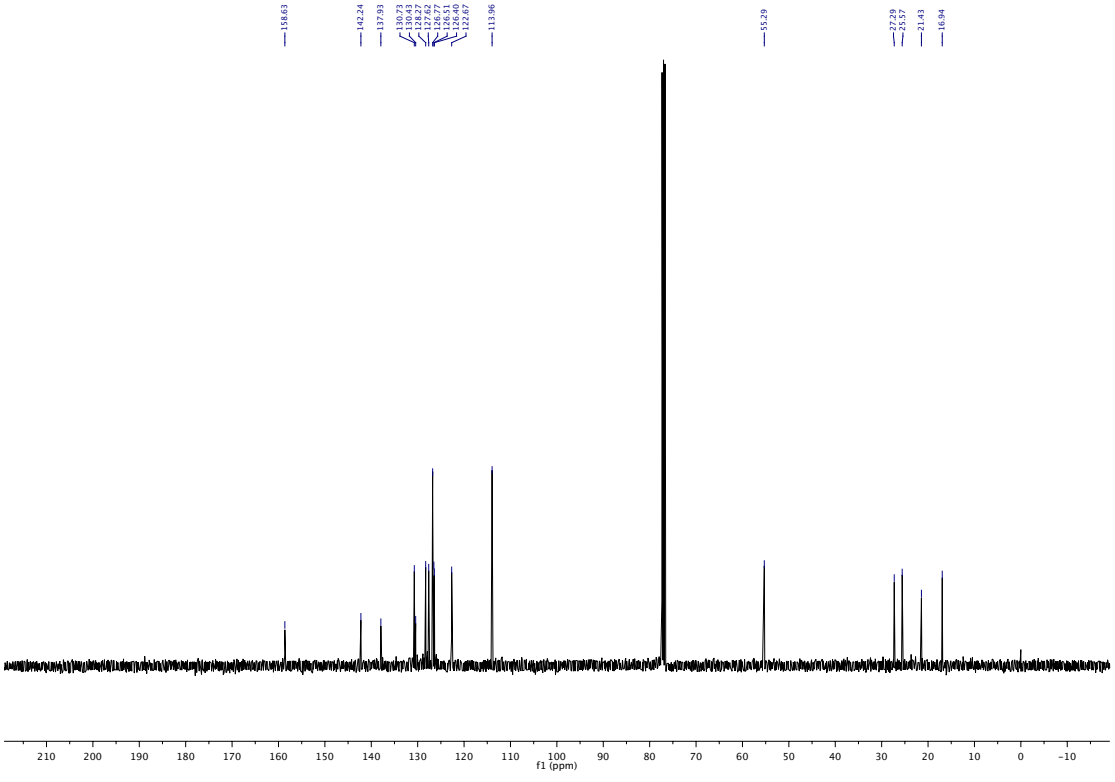

BHE-X-358_1H.10.fid
ResearchGroup Echavarren
ICIQ_1H20p8s CDCl3 /opt/topspin bberle 52
f1 (ppm)

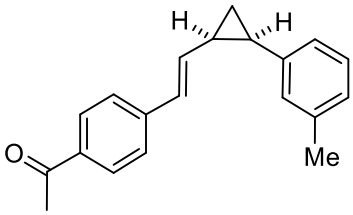

154.34
131.41
126.32
121.56
65.53
57.98
33.15
29.68
f1 (ppm)



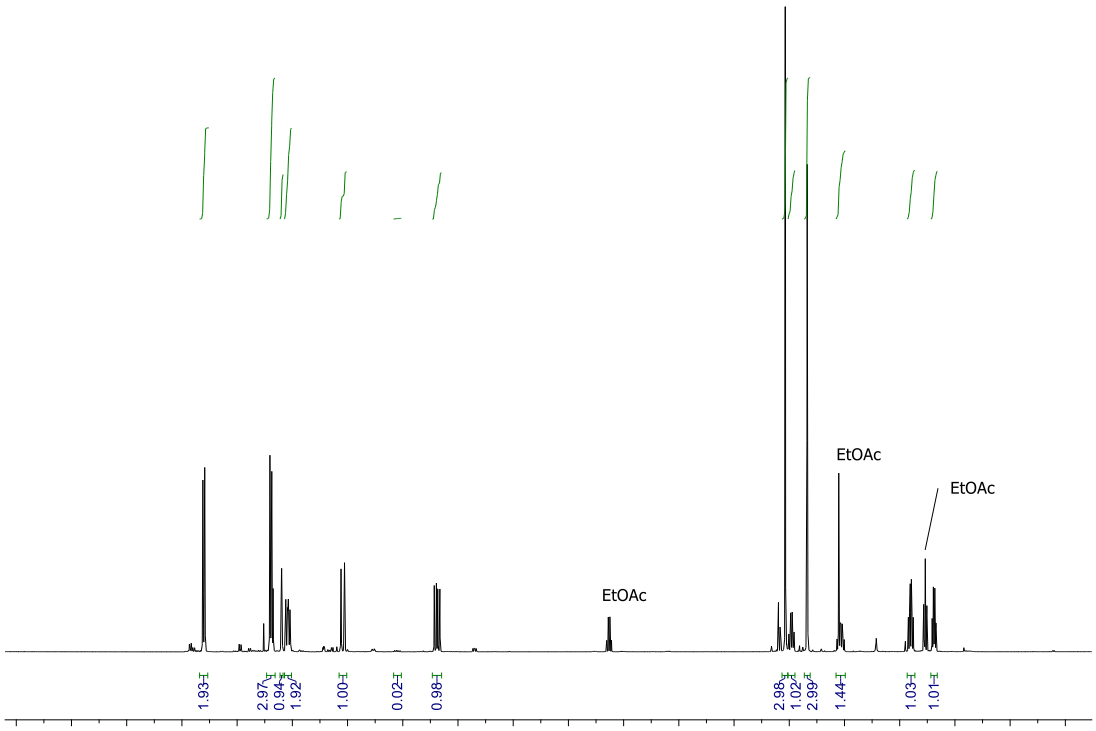
3ad

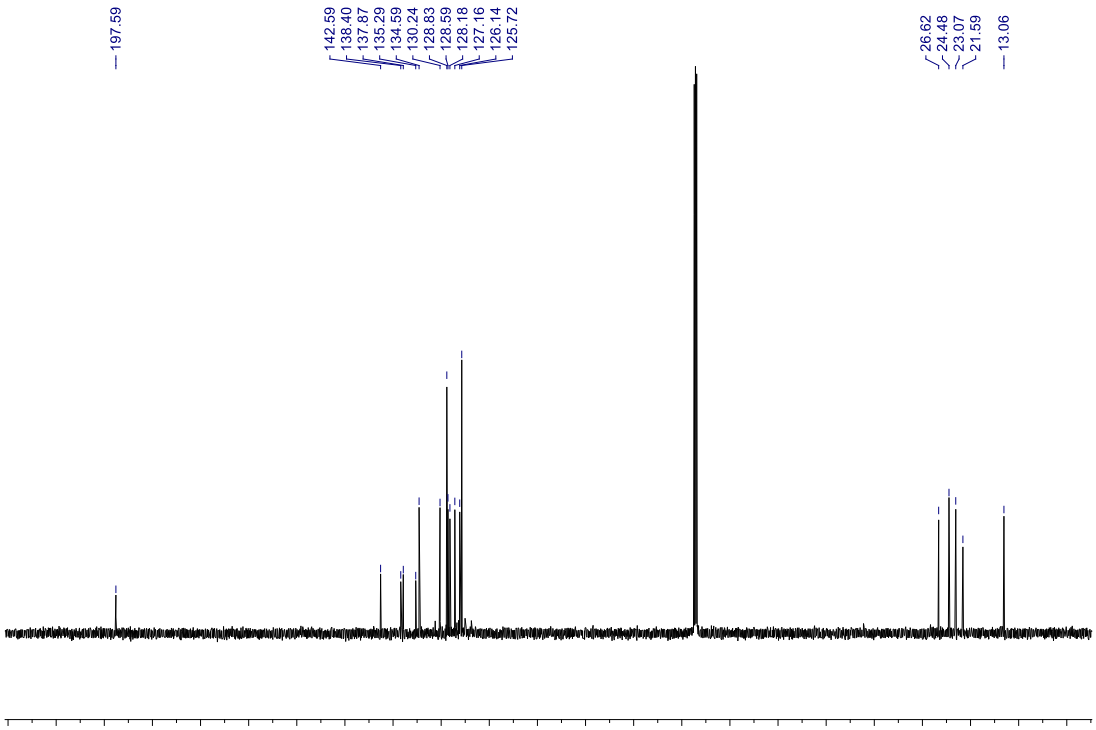


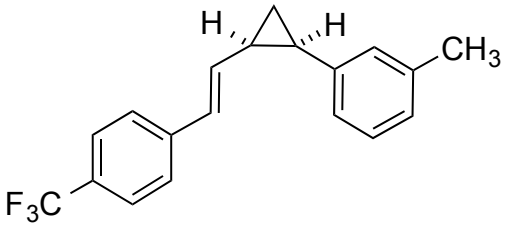



H
H
O
Me

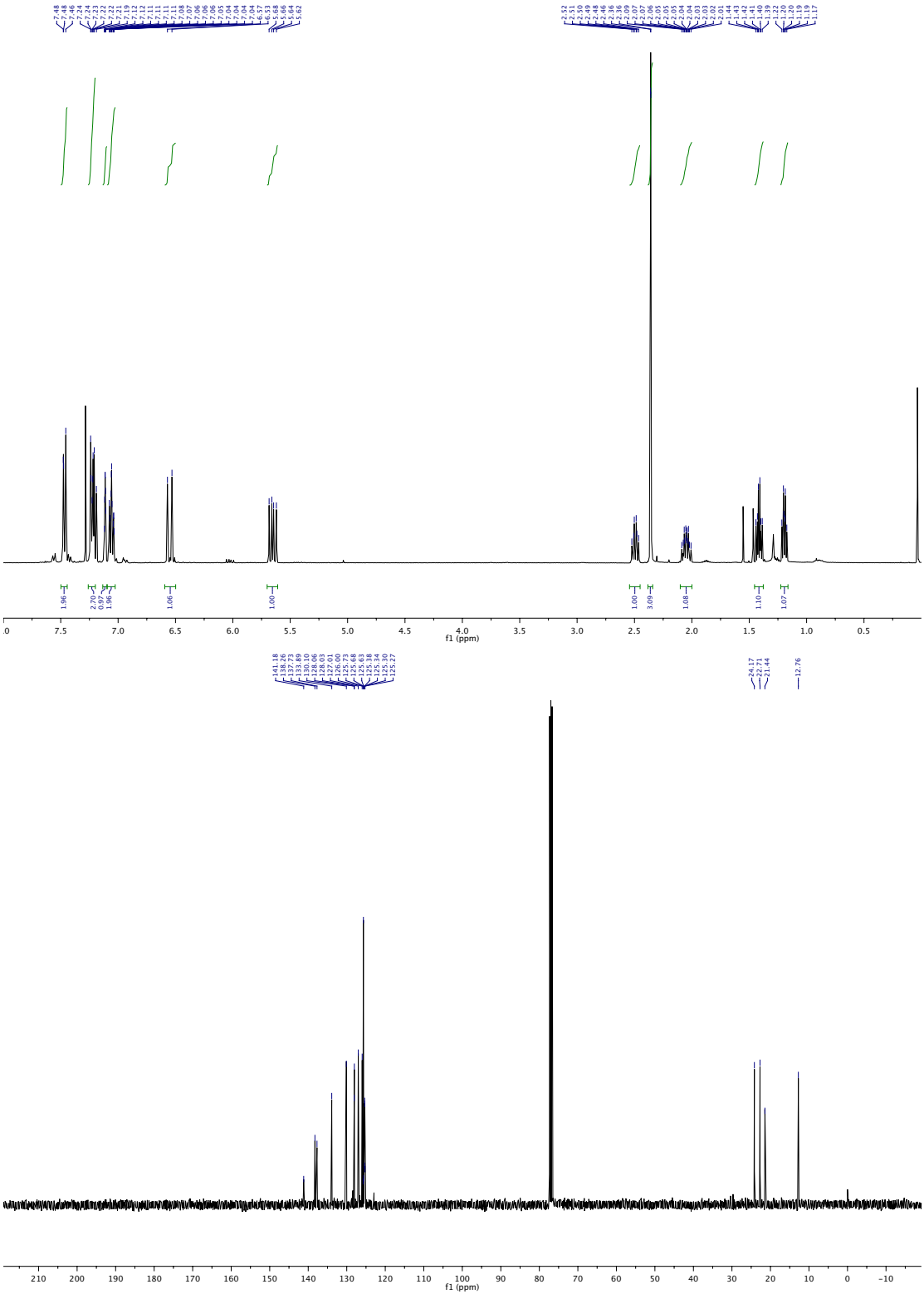
3ae

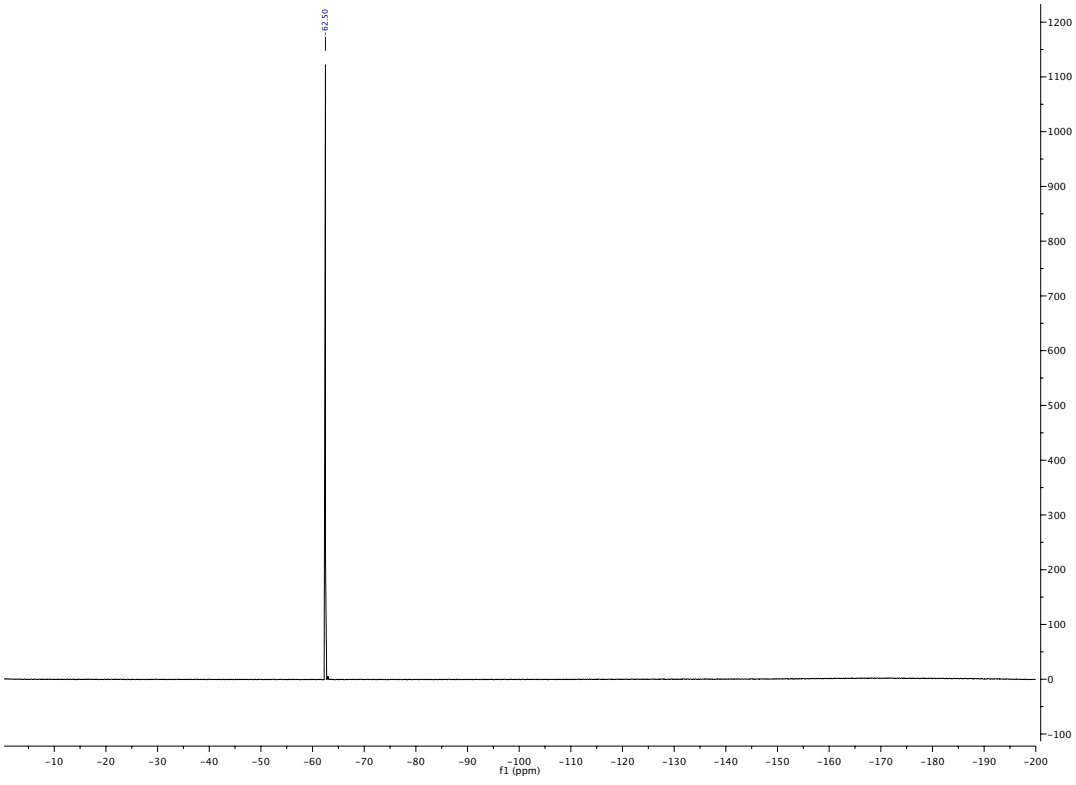

EtOAc
EtOAc
EtOAc
1.93
2.97
0.94
1.92
1.00
0.02
0.98
2.98
1.02
2.99
1.44
1.03
1.01

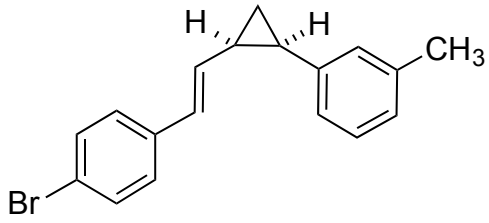

197.59
142.59
138.40
137.87
135.29
134.59
130.24
128.83
128.59
128.18
127.16
126.14
125.72
26.62
24.48
23.07
21.59
13.06



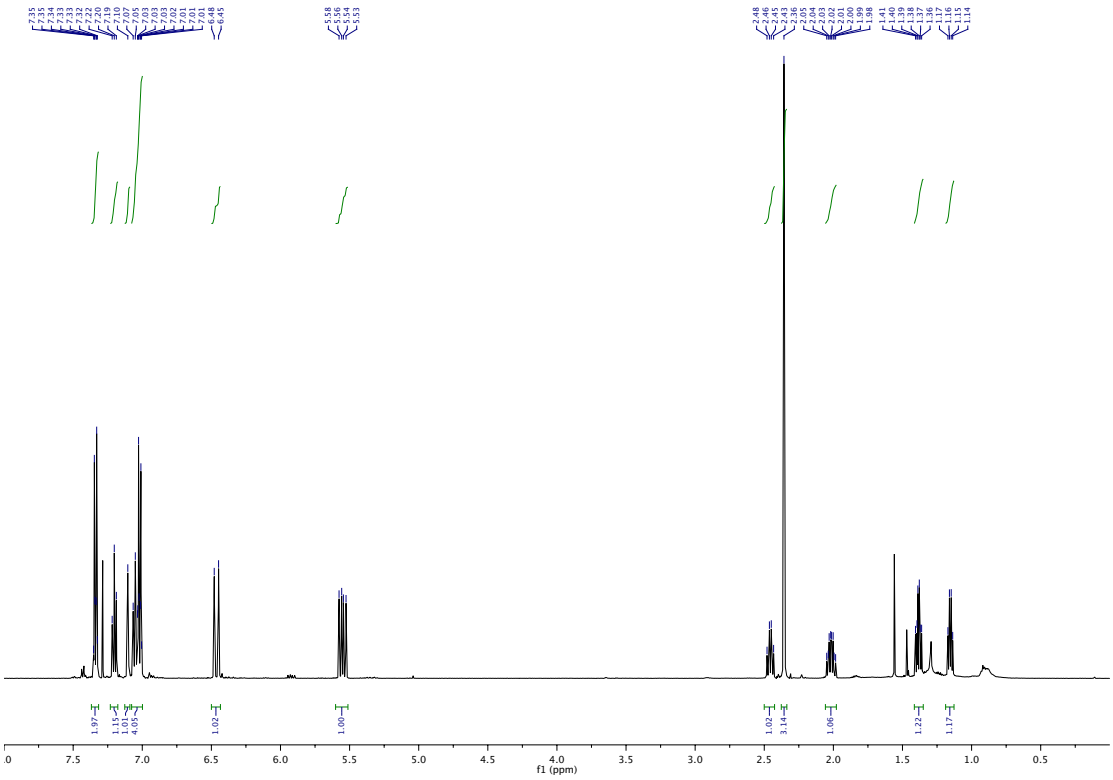
3af

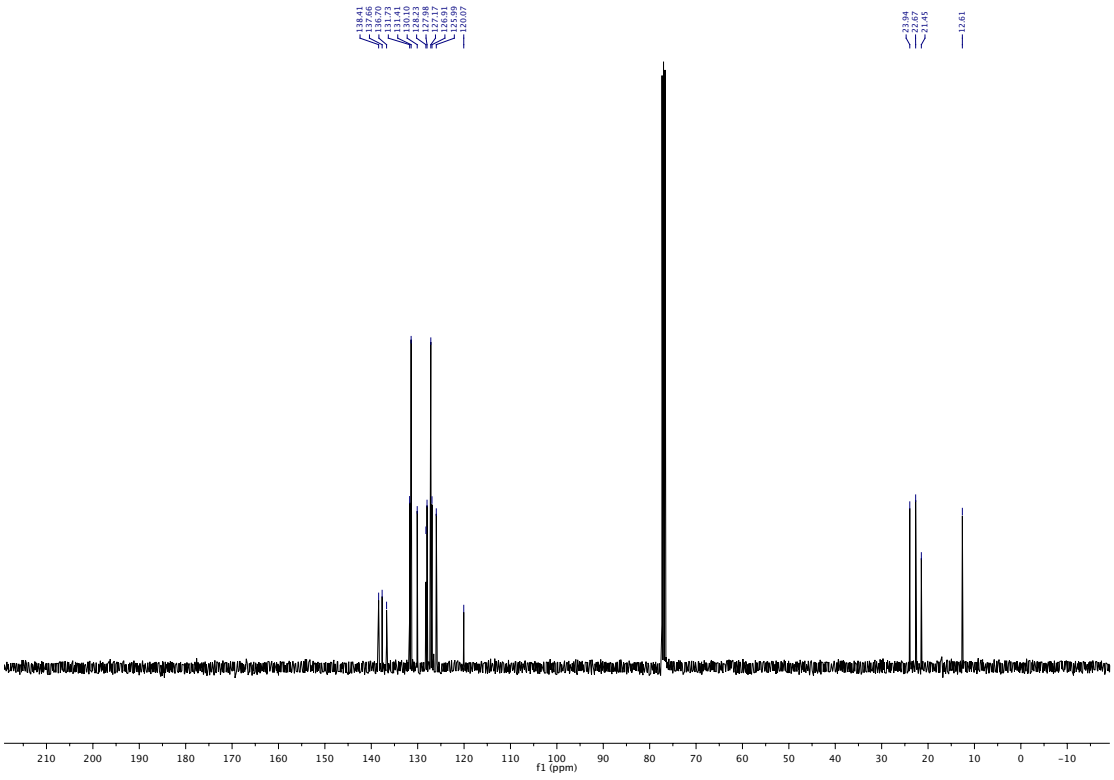


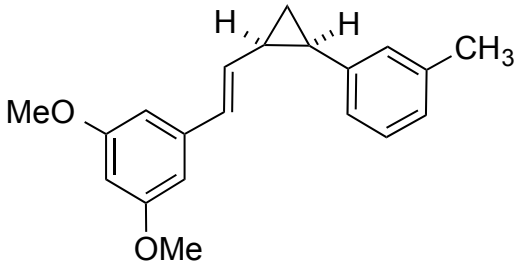

-62.50
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)



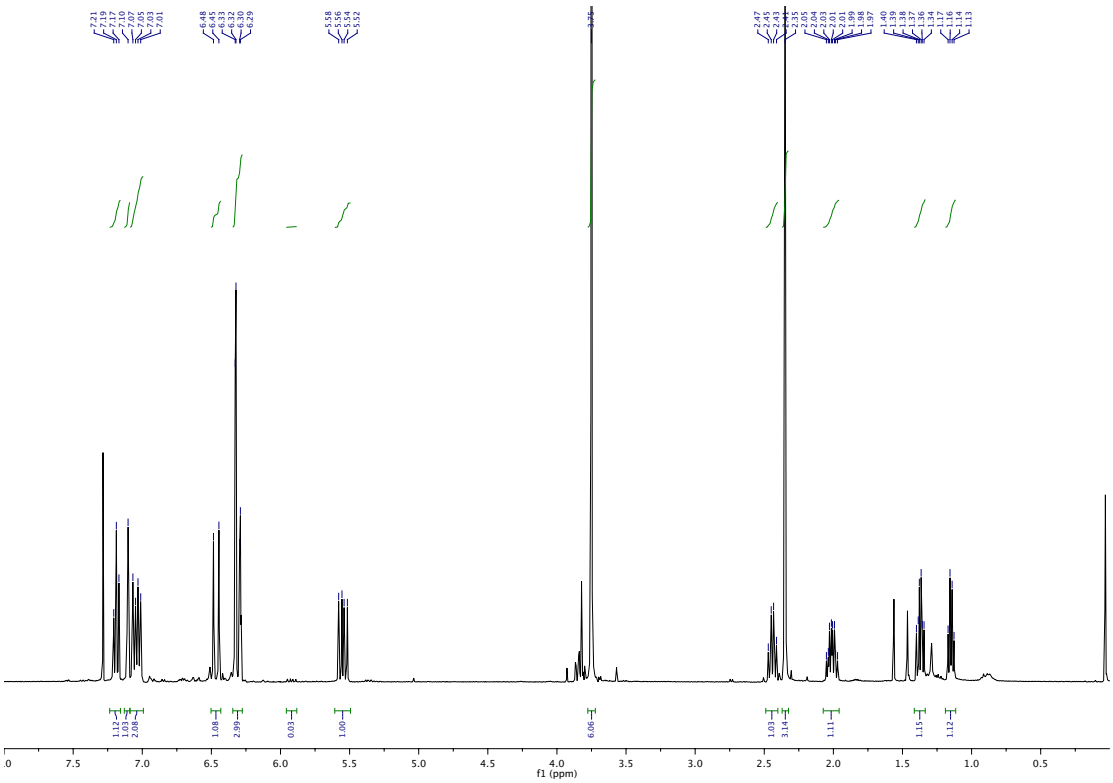
3ag

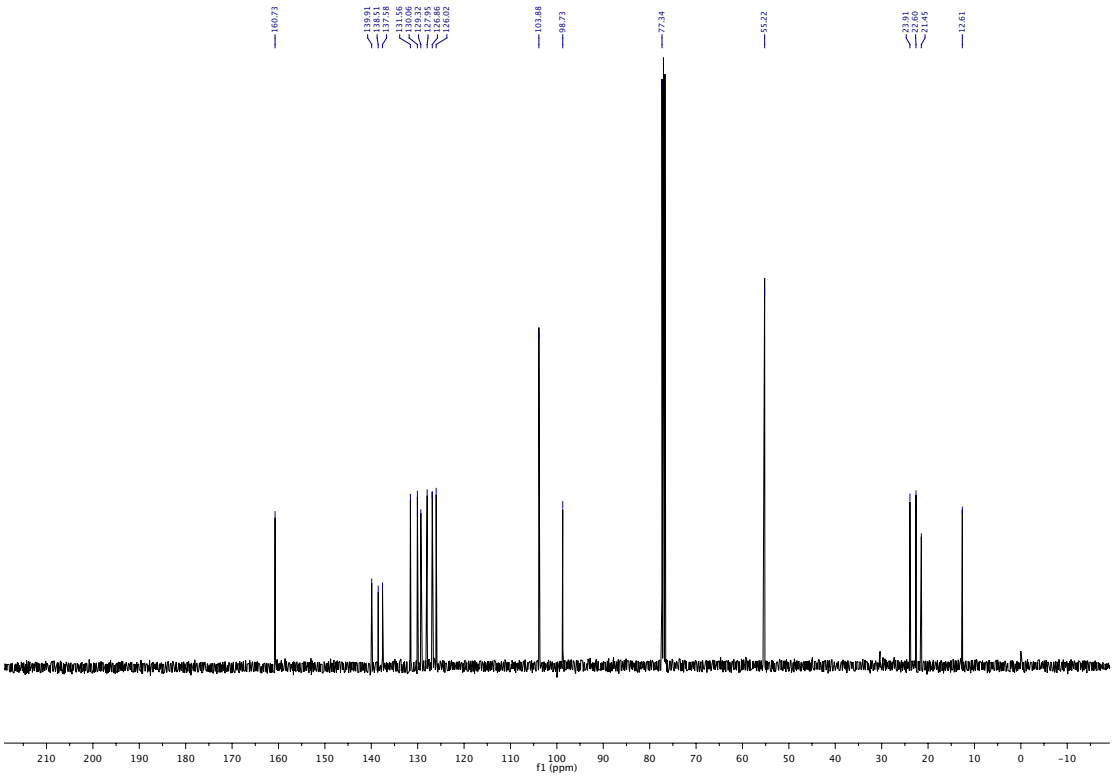


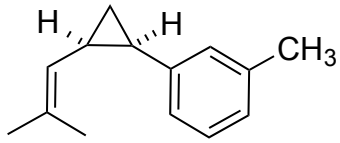




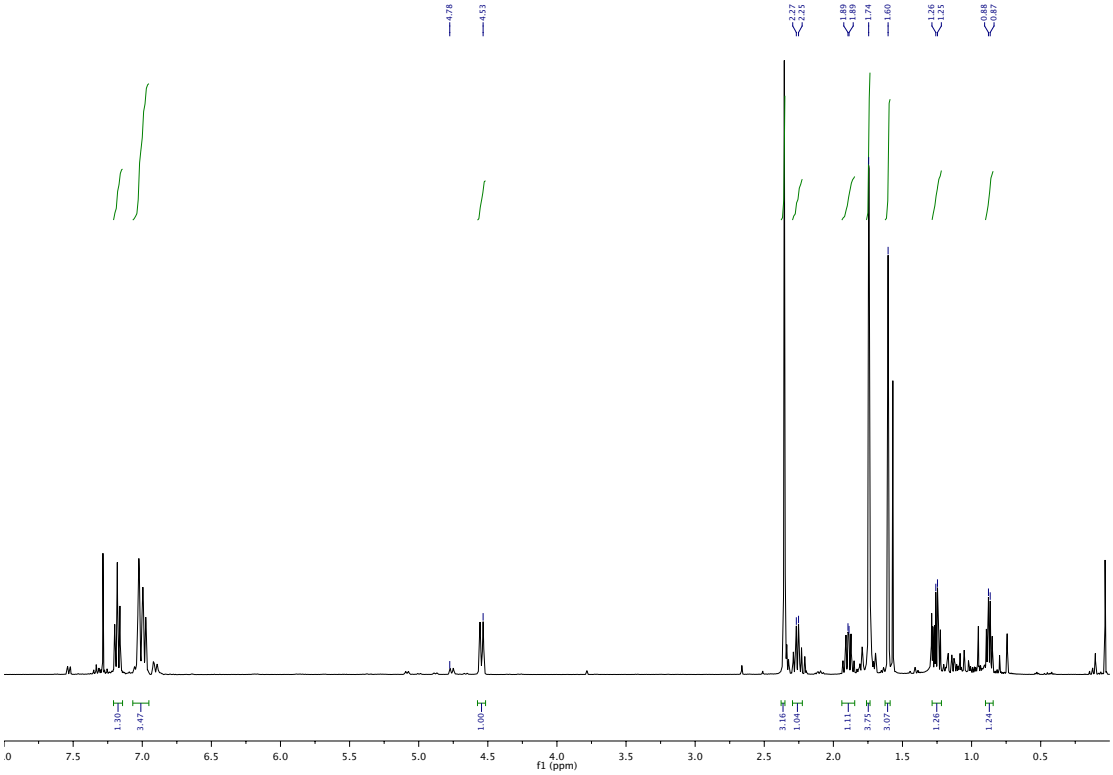
3ah

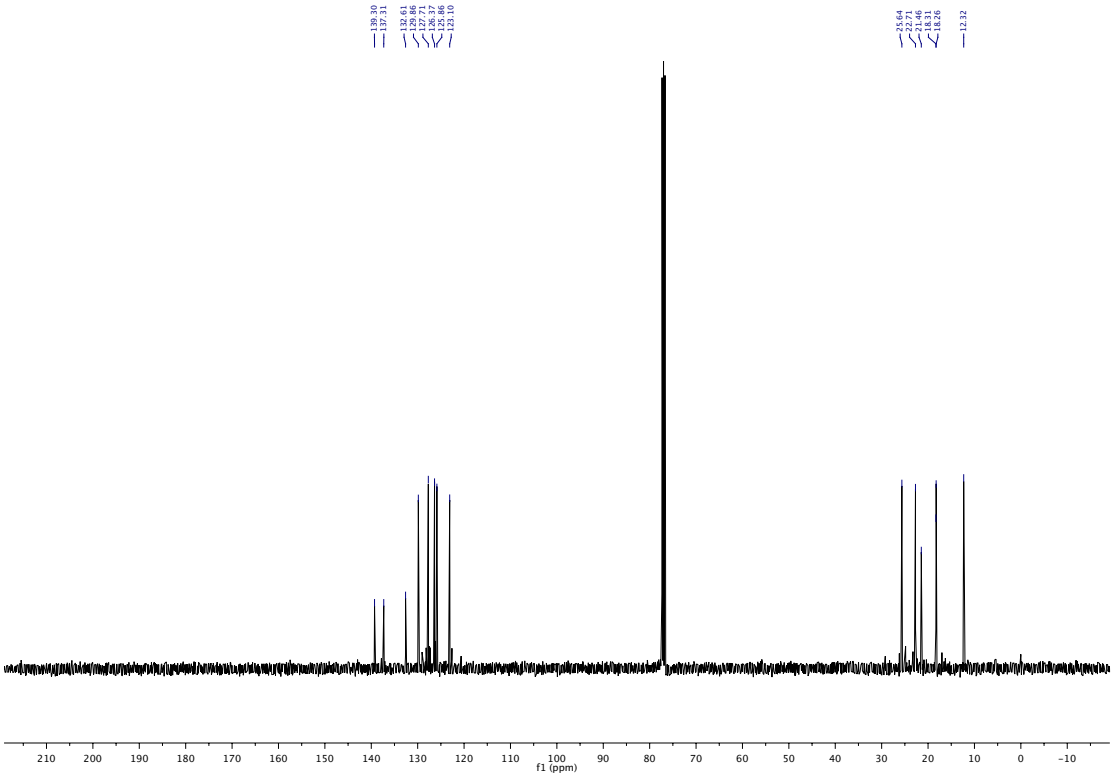


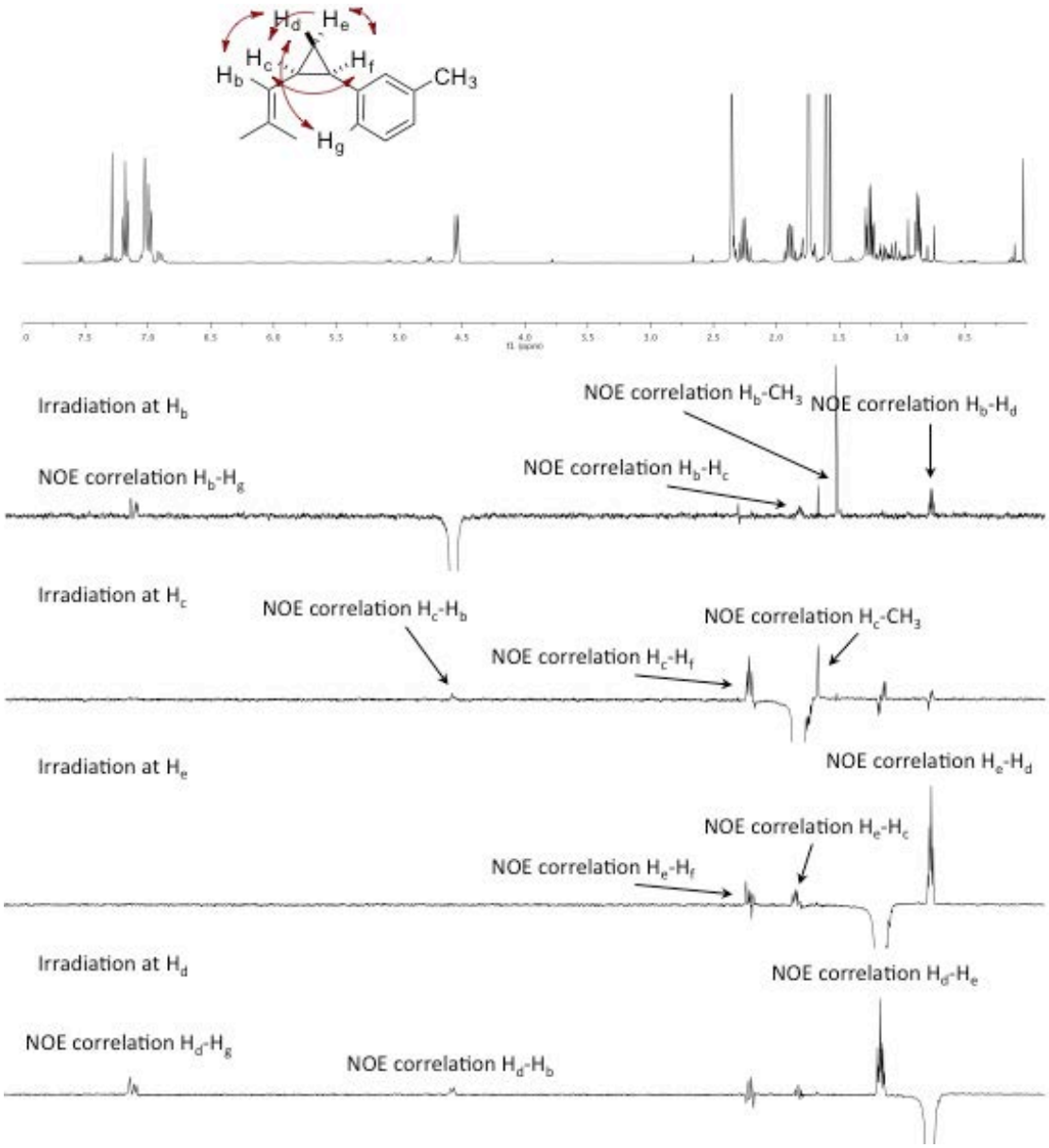


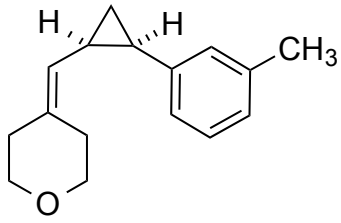

H
H
CH3

3ai

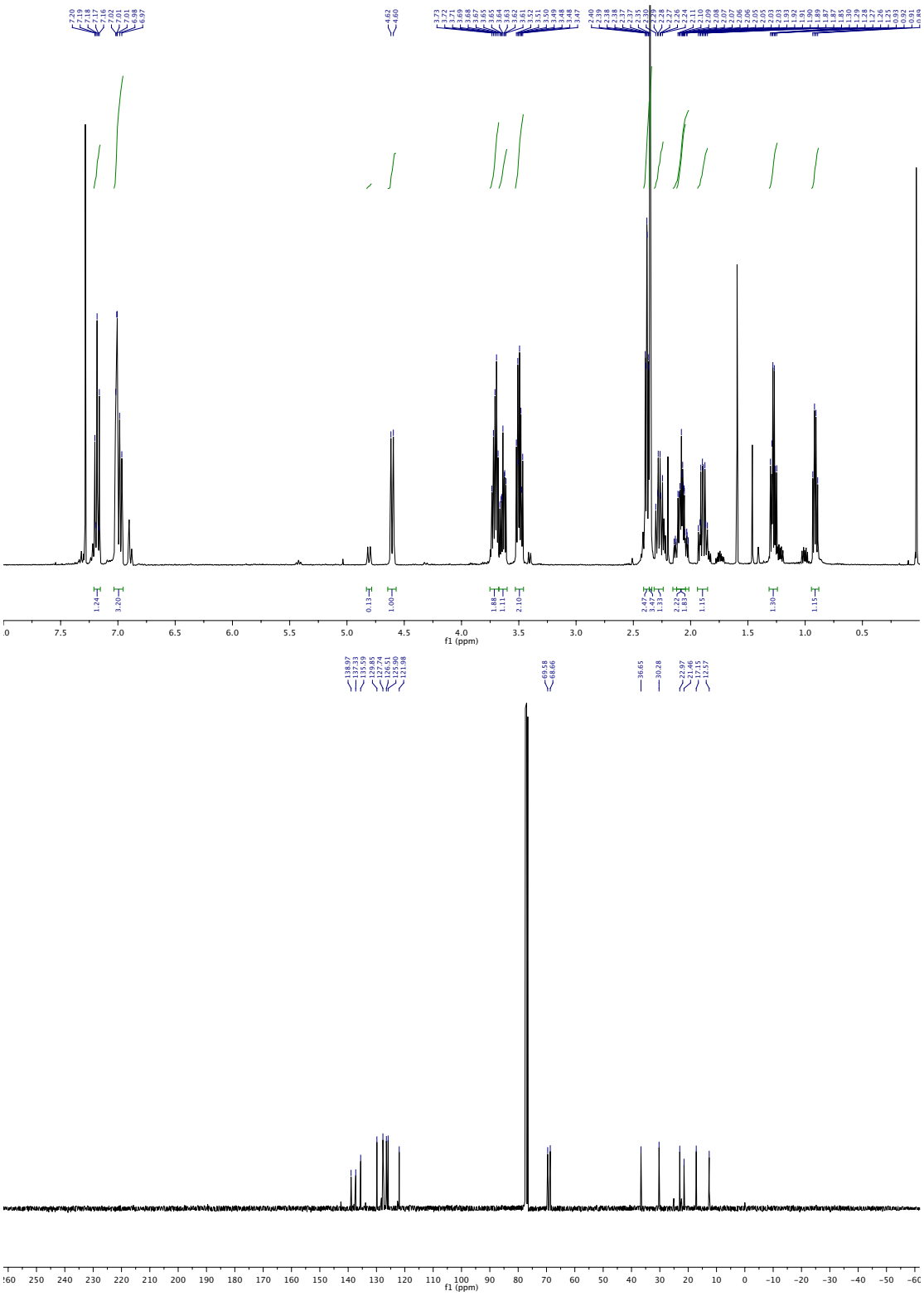

4.78
4.53
2.27
2.25
1.89
1.89
1.74
1.60
1.26
1.25
0.88
0.87
1.30
3.47
1.00
3.16
1.04
1.11
3.75
3.07
1.26
1.24
f1 (ppm)

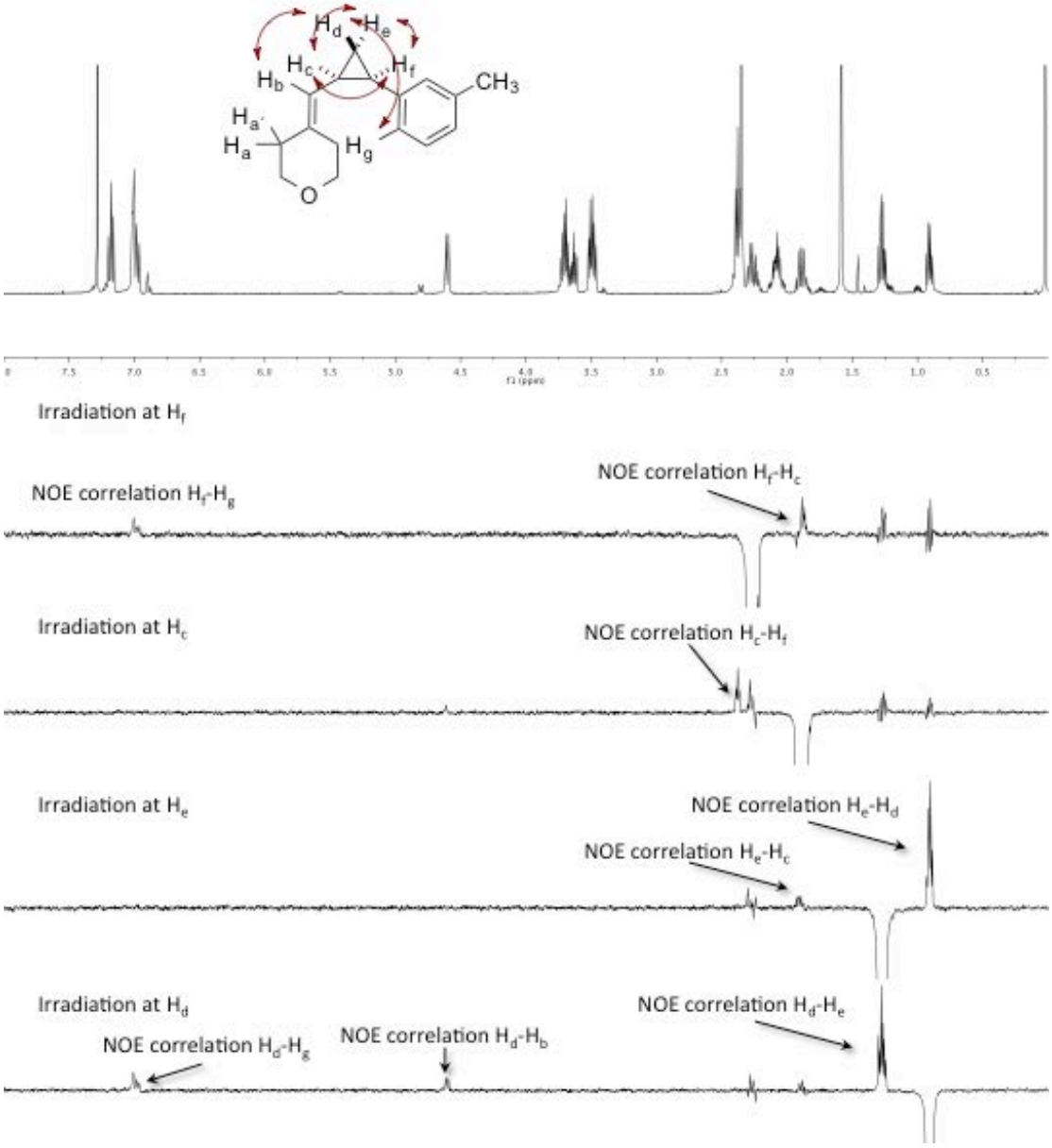

139.30
137.31
132.61
129.86
127.77
126.17
125.86
123.10
25.64
22.67
21.46
18.31
14.26
12.32
f1 (ppm)

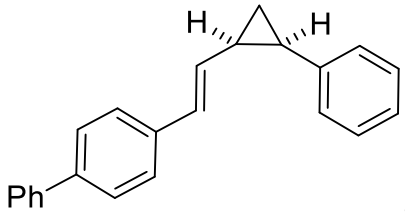

Hd
He
Hc
Hf
Hb
CH3
Hg
Irradiation at Hb
NOE correlation Hb-CH3
NOE correlation Hb-Hd
NOE correlation Hb-Hg
NOE correlation Hb-Hc
Irradiation at Hc
NOE correlation Hc-Hb
NOE correlation Hc-CH3
NOE correlation Hc-Hf
Irradiation at He
NOE correlation He-Hd
NOE correlation He-Hc
NOE correlation He-Hf
Irradiation at Hd
NOE correlation Hd-He
NOE correlation Hd-Hg
NOE correlation Hd-Hb



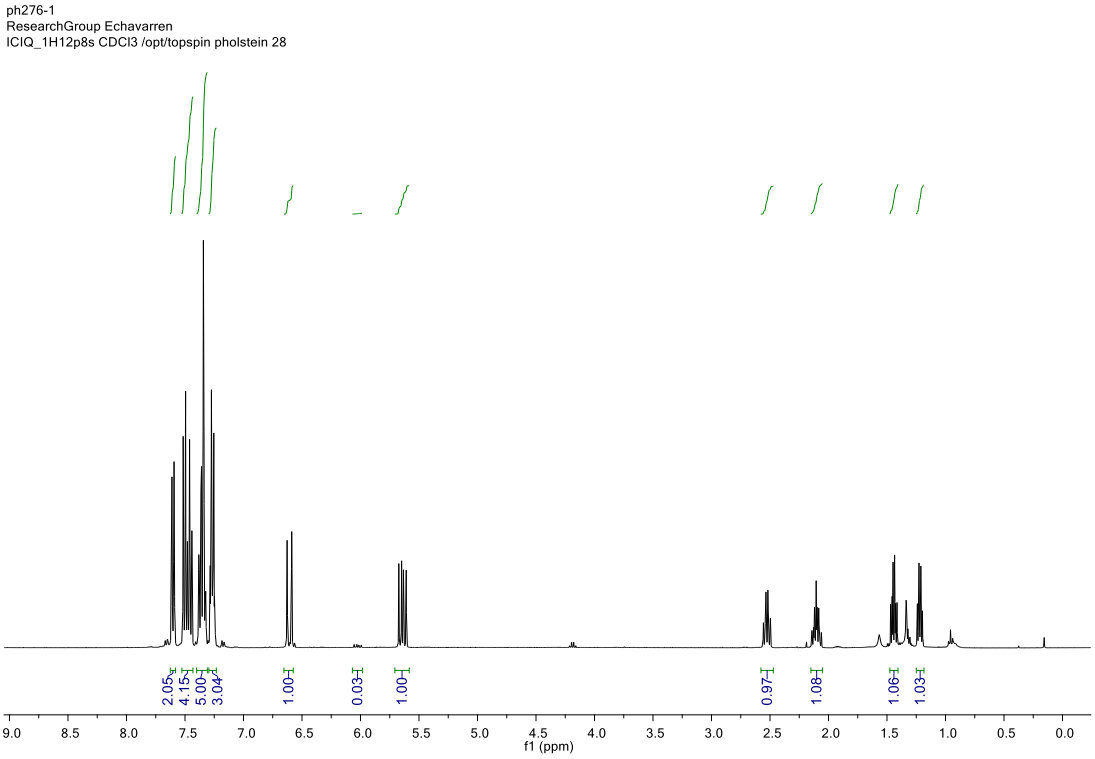
3aj

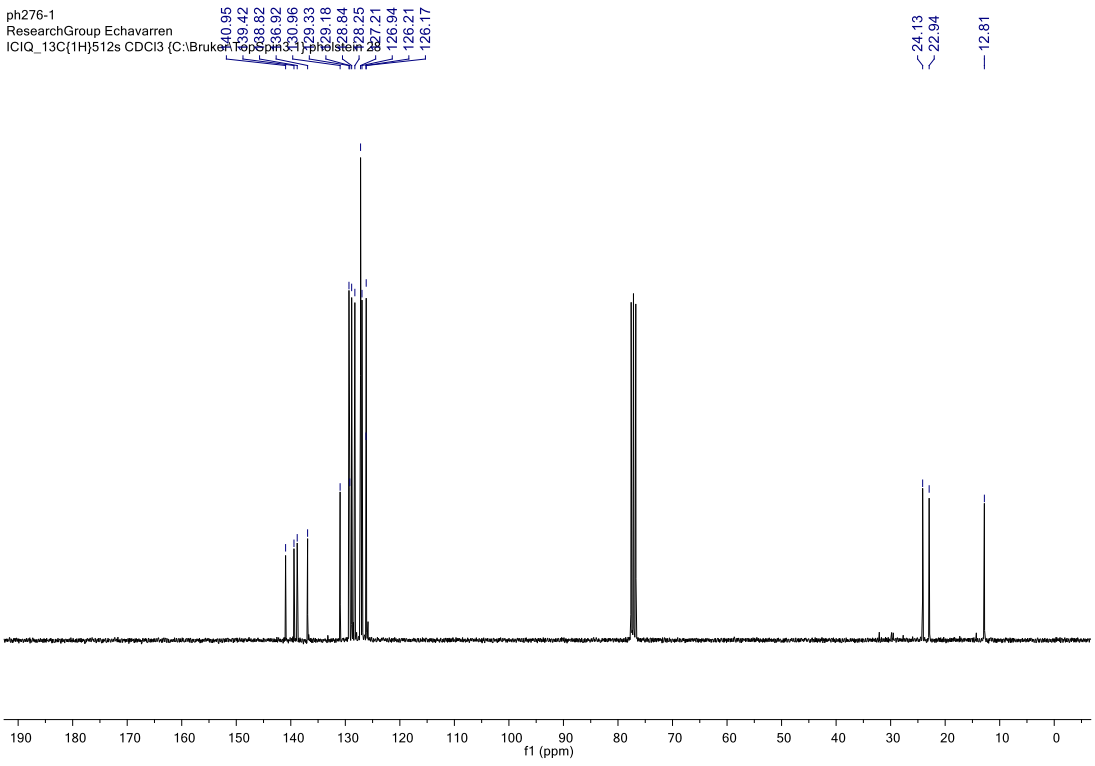


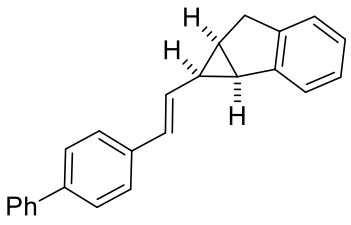

Hd
He
Hc
Hf
Hb
CH3
Ha'
Ha
Hg
O
Irradiation at Hf
NOE correlation Hf-Hg
NOE correlation Hf-Hc
Irradiation at Hc
NOE correlation Hc-Hf
Irradiation at He
NOE correlation He-Hd
NOE correlation He-Hc
Irradiation at Hd
NOE correlation Hd-Hg
NOE correlation Hd-Hb
NOE correlation Hd-He


H
H
Ph

3ak

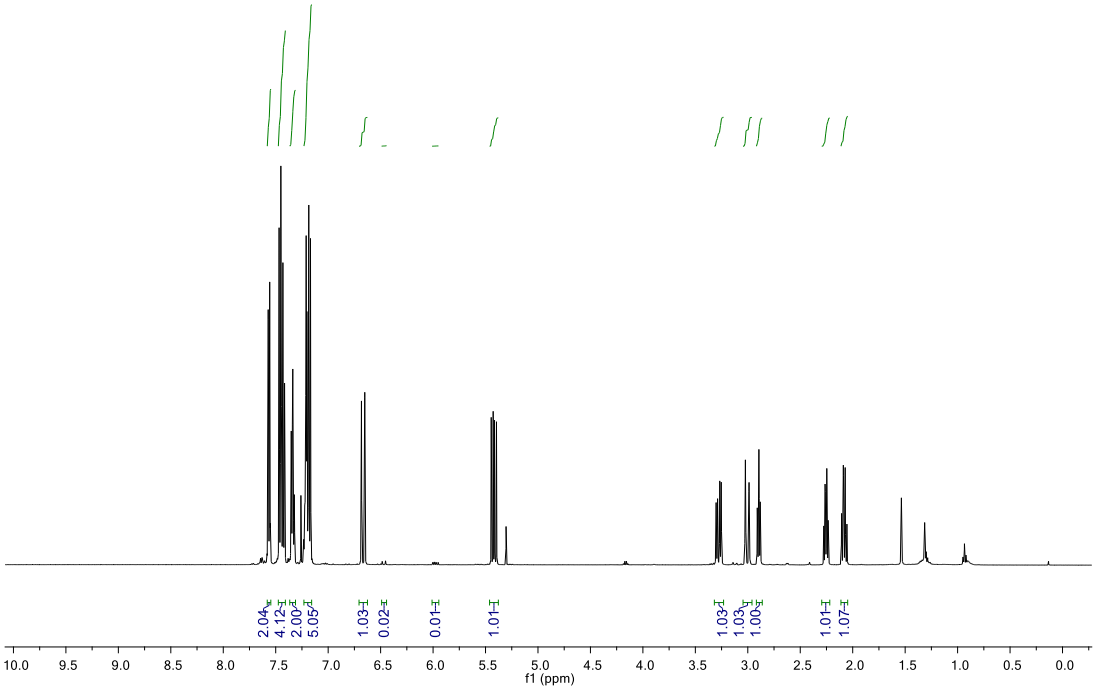

ph276-1
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 28
2.05
4.15
5.00
3.04
1.00
0.03
1.00
0.97
1.08
1.06
1.03
f1 (ppm)

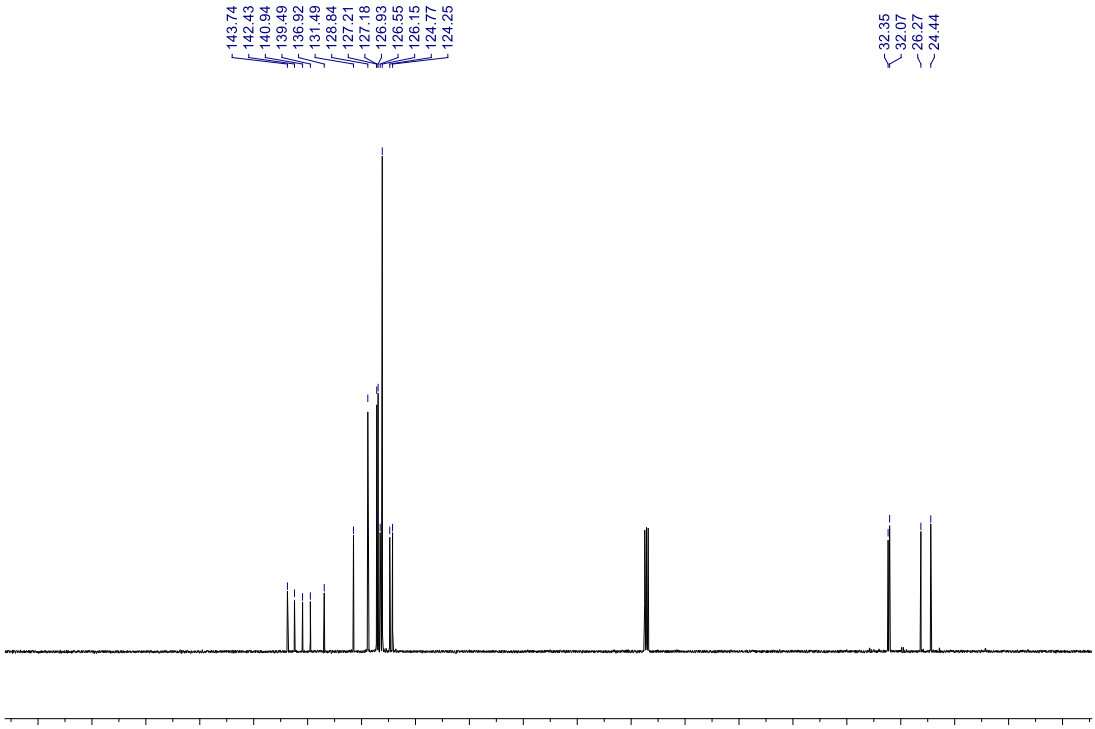

ph276-1
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1}-pholstein 28
140.95
139.42
138.82
136.92
130.96
129.33
129.18
128.84
128.25
127.21
126.94
126.21
126.17
24.13
22.94
12.81
f1 (ppm)

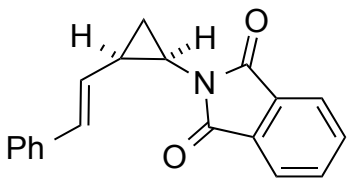


3al

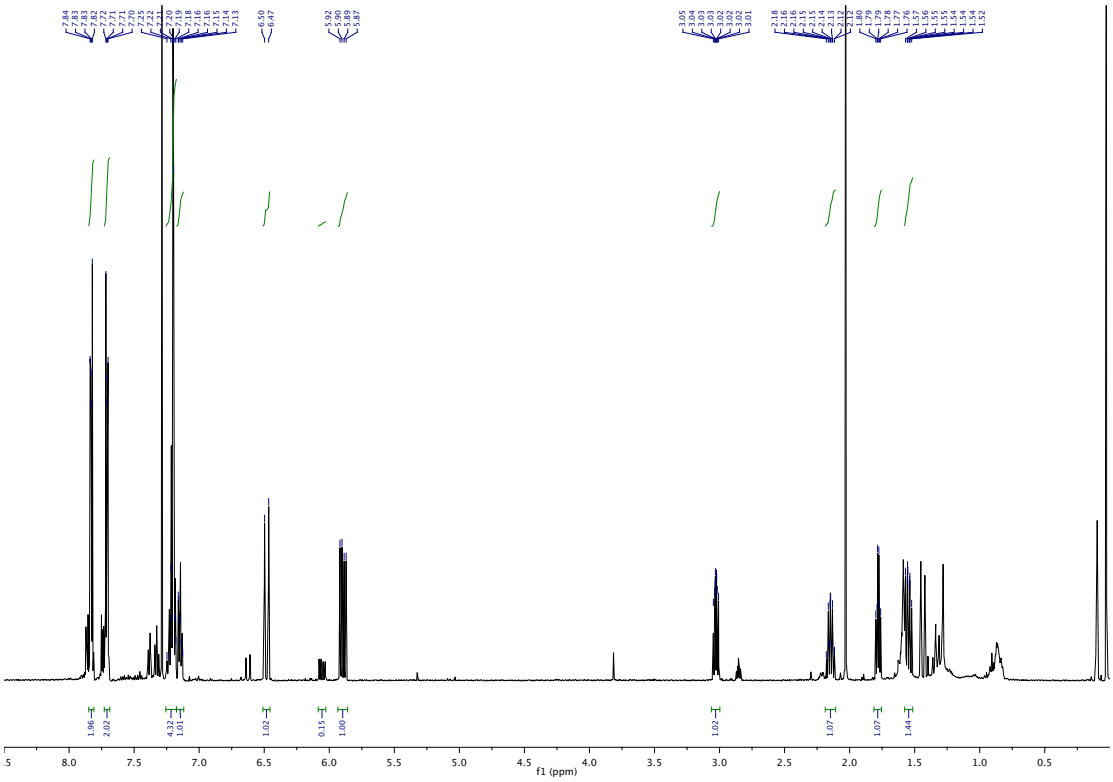
ph272-2
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin pholstein 30

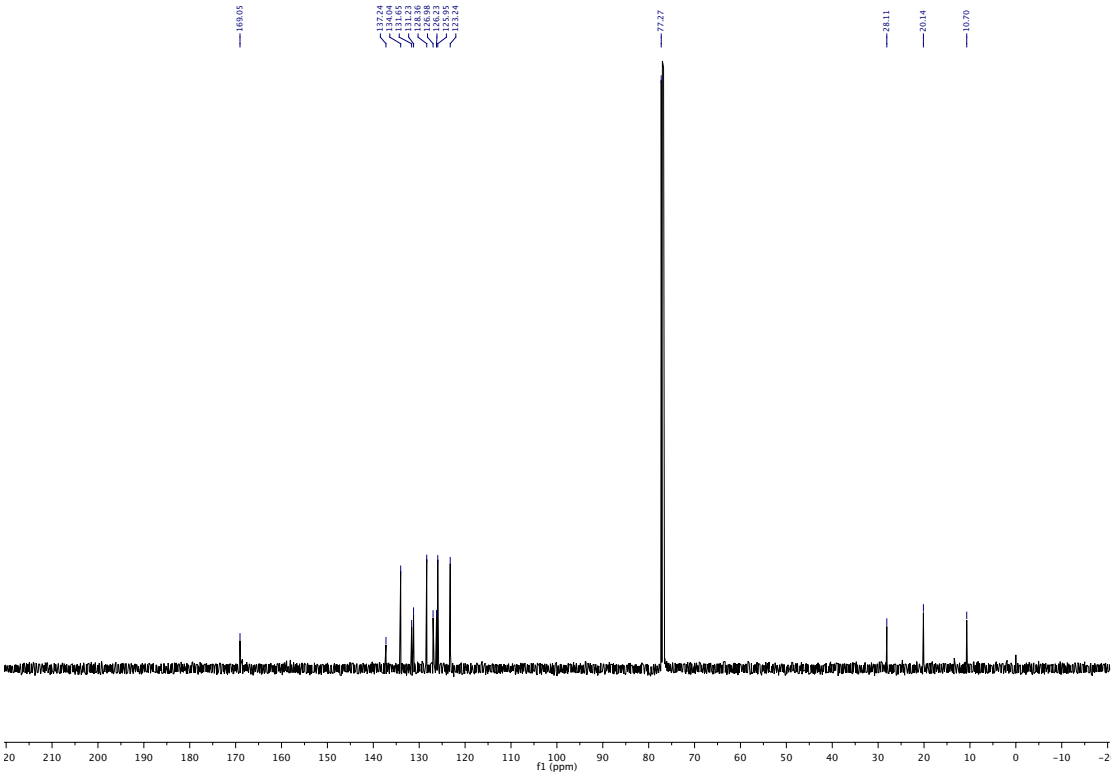


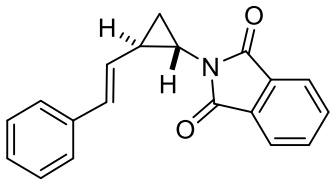




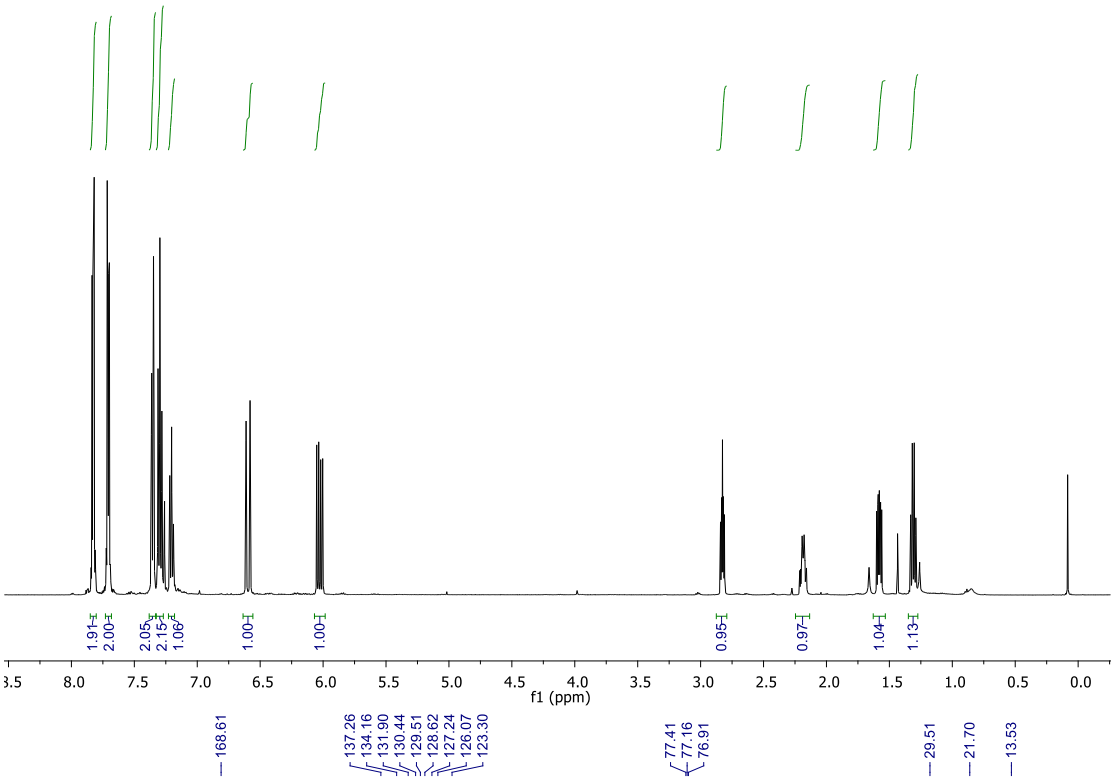
***cis*-6a**

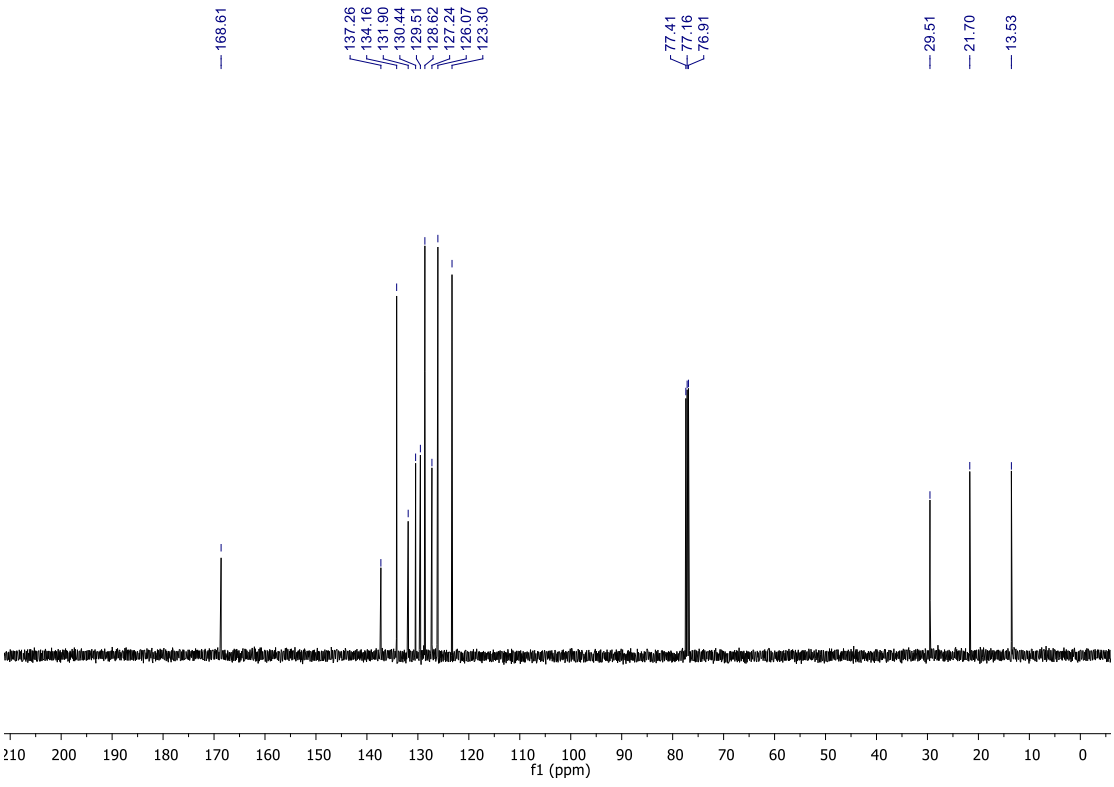


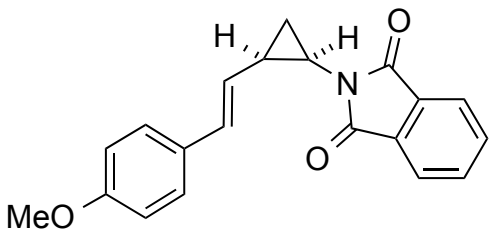



H
H
N
O
O

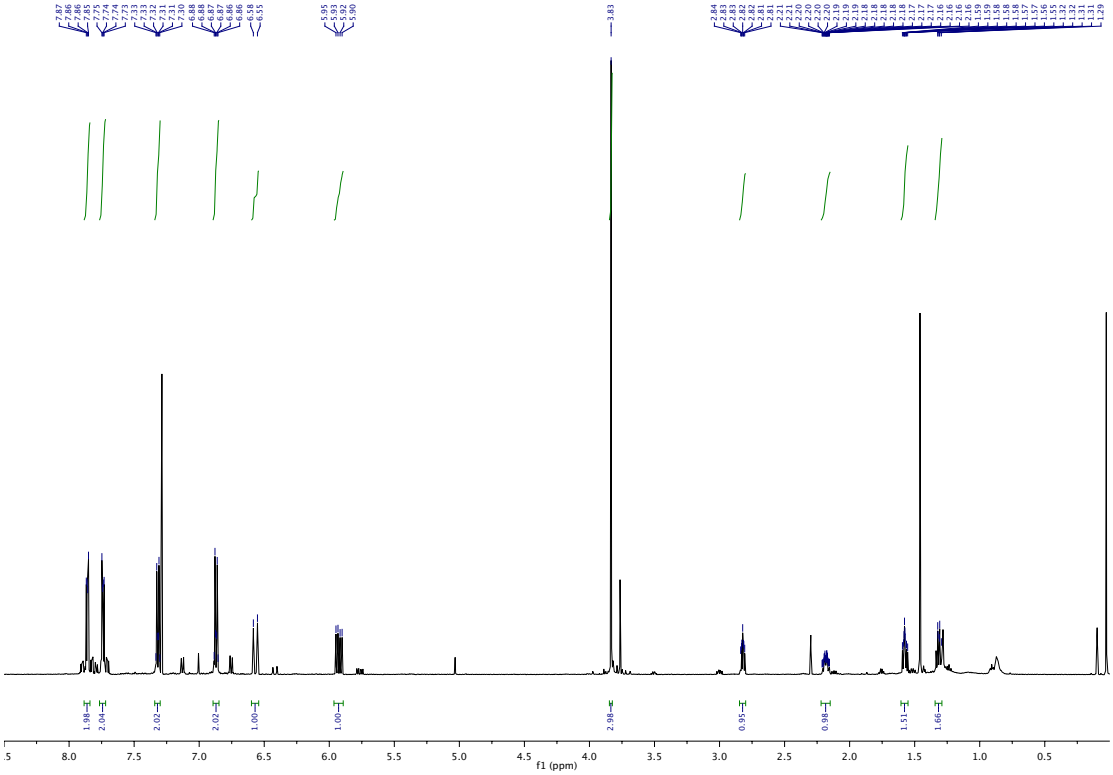
***trans*-6a**

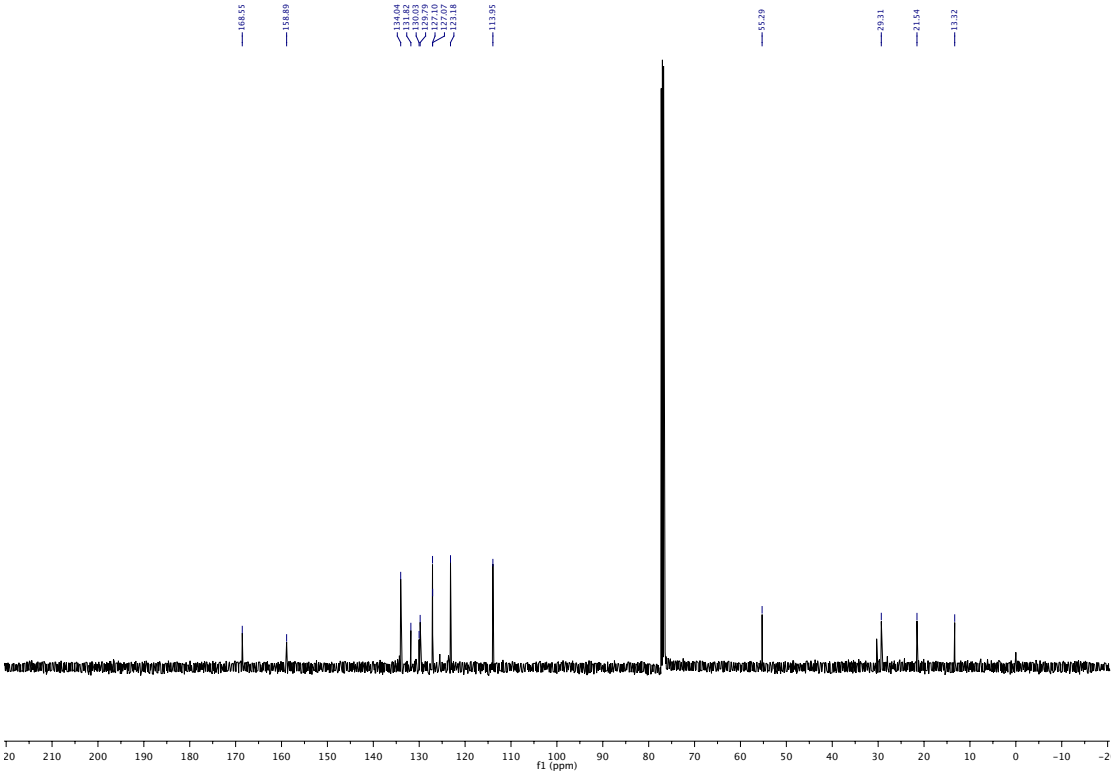

1.91
2.00
2.05
2.15
1.06
1.00
1.00
0.95
0.97
1.04
1.13
f1 (ppm)

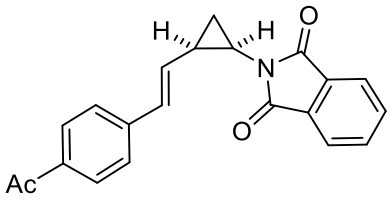

168.61
137.26
134.16
131.90
130.44
129.51
128.62
127.24
126.07
123.30
77.41
77.16
76.91
29.51
21.70
13.53
f1 (ppm)



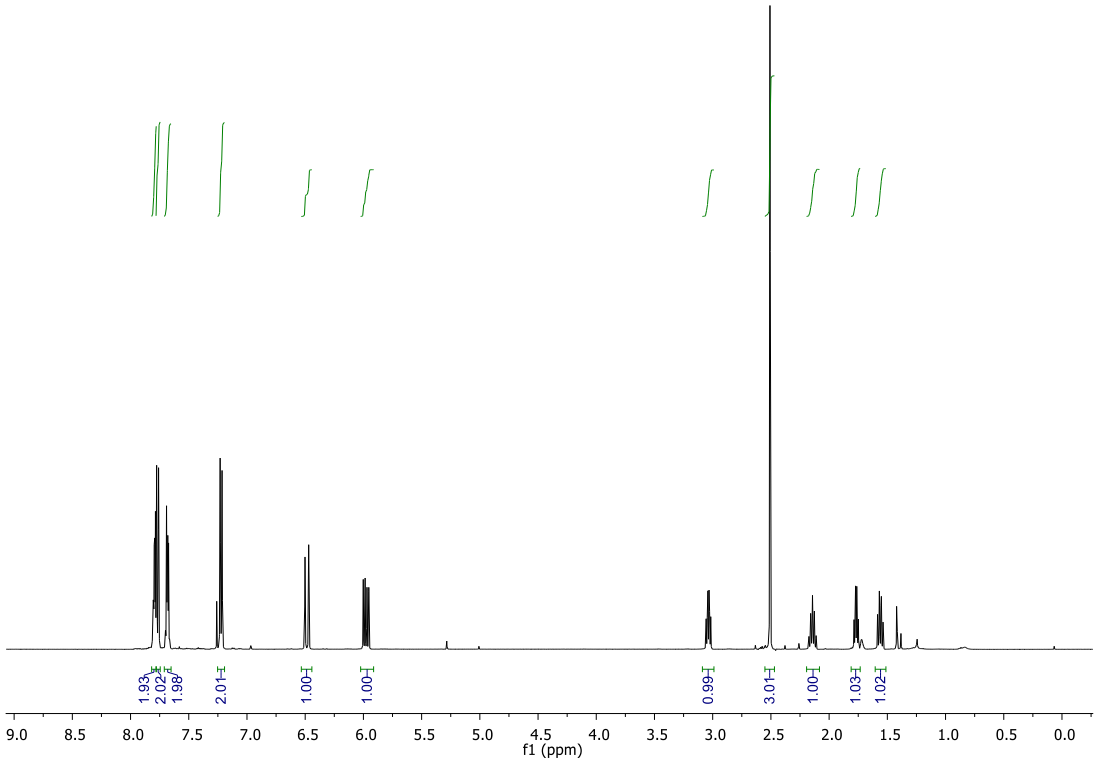
6b

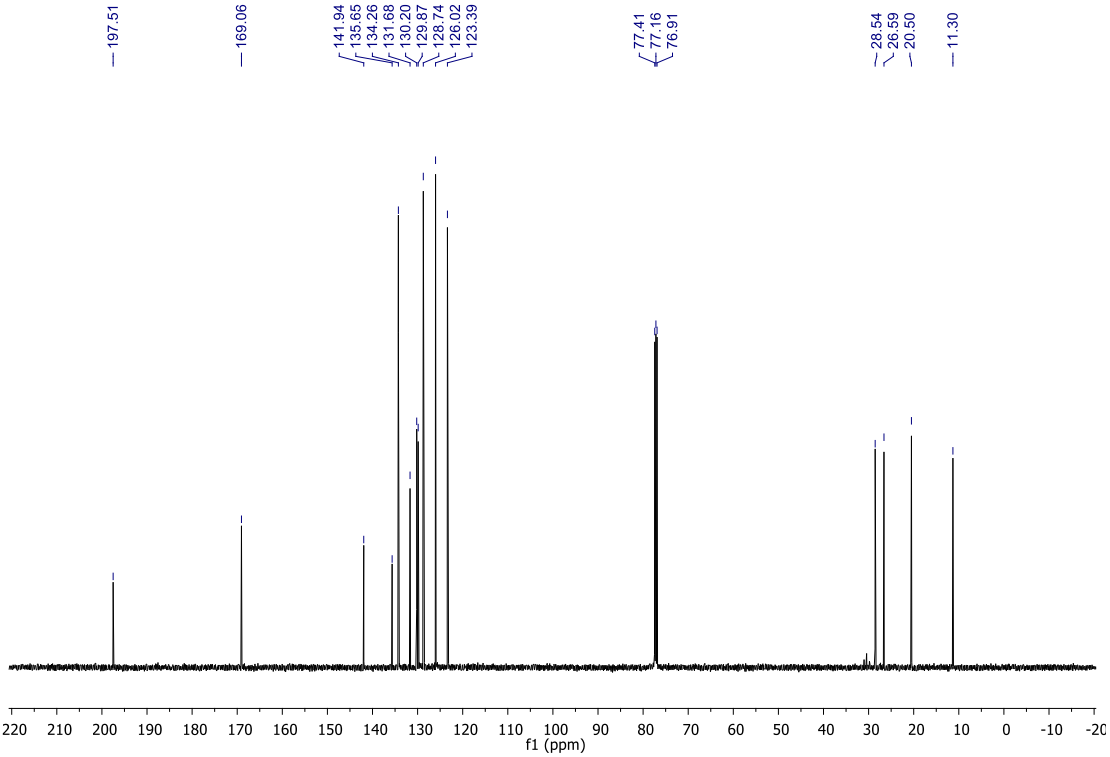


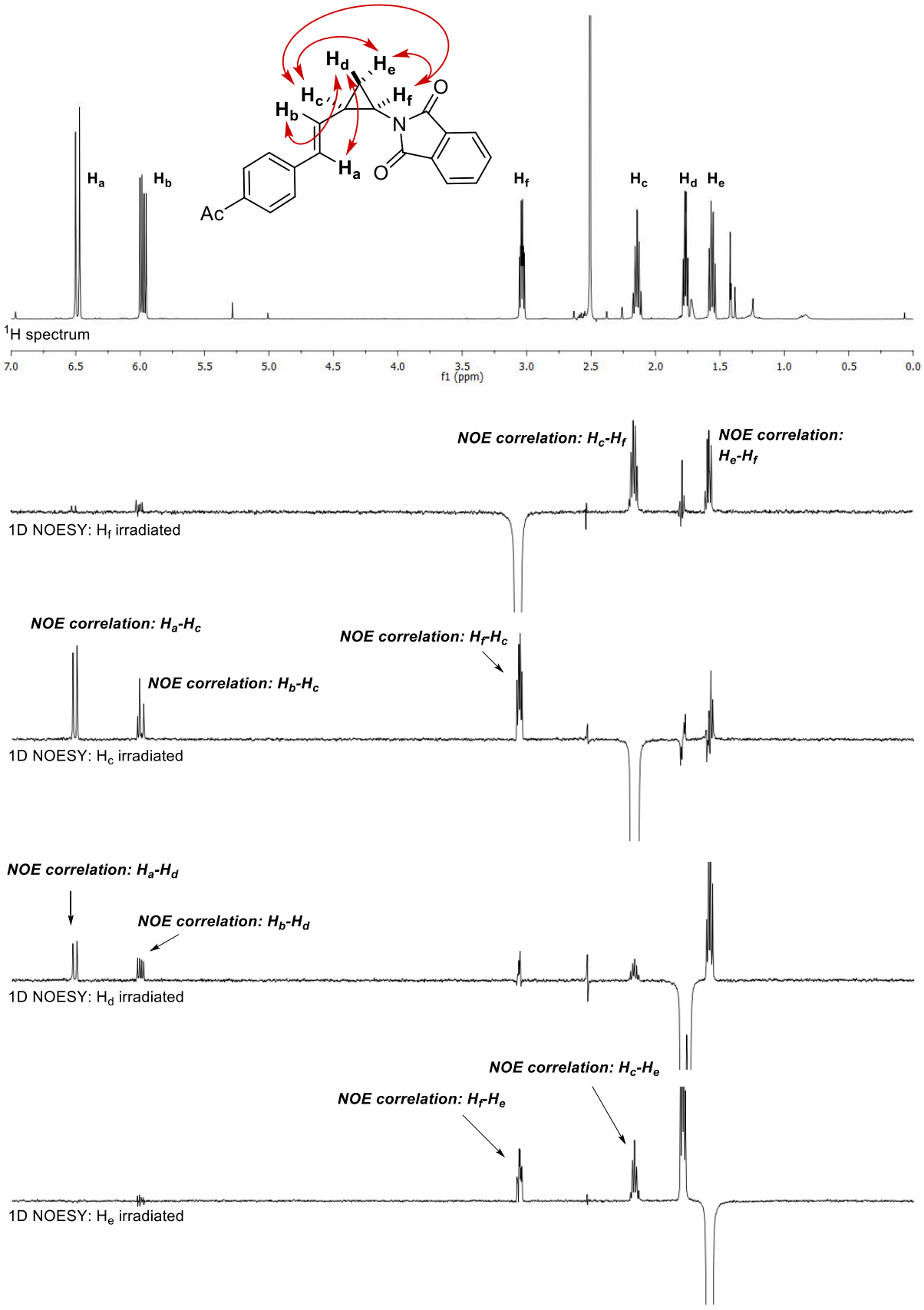


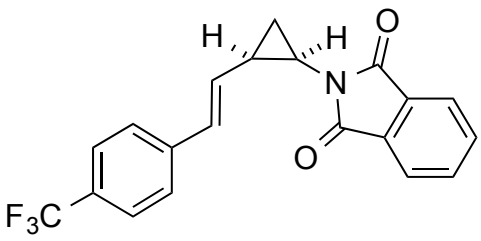

H
H
O
N
O
Ac

6c

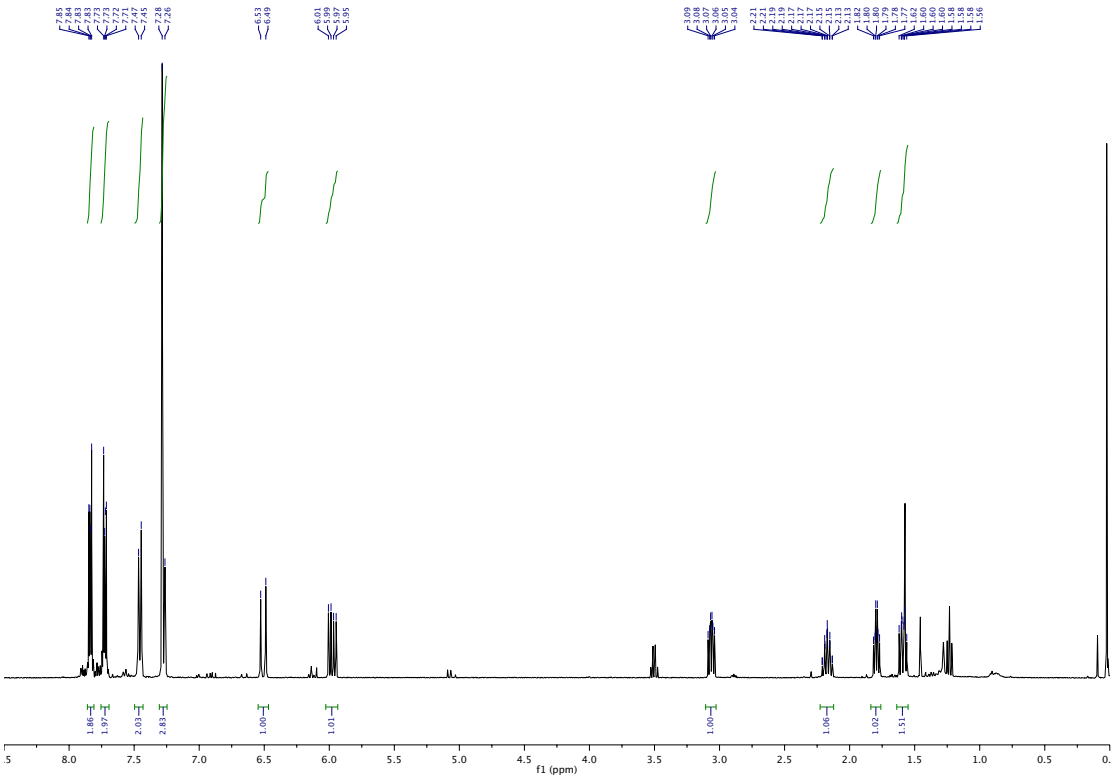

1.93
2.02
1.98
2.01
1.00
1.00
0.99
3.01
1.00
1.03
1.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

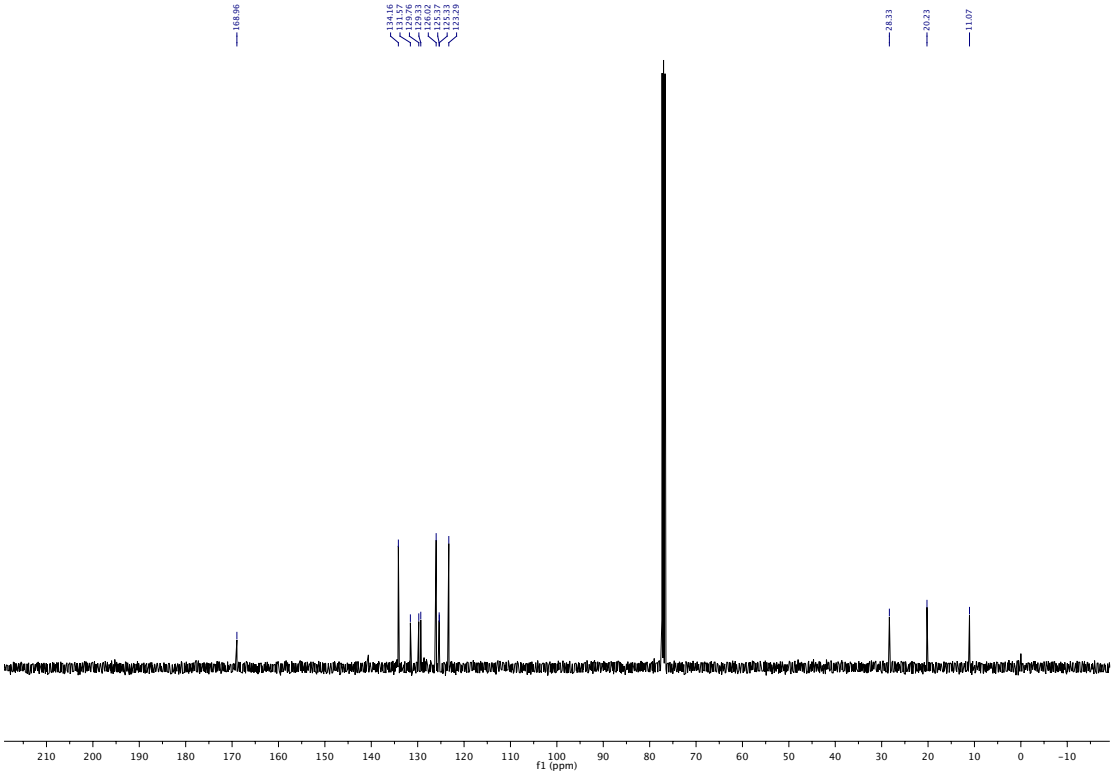

197.51
169.06
141.94
135.65
134.26
131.68
130.20
129.87
128.74
126.02
123.39
77.41
77.16
76.91
28.54
26.59
20.50
11.30
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

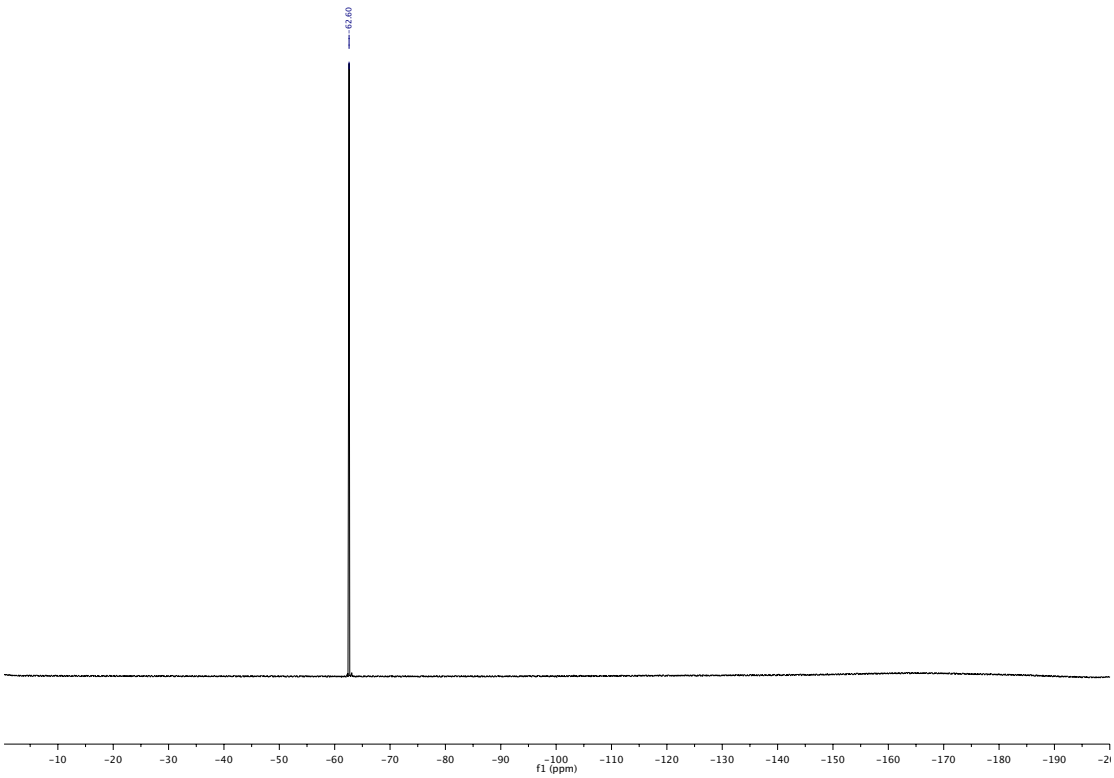

Hd
He
Hc
Hf
Hb
Ha
O
N
O
Ac
Ha
Hb
Hf
Hc
Hd
He
1H spectrum
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
NOE correlation: Hc-Hf
NOE correlation: He-Hf
1D NOESY: Hf irradiated
NOE correlation: Ha-Hc
NOE correlation: Hf-Hc
NOE correlation: Hb-Hc
1D NOESY: Hc irradiated
NOE correlation: Ha-Hd
NOE correlation: Hb-Hd
1D NOESY: Hd irradiated
NOE correlation: Hc-He
NOE correlation: Hf-He
1D NOESY: He irradiated

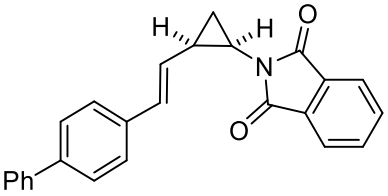


6d

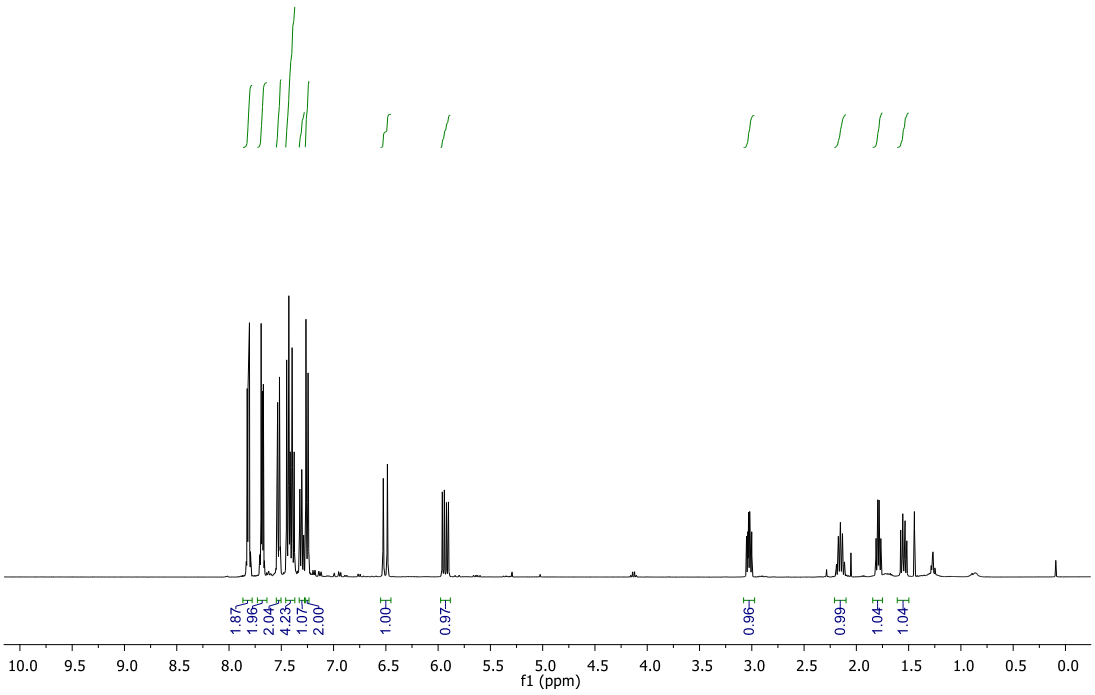


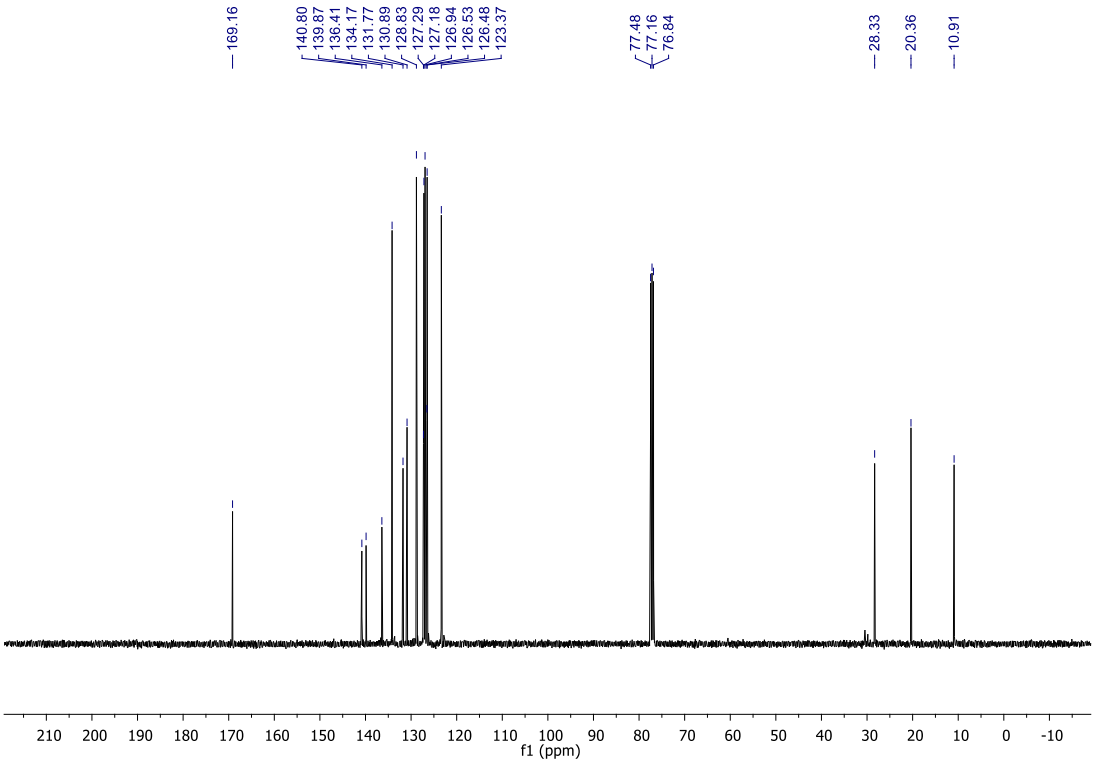


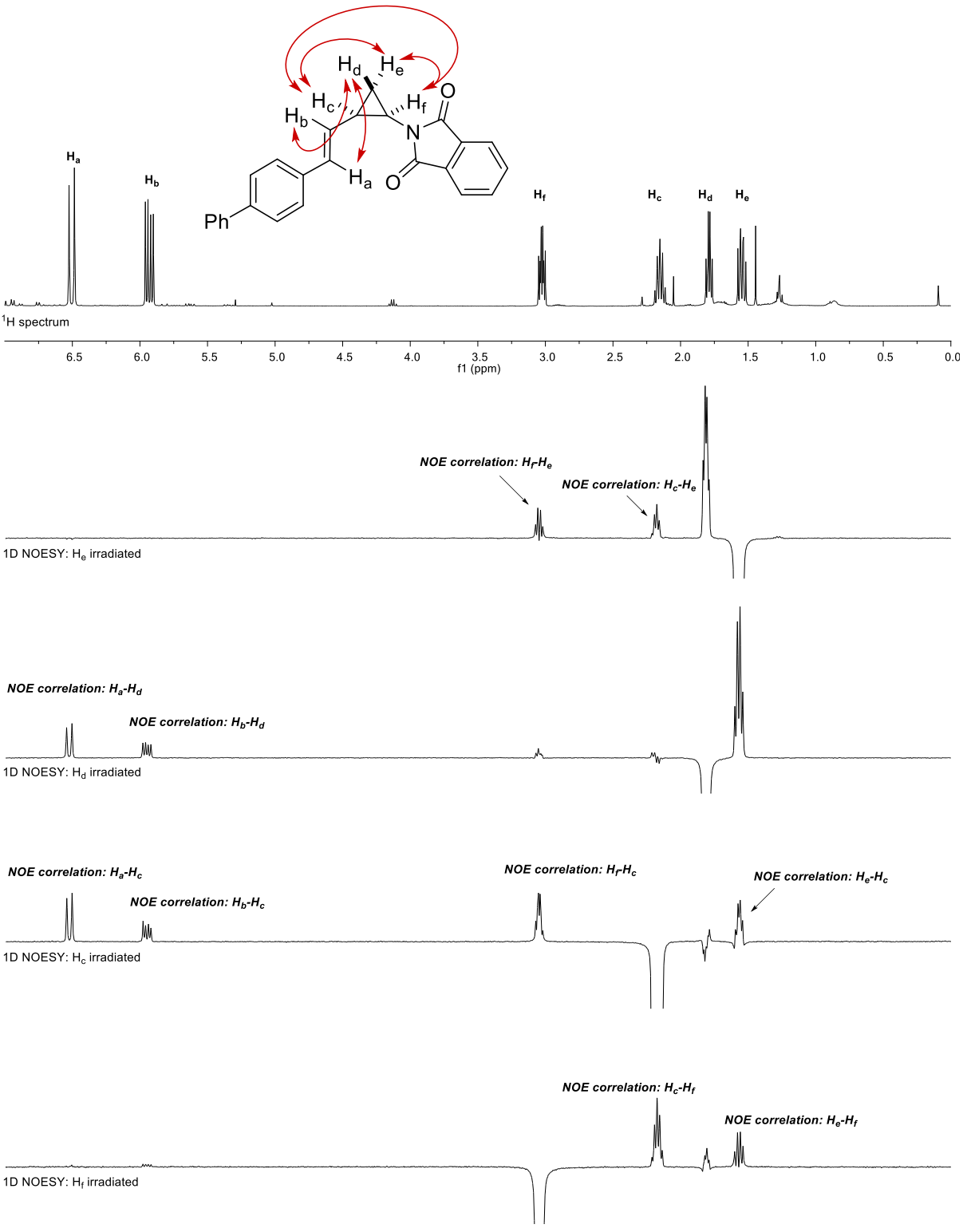

-62.60
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

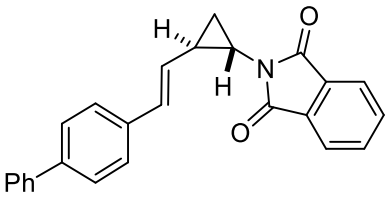

H
H
O
N
O
Ph

***cis*-6e**

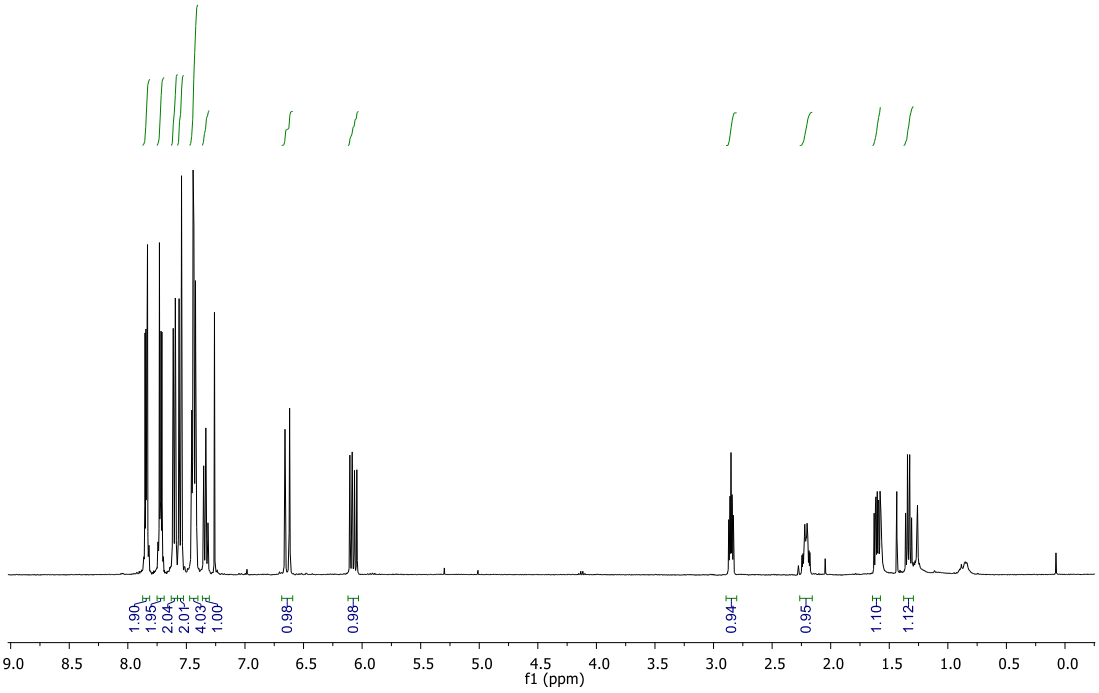

1.87
1.96
2.04
4.25
1.07
2.00
1.00
0.97
0.96
0.99
1.04
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

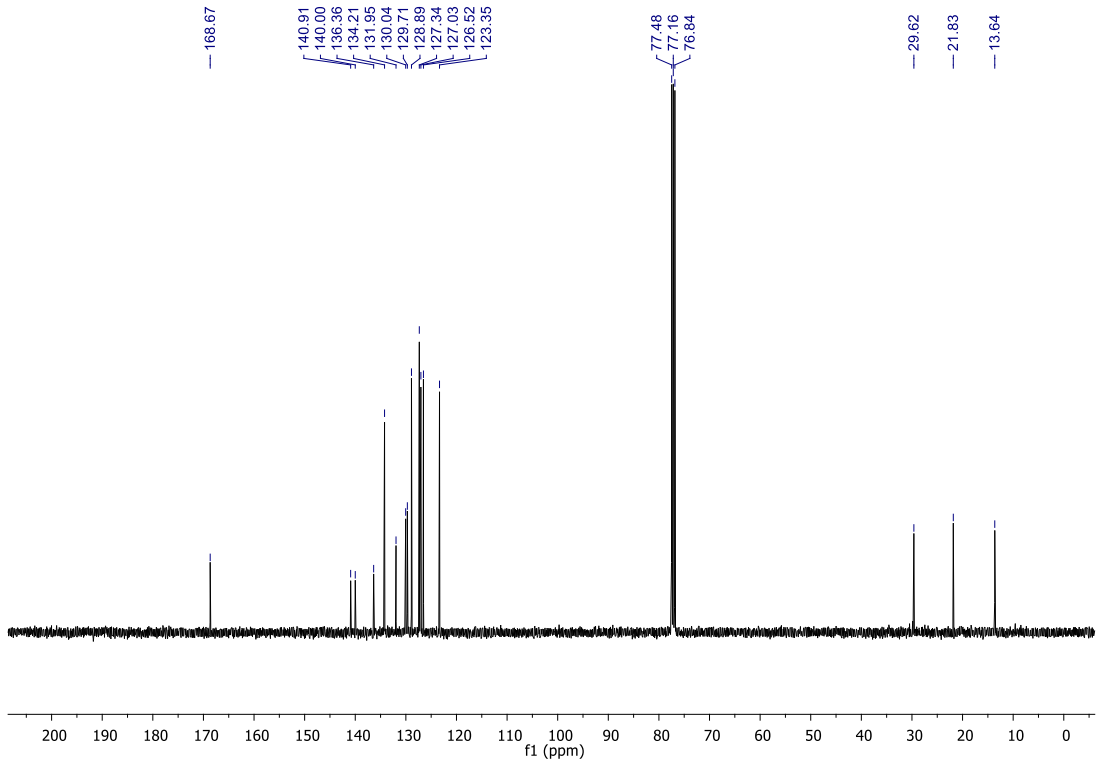

169.16
140.80
139.87
136.41
134.17
131.77
130.89
128.83
127.29
127.18
126.94
126.53
126.48
123.37
77.48
77.16
76.84
28.33
20.36
10.91
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

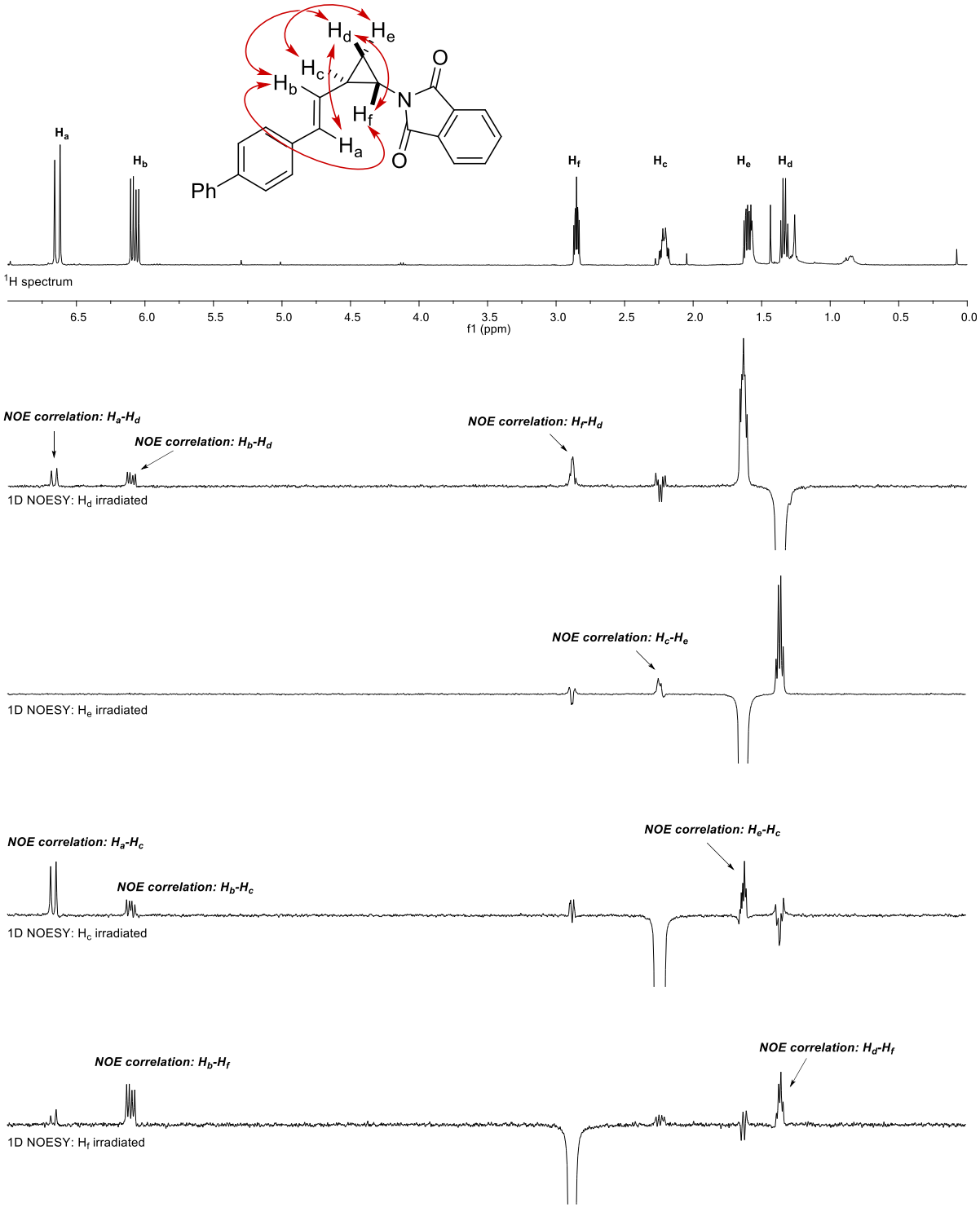

Hd
He
Hc
Hf
Hb
N
O
O
Ha
Ph
Ha
Hb
Hf
Hc
Hd
He
1H spectrum
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
NOE correlation: HfHe
NOE correlation: Hc-He
1D NOESY: He irradiated
NOE correlation: Ha-Hd
NOE correlation: Hb-Hd
1D NOESY: Hd irradiated
NOE correlation: Ha-Hc
NOE correlation: Hb-Hc
NOE correlation: HfHc
NOE correlation: He-Hc
1D NOESY: Hc irradiated
NOE correlation: Hc-Hf
NOE correlation: He-Hf
1D NOESY: Hf irradiated

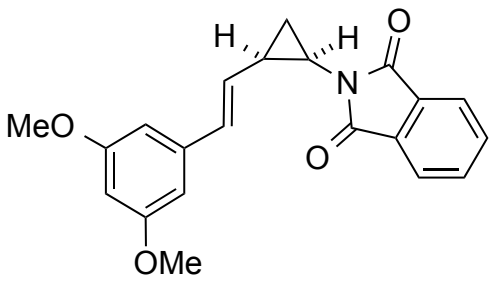

H
O
N
H
O
Ph

***trans*-6e**

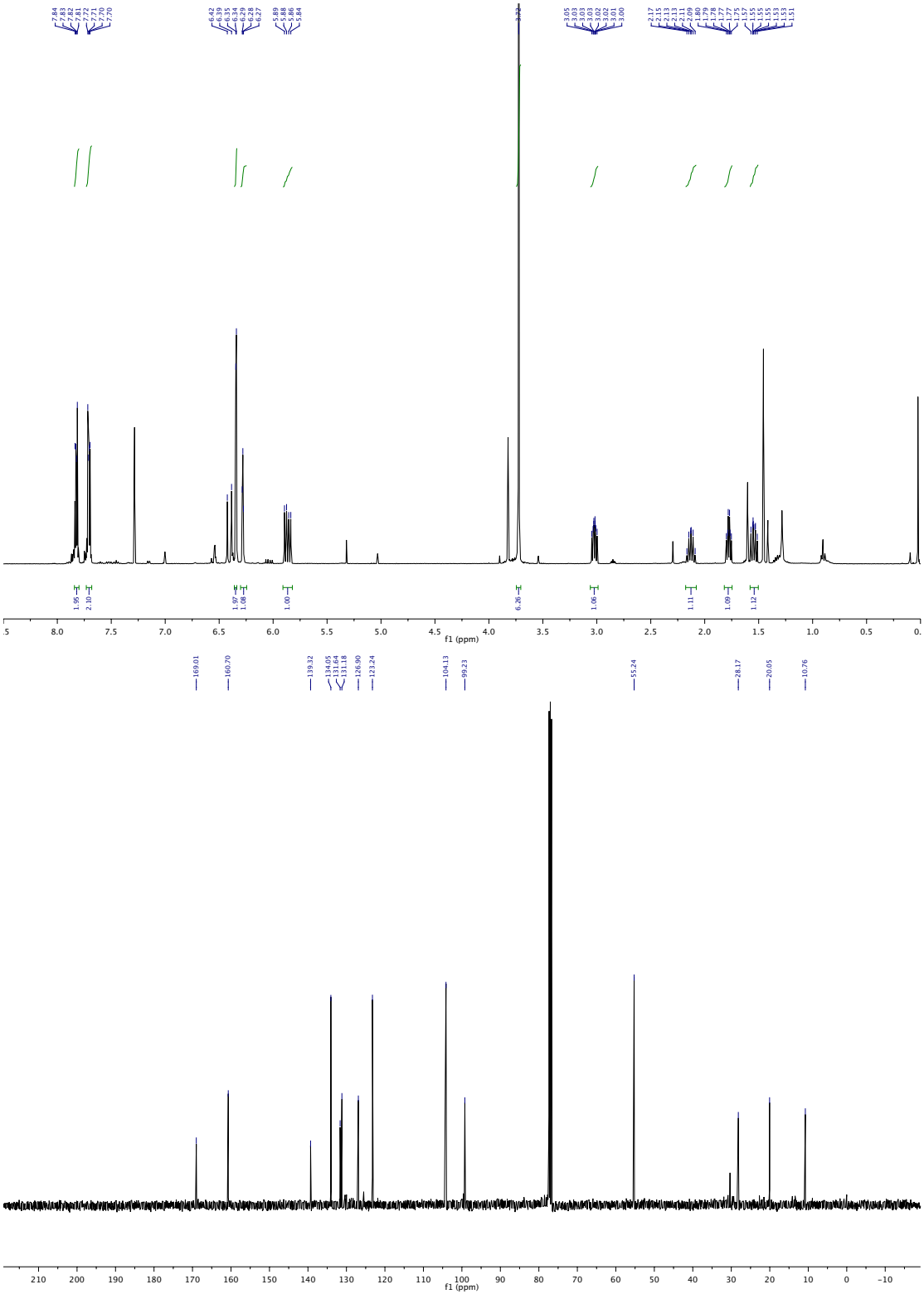

1.90
1.95
2.04
2.01
4.03
1.00
0.98
0.98
0.94
0.95
1.10
1.12
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

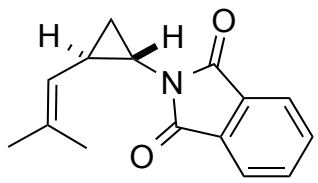

168.67
140.91
140.00
136.36
134.21
131.95
130.04
129.71
128.89
127.34
127.03
126.52
123.35
77.48
77.16
76.84
29.62
21.83
13.64
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Hd
He
Hc
Hb
Hf
Ha
O
N
O
Ph
Ha
Hb
Hf
Hc
He
Hd
1H spectrum
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
NOE correlation: Ha-Hd
NOE correlation: Hb-Hd
NOE correlation: Hf-Hd
1D NOESY: Hd irradiated
NOE correlation: Hc-He
1D NOESY: He irradiated
NOE correlation: Ha-Hc
NOE correlation: Hb-Hc
NOE correlation: He-Hc
1D NOESY: Hc irradiated
NOE correlation: Hb-Hf
NOE correlation: Hd-Hf
1D NOESY: Hf irradiated

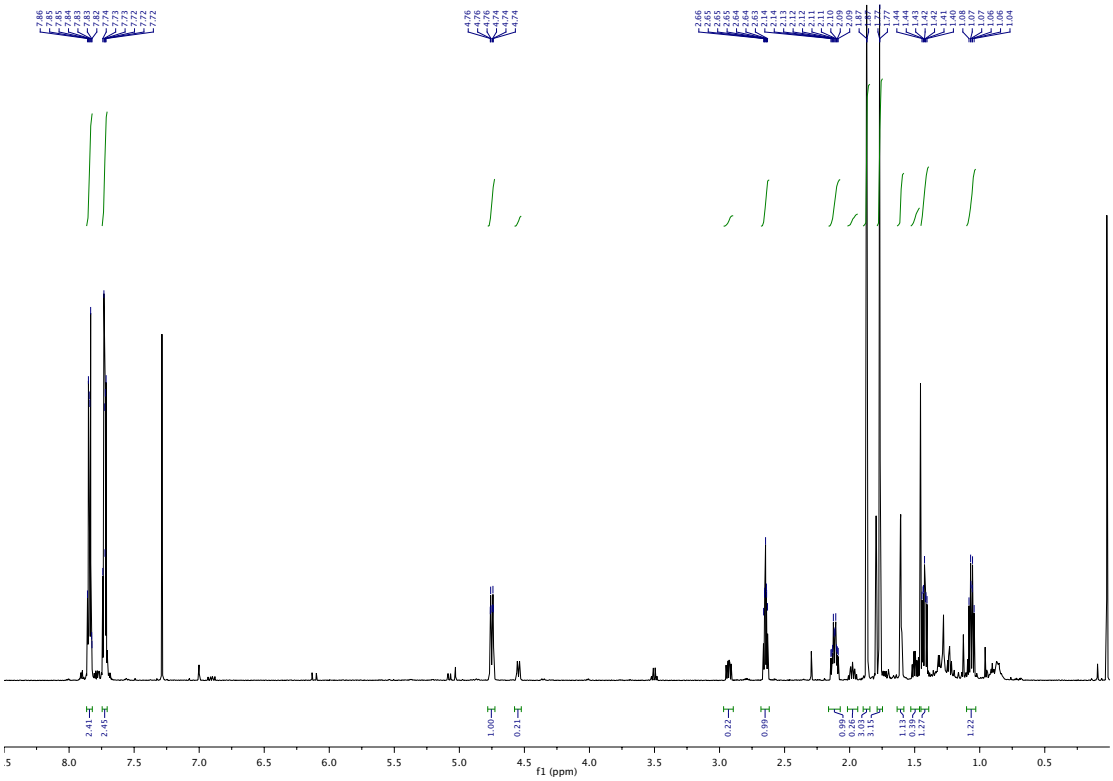


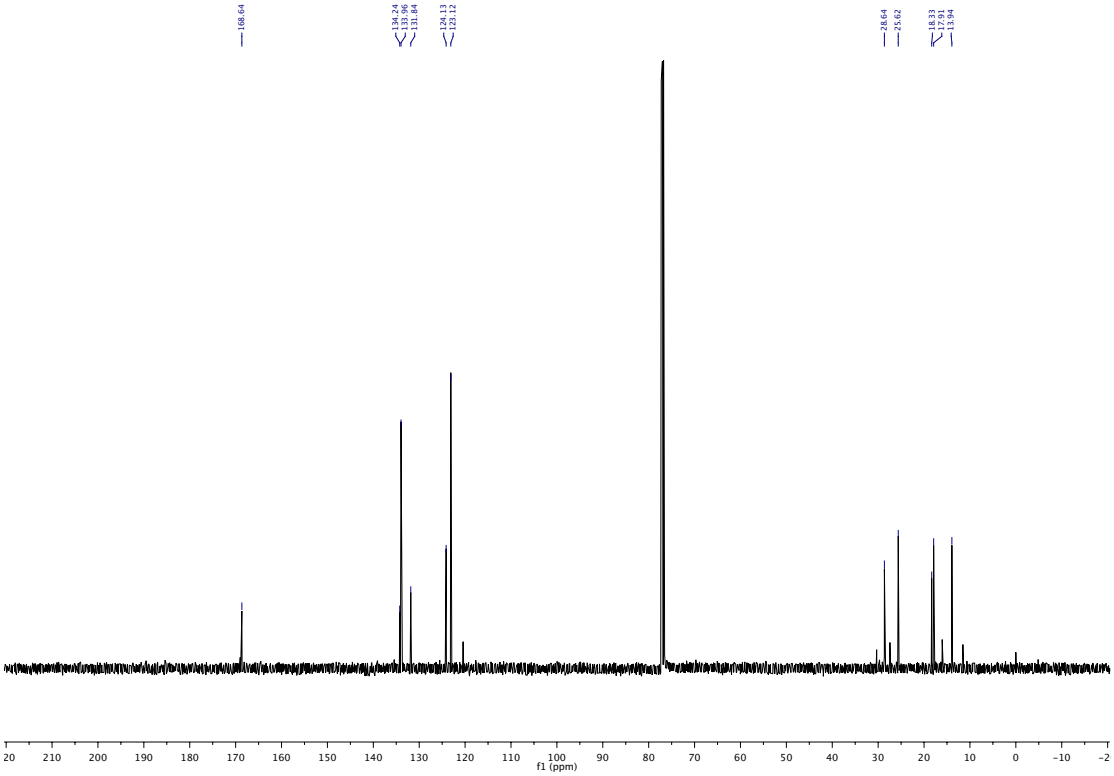
6f

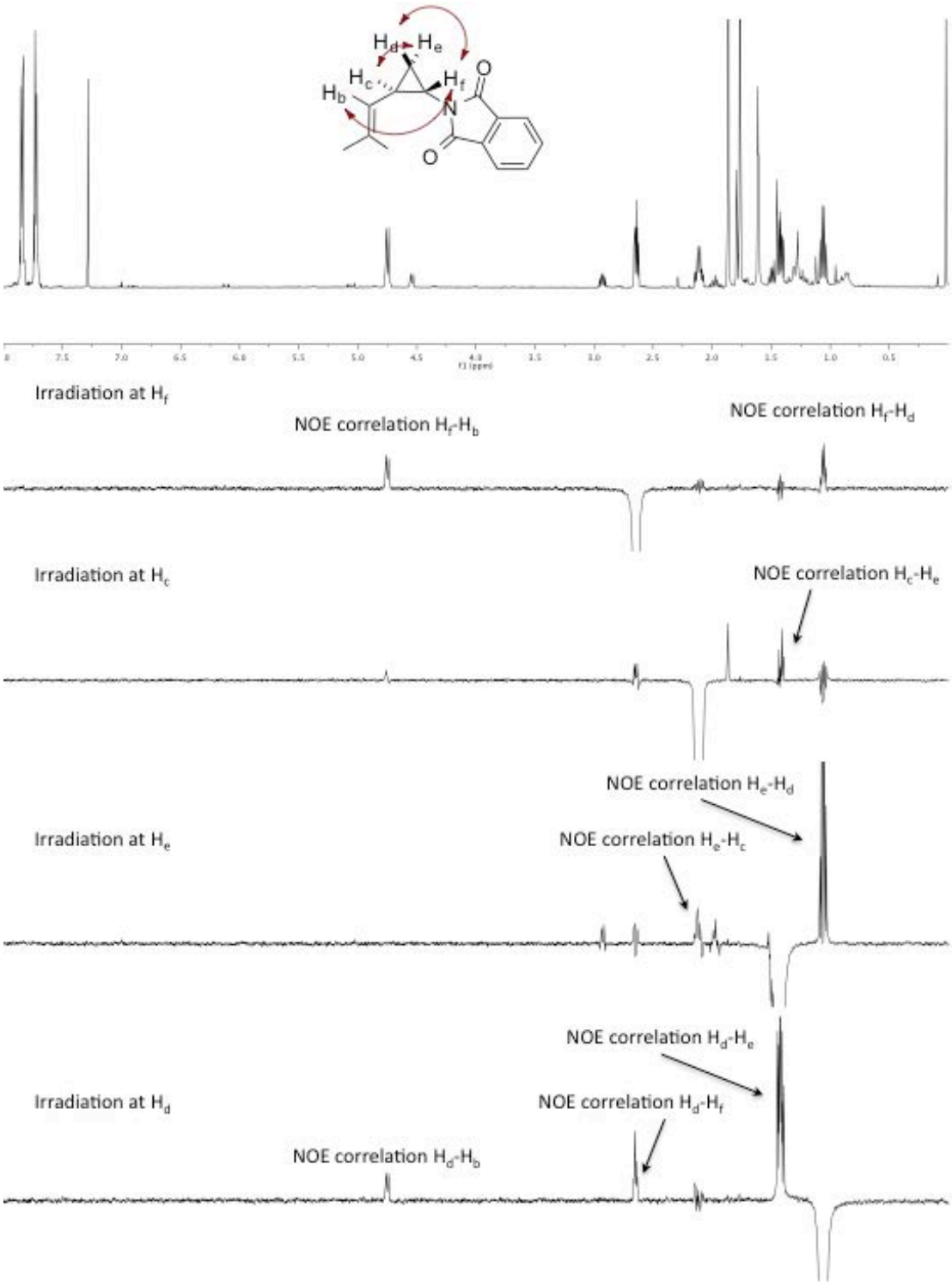


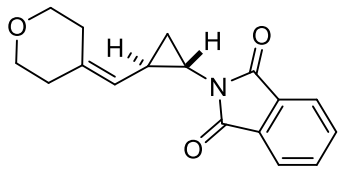


6g

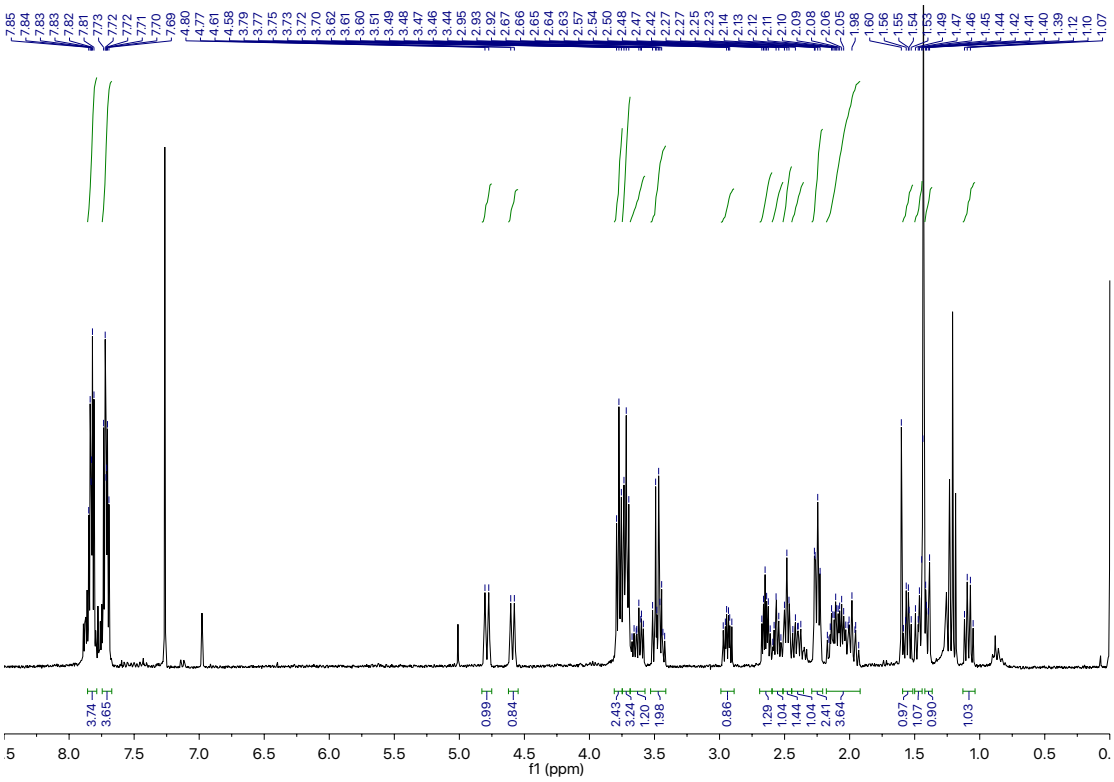


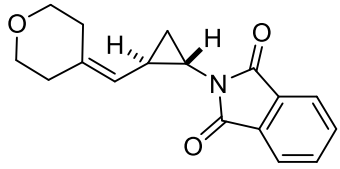



Hd
He
Hc
Hf
Hb
O
N
O
Irradiation at Hf
NOE correlation Hf-Hb
NOE correlation Hf-Hd
Irradiation at Hc
NOE correlation Hc-He
NOE correlation He-Hd
Irradiation at He
NOE correlation He-Hc
NOE correlation Hd-He
Irradiation at Hd
NOE correlation Hd-Hf
NOE correlation Hd-Hb

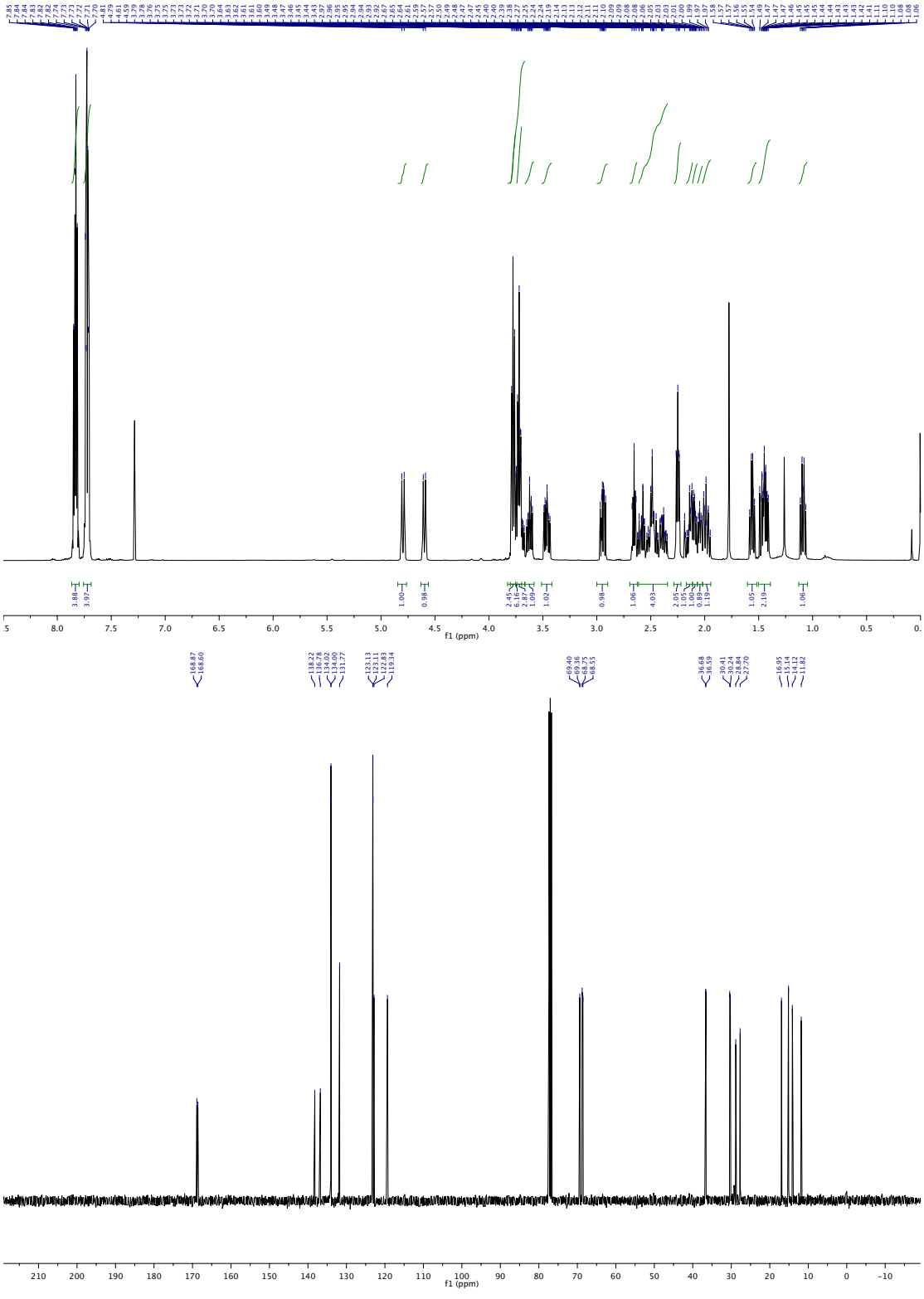


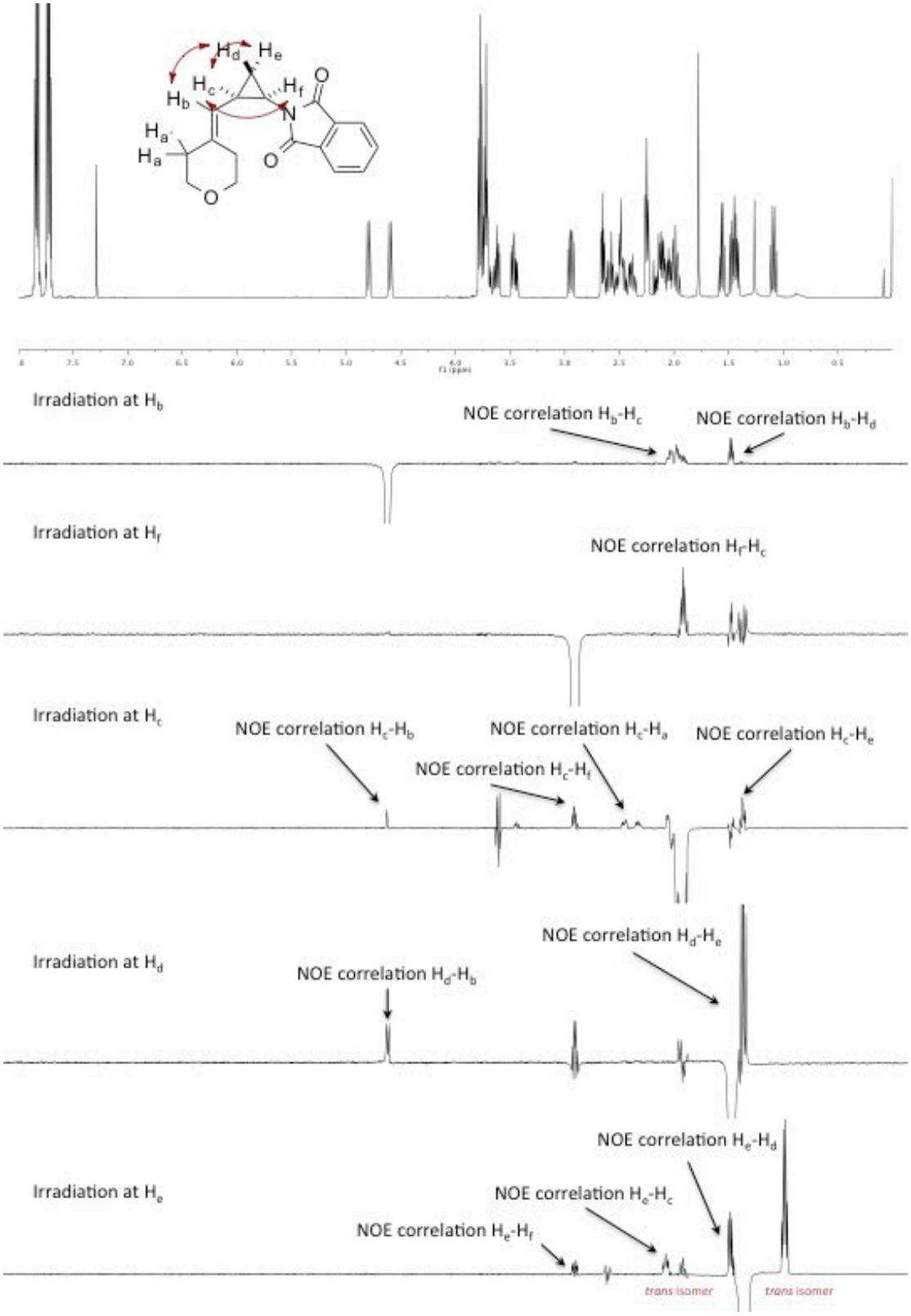
6h (d.r. 1.2:1)

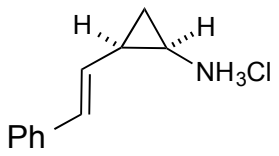




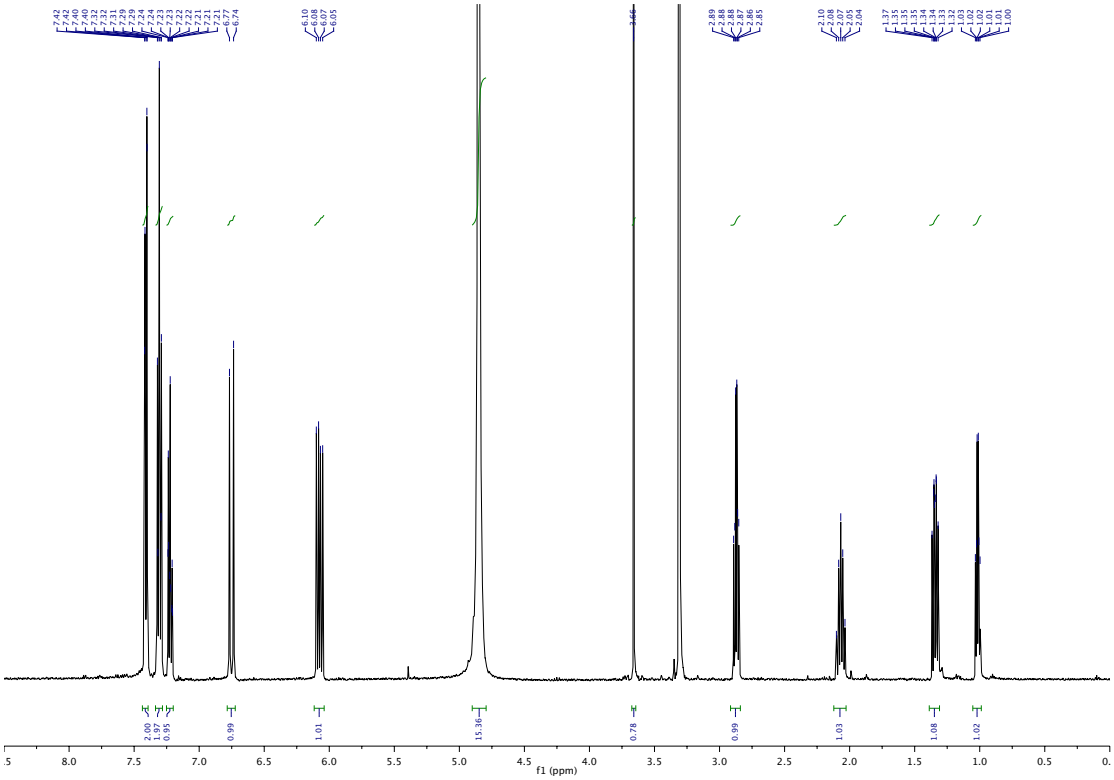
6h (recrystallized sample, d.r. 1:1)

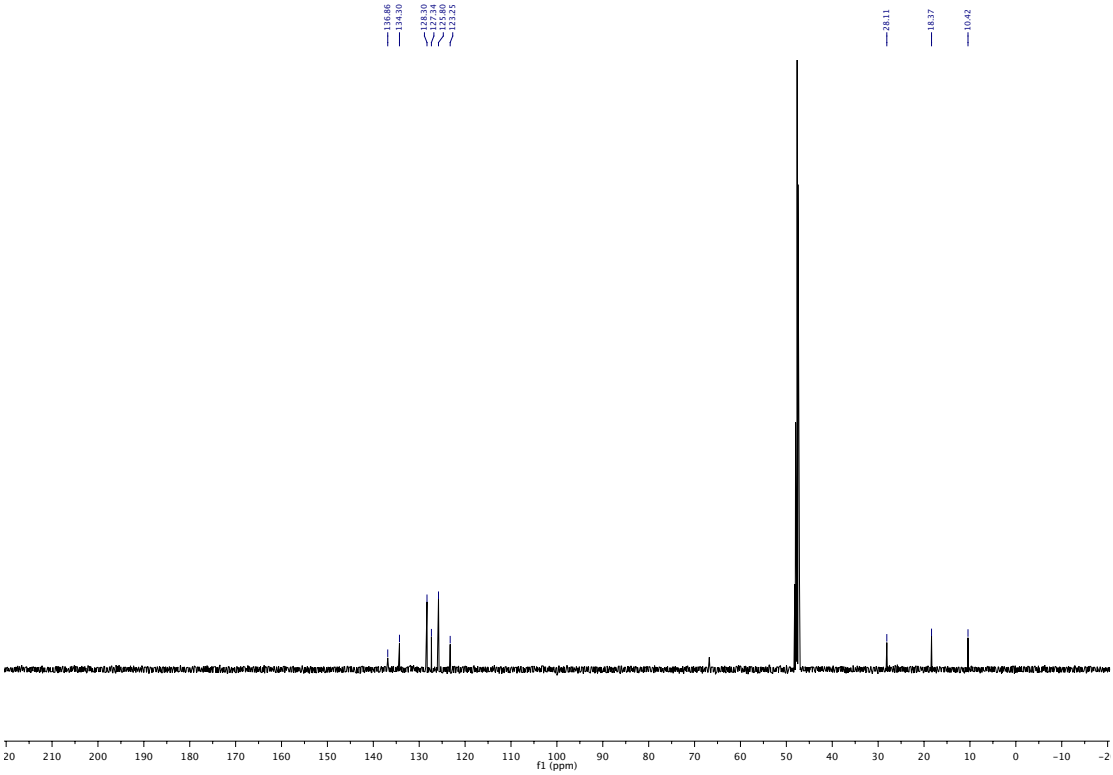


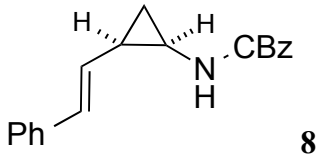

Irradiation at H_b
NOE correlation H_b-H_c
NOE correlation H_b-H_d
Irradiation at H_f
NOE correlation H_f-H_c
Irradiation at H_c
NOE correlation H_c-H_b
NOE correlation H_c-H_a
NOE correlation H_c-H_e
NOE correlation H_c-H_f
Irradiation at H_d
NOE correlation H_d-H_e
NOE correlation H_d-H_b
Irradiation at H_e
NOE correlation H_e-H_d
NOE correlation H_e-H_c
NOE correlation H_e-H_f
trans isomer
trans isomer



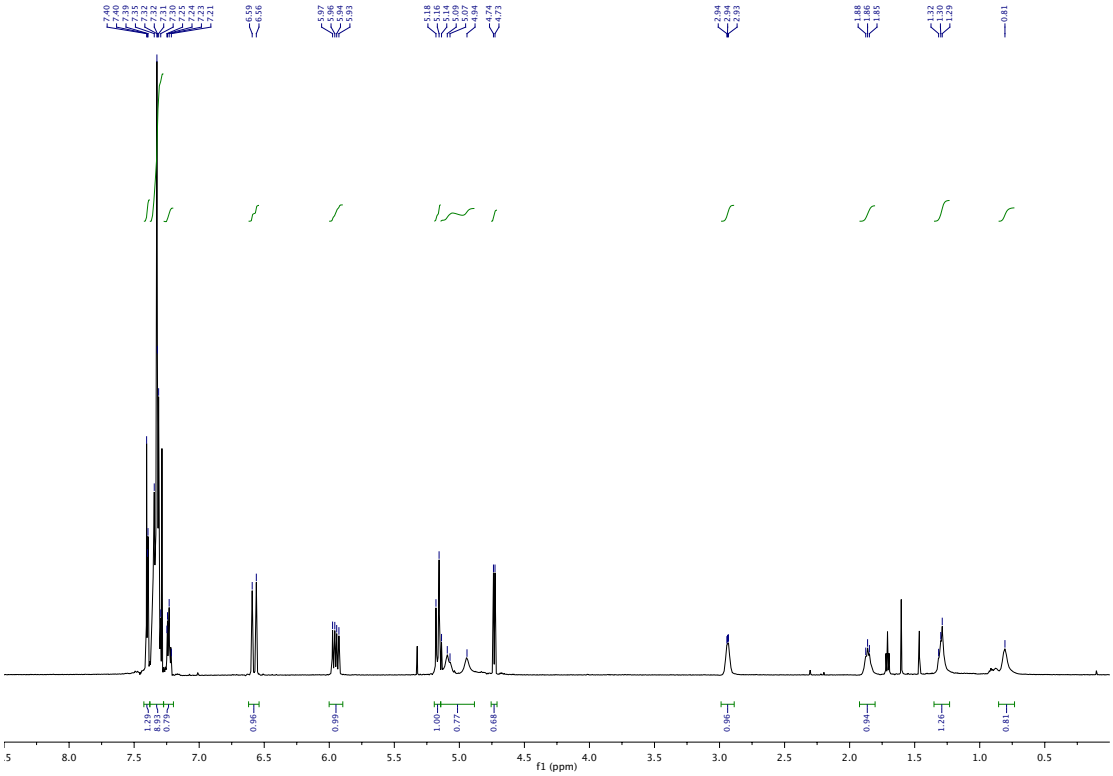
7

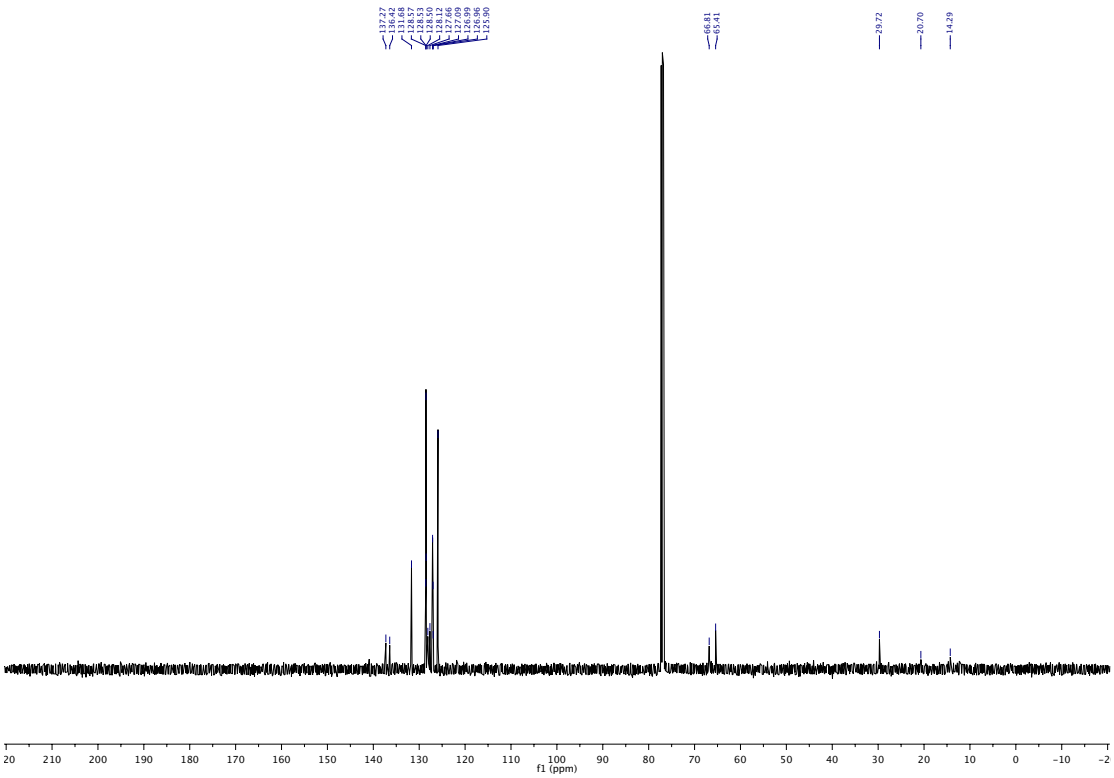


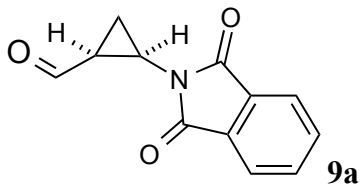



H
H
CBz
N
H
Ph

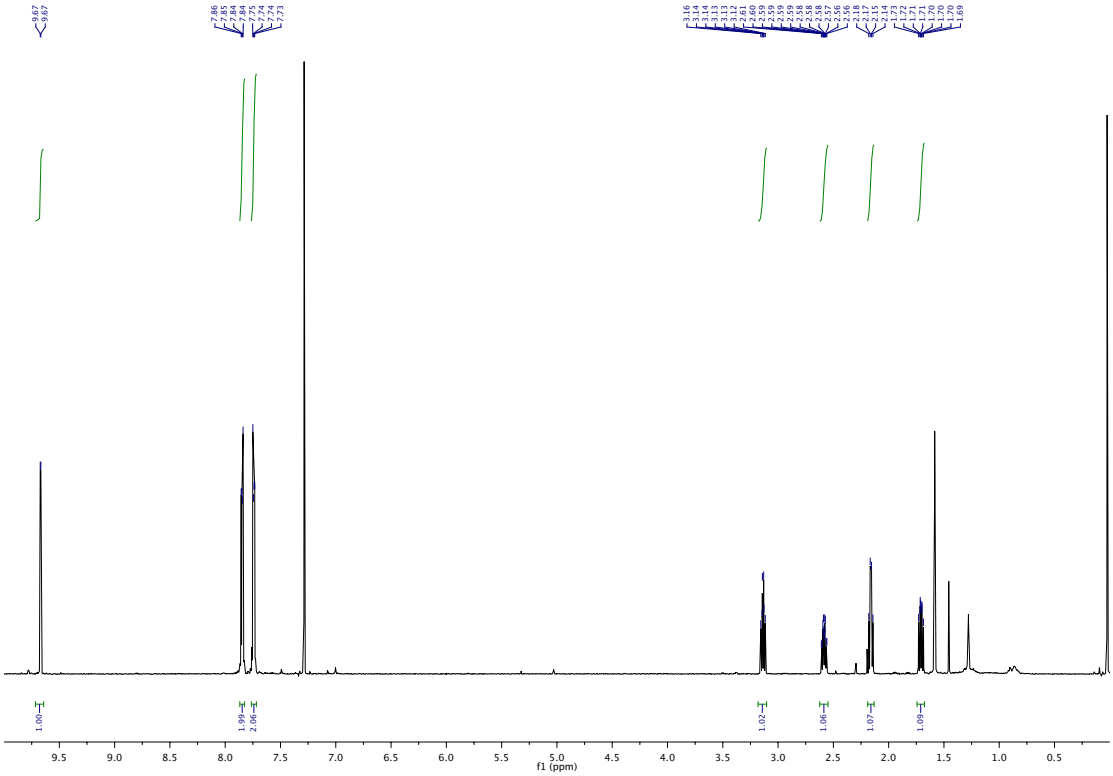
8

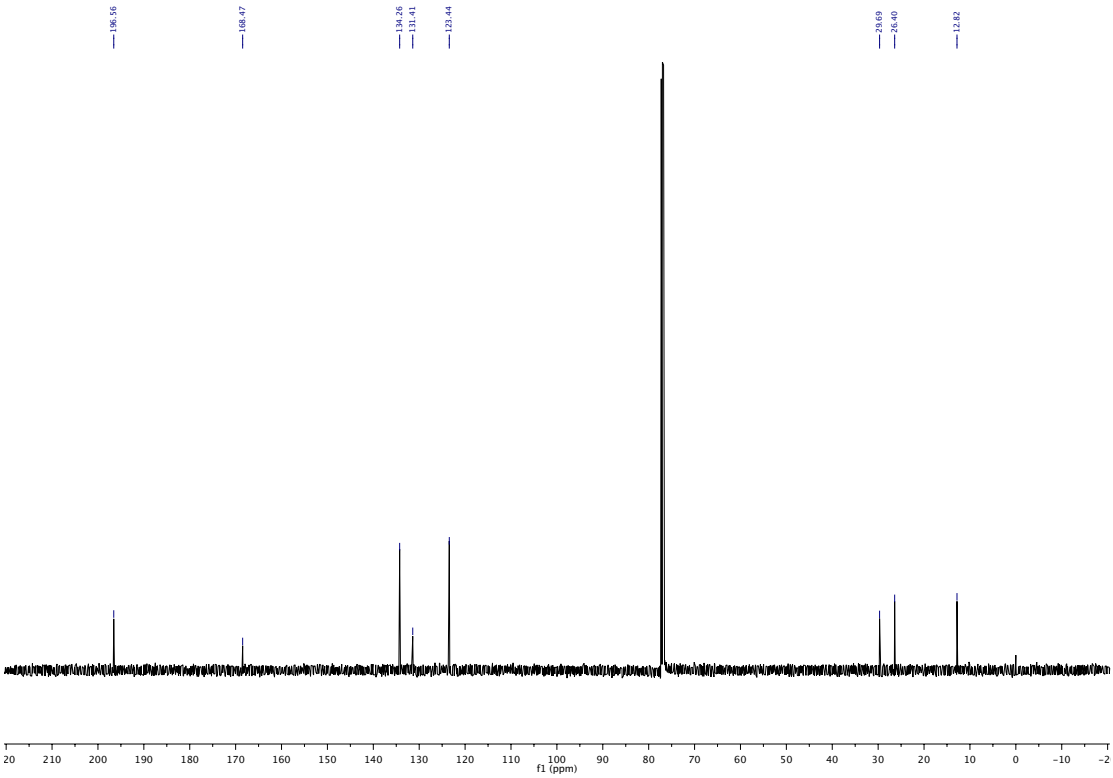

7.40
7.40
7.39
7.35
7.32
7.32
7.31
7.30
7.25
7.24
7.23
7.21
6.59
6.56
5.97
5.96
5.94
5.93
5.18
5.16
5.14
5.09
5.07
4.94
4.74
4.73
2.94
2.94
2.93
1.88
1.86
1.85
1.32
1.30
1.29
0.81
1.29
1.03
0.72
0.96
0.99
1.00
0.77
0.68
0.96
0.94
1.26
0.81
f1 (ppm)

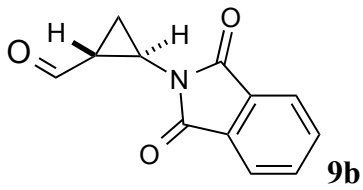

137.27
136.42
131.68
124.57
124.53
128.50
128.12
127.66
127.09
126.99
126.86
125.90
66.81
65.41
29.72
20.70
14.29
f1 (ppm)


H
H
O
O
N
O

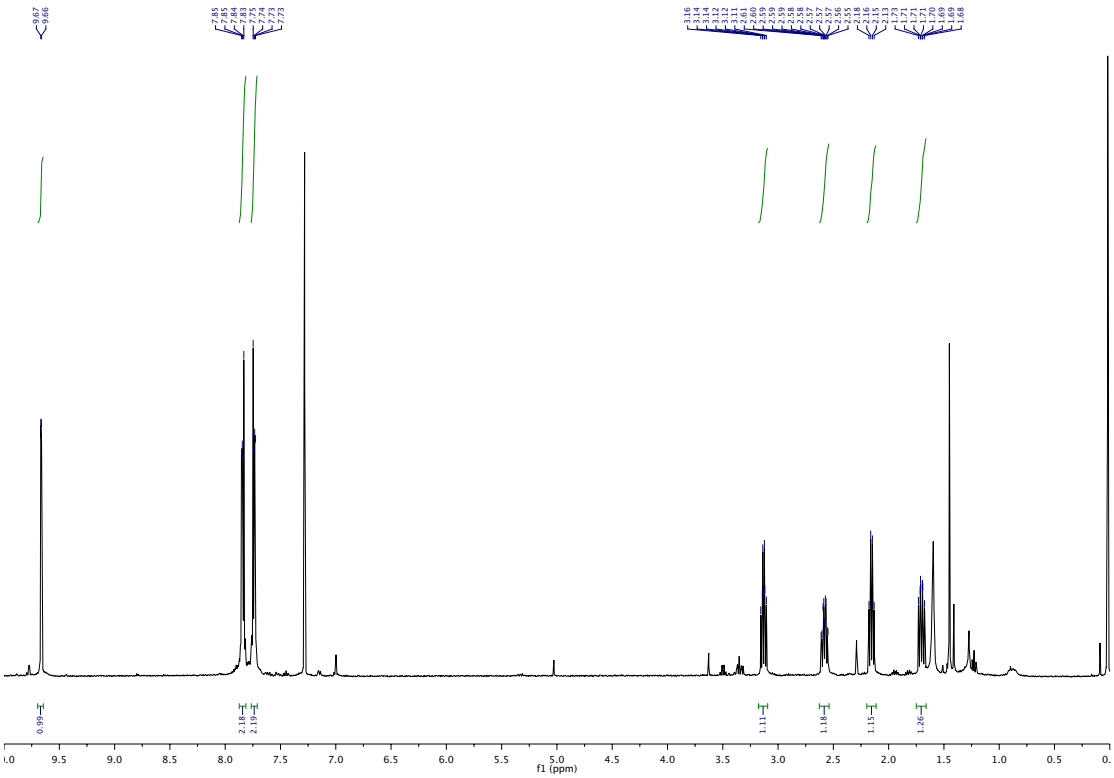
9a

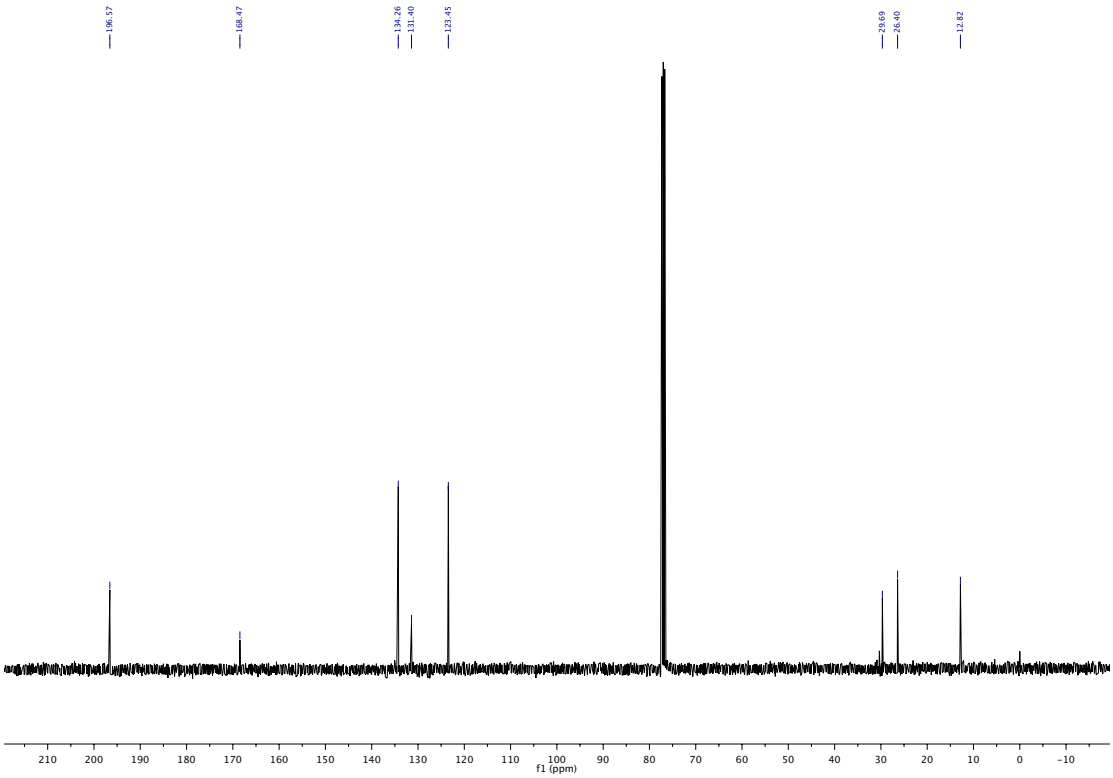

9.67
9.67
7.86
7.85
7.84
7.84
7.75
7.74
7.74
7.73
3.16
3.14
3.14
3.13
3.13
3.12
3.12
2.61
2.60
2.59
2.59
2.59
2.59
2.58
2.58
2.57
2.57
2.56
2.56
2.18
2.17
2.15
2.14
1.73
1.72
1.71
1.71
1.70
1.70
1.70
1.69
1.00
1.90
2.00
1.02
1.06
1.07
1.09
f1 (ppm)

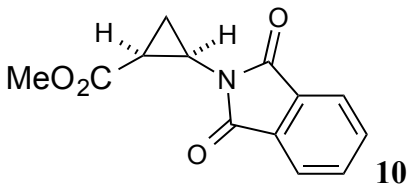

196.56
168.47
134.26
131.41
123.44
29.69
26.40
12.82
f1 (ppm)


H
O
H
O
N
O

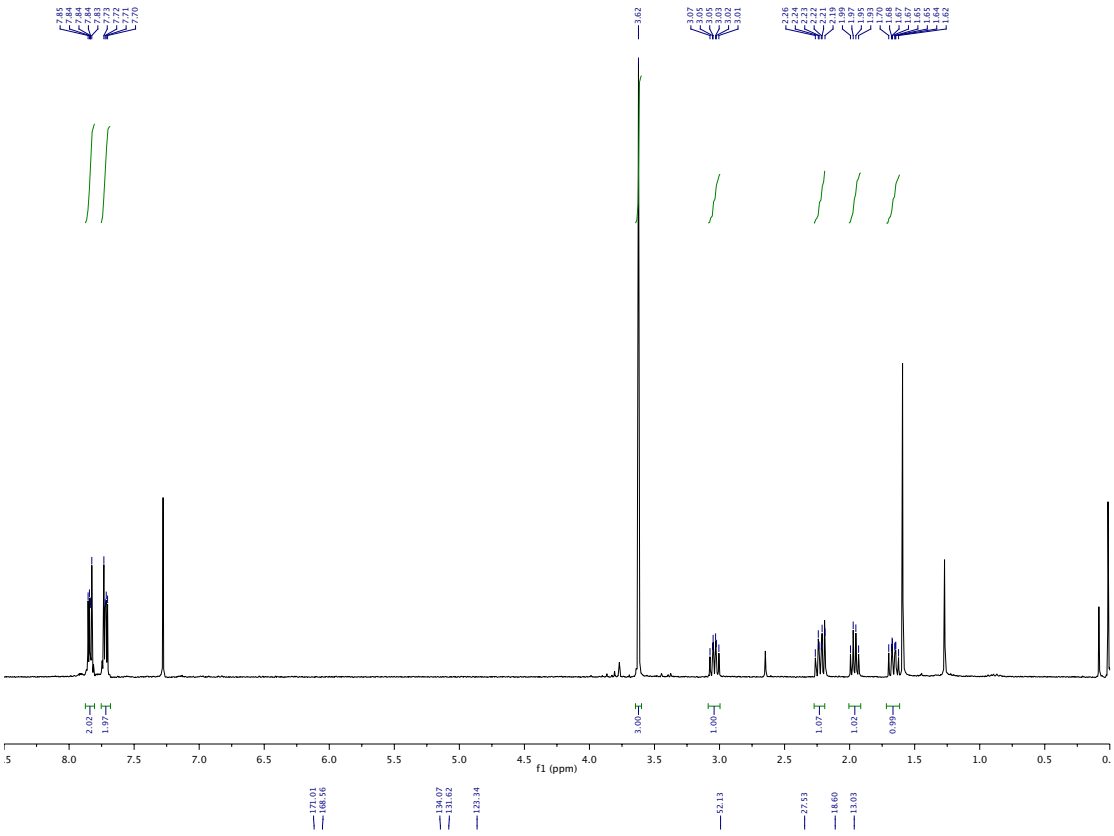
9b

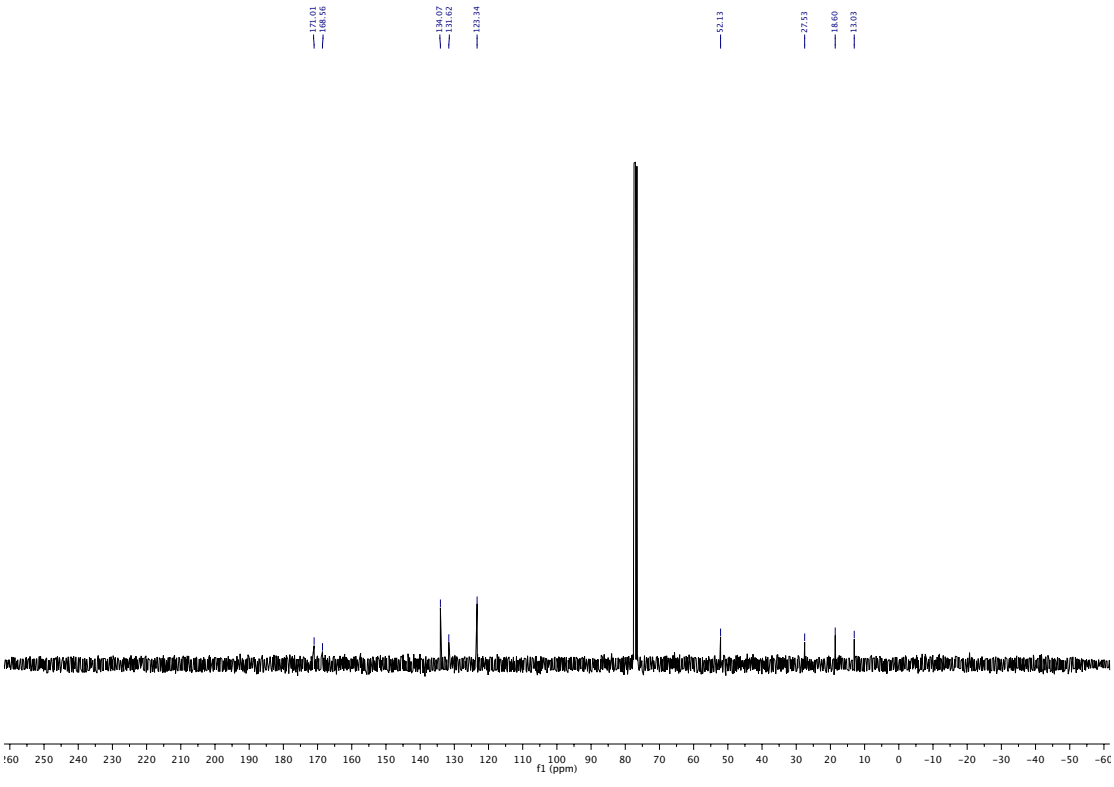

9.67
9.66
7.85
7.85
7.84
7.83
7.75
7.74
7.73
7.73
3.16
3.14
3.14
3.12
3.12
3.11
3.11
2.61
2.60
2.59
2.59
2.59
2.58
2.58
2.57
2.57
2.57
2.56
2.55
2.18
2.16
2.15
2.13
1.75
1.71
1.71
1.70
1.69
1.69
1.68
0.99
2.18
2.19
1.11
1.18
1.15
1.26
f1 (ppm)

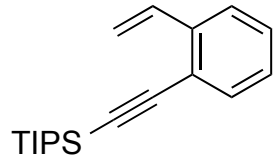

196.57
168.47
134.26
131.40
123.45
29.69
26.40
12.82
f1 (ppm)


H
H
O
MeO2C
N
O

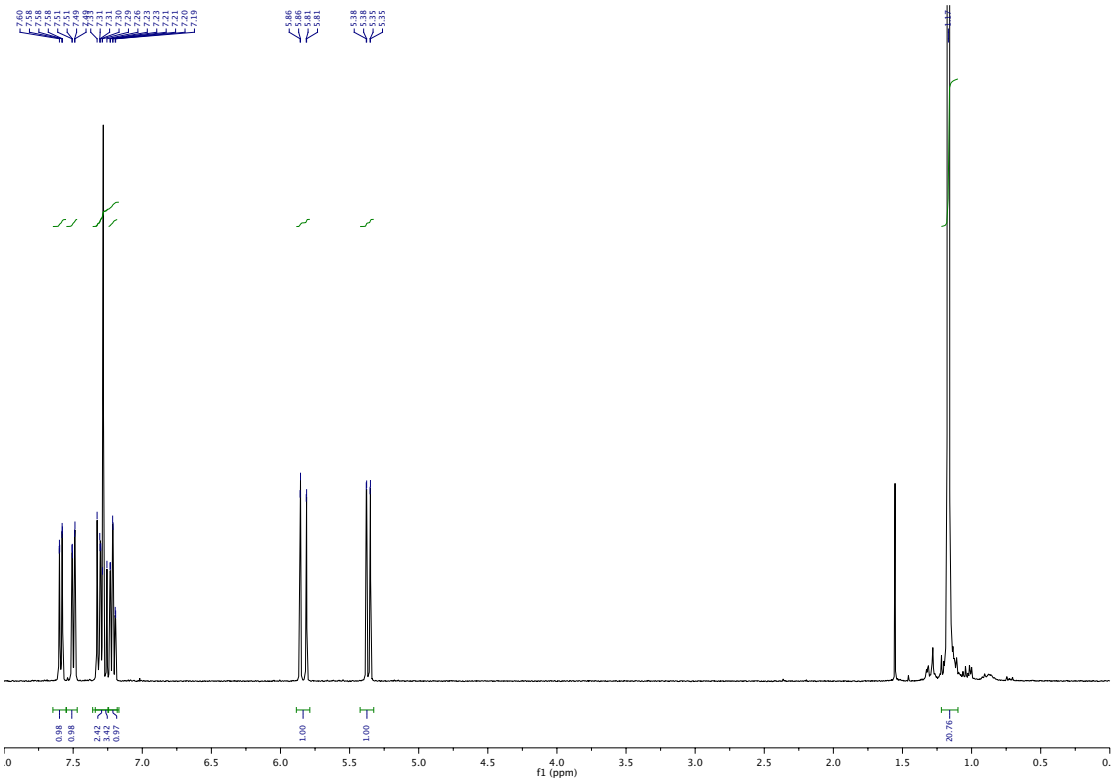
10

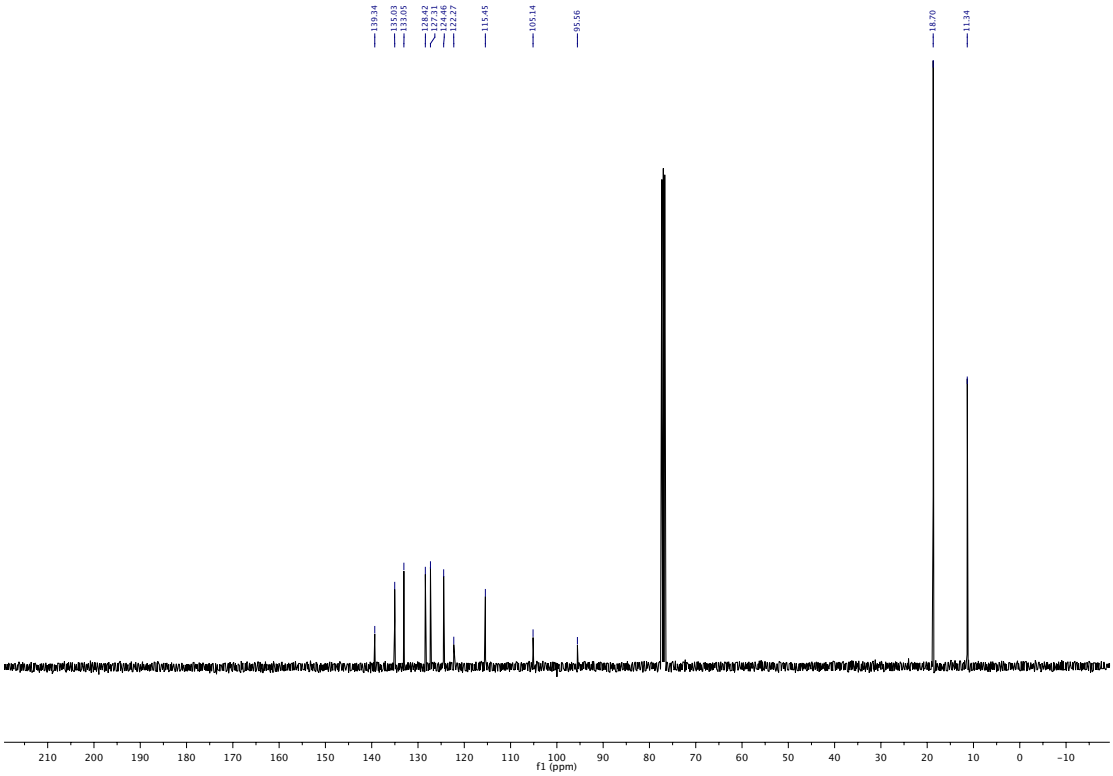

7.85
7.84
7.84
7.84
7.84
7.73
7.72
7.71
7.70
3.62
3.07
3.05
3.03
3.02
3.01
2.26
2.24
2.23
2.22
2.21
2.19
1.99
1.97
1.95
1.93
1.70
1.68
1.67
1.65
1.65
1.64
1.62
2.02
1.97
3.00
1.00
1.07
1.02
0.99
f1 (ppm)

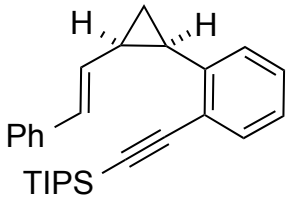

171.01
168.56
134.07
131.62
123.34
52.13
27.53
18.60
13.03
f1 (ppm)



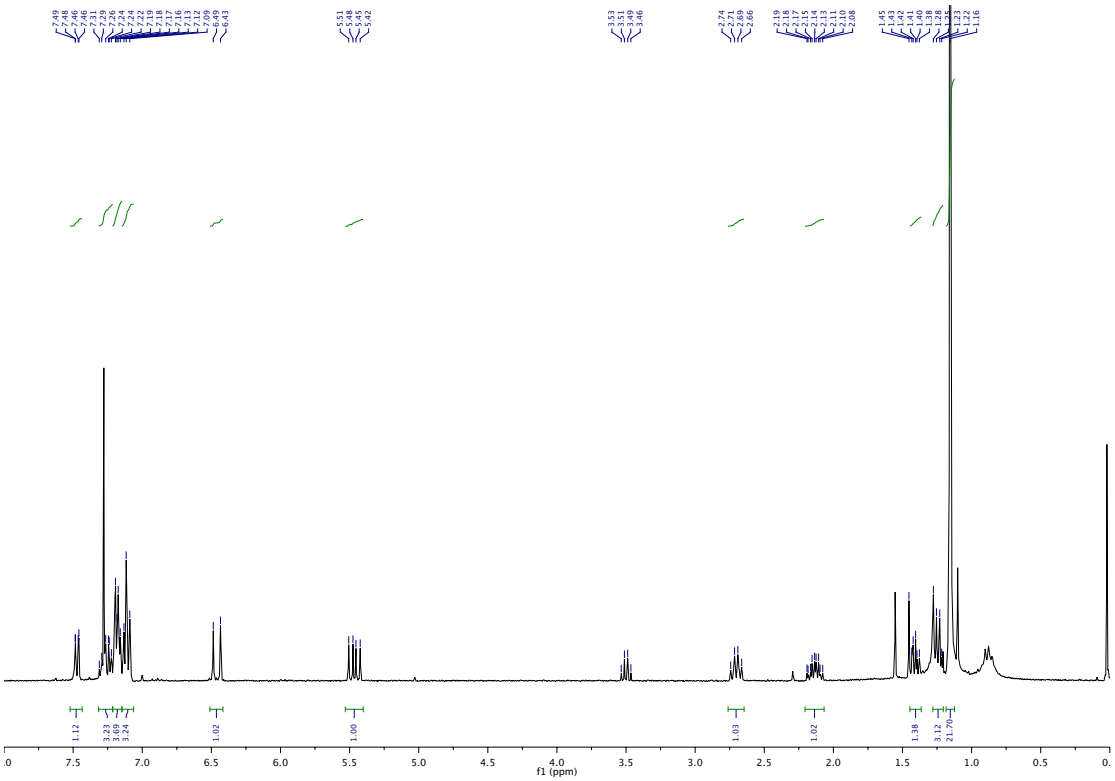
11

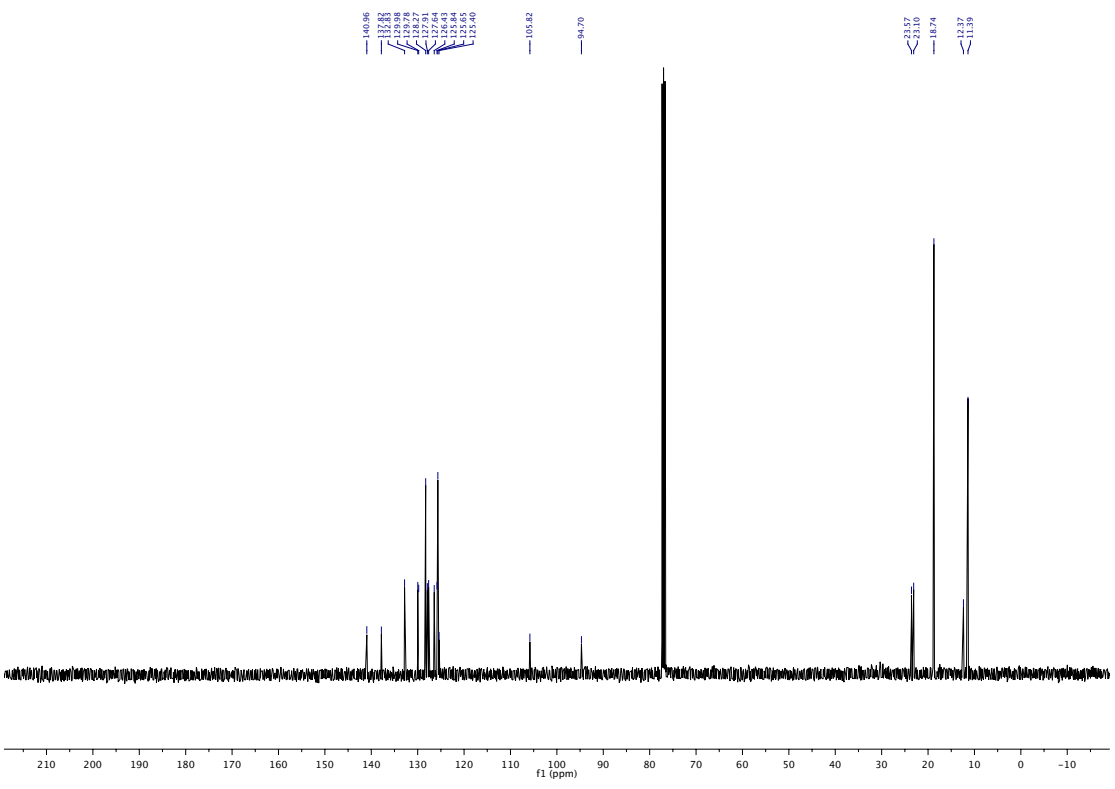


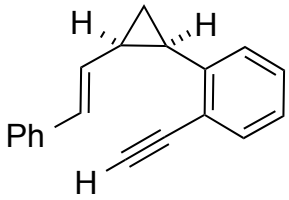



H
H
Ph
TIPS

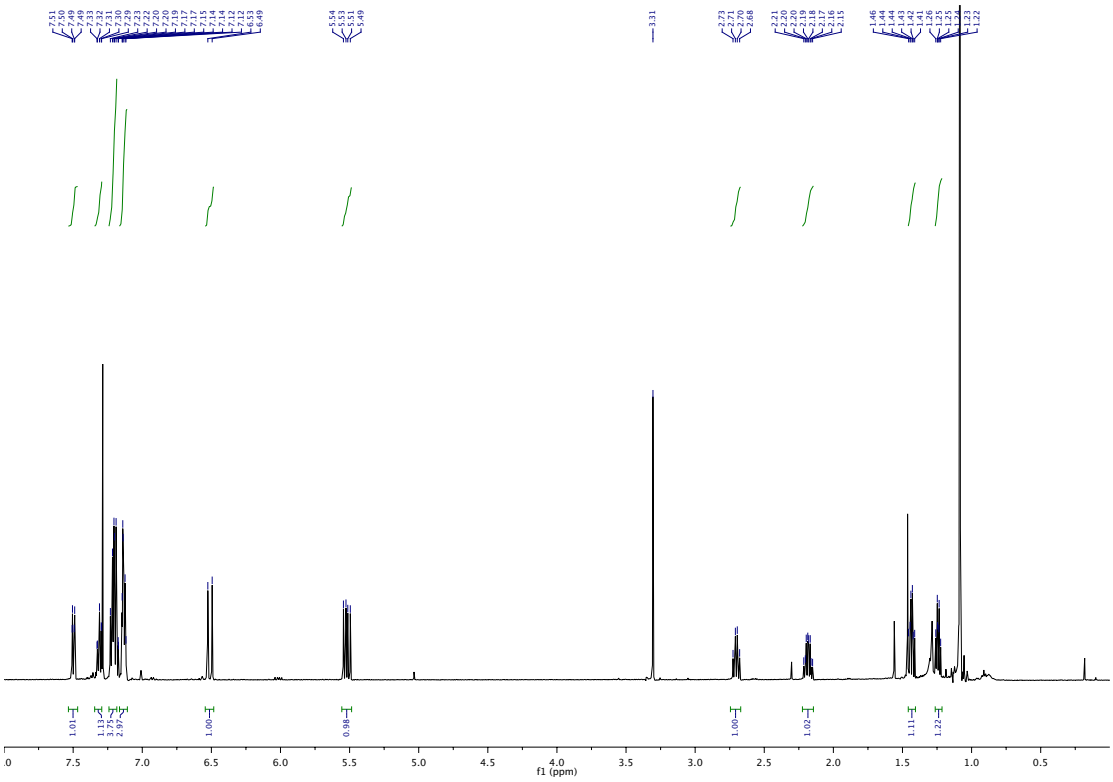
12a

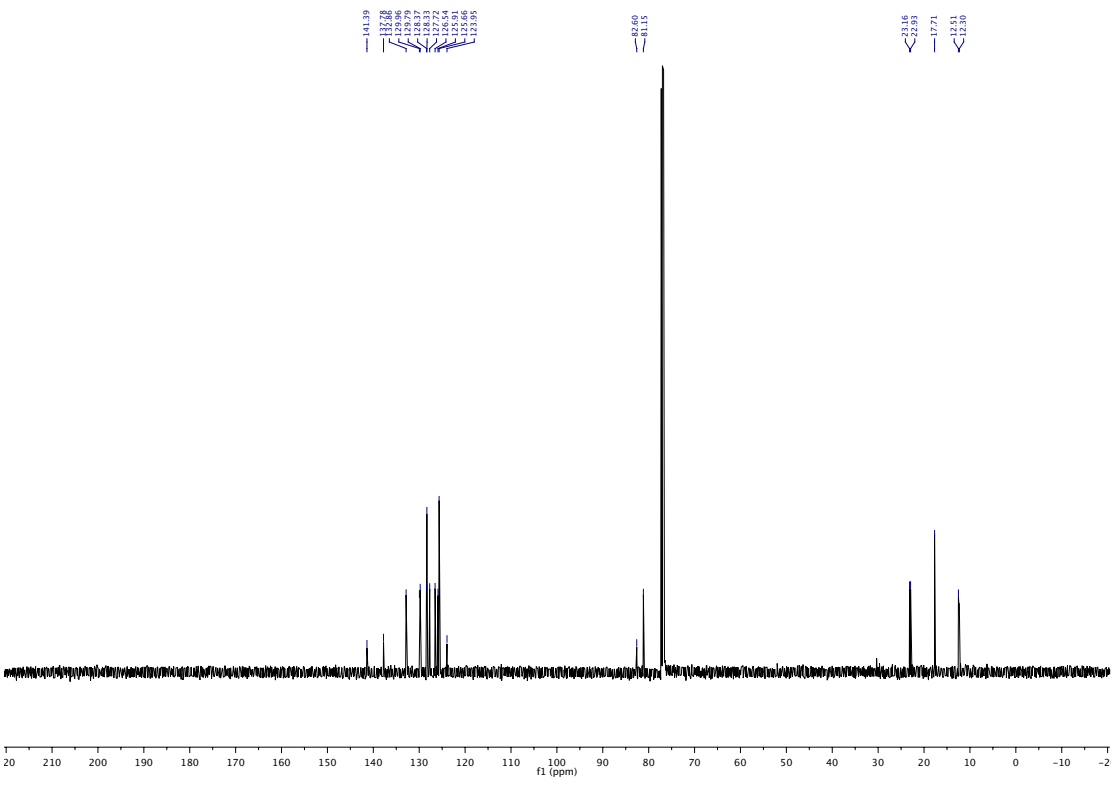

7.49
7.48
7.46
7.46
7.31
7.29
7.26
7.24
7.22
7.19
7.18
7.17
7.16
7.13
7.12
7.09
6.49
6.43
5.51
5.48
5.45
5.42
3.53
3.51
3.49
3.46
2.74
2.71
2.69
2.66
2.19
2.18
2.17
2.15
2.14
2.13
2.11
2.10
2.08
1.45
1.43
1.42
1.41
1.40
1.38
1.38
1.25
1.23
1.22
1.16
1.12
3.23
3.69
3.24
1.02
1.00
1.03
1.02
1.38
3.12
21.70
f1 (ppm)

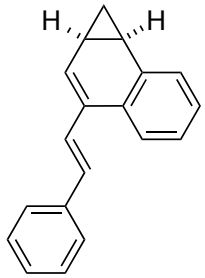

140.96
132.83
132.83
129.98
129.98
128.27
127.91
127.64
126.43
125.84
125.55
125.40
105.82
94.70
23.57
23.10
18.74
12.37
11.39
f1 (ppm)


H
H
Ph
H

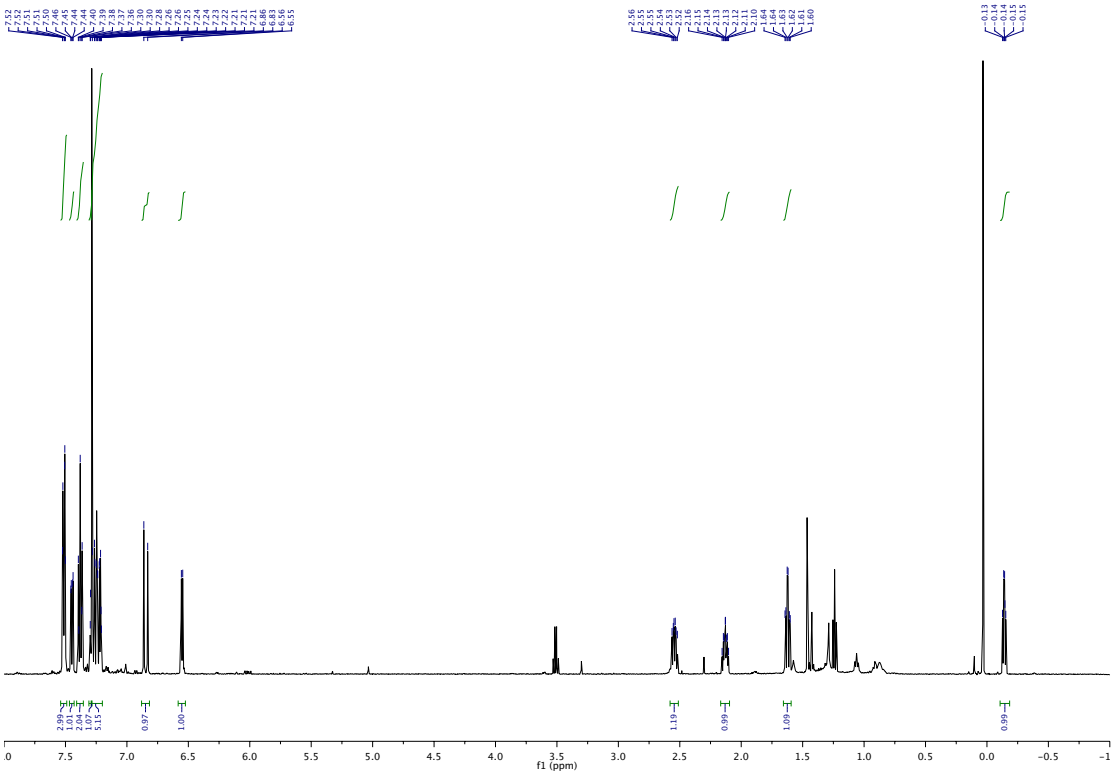
12b

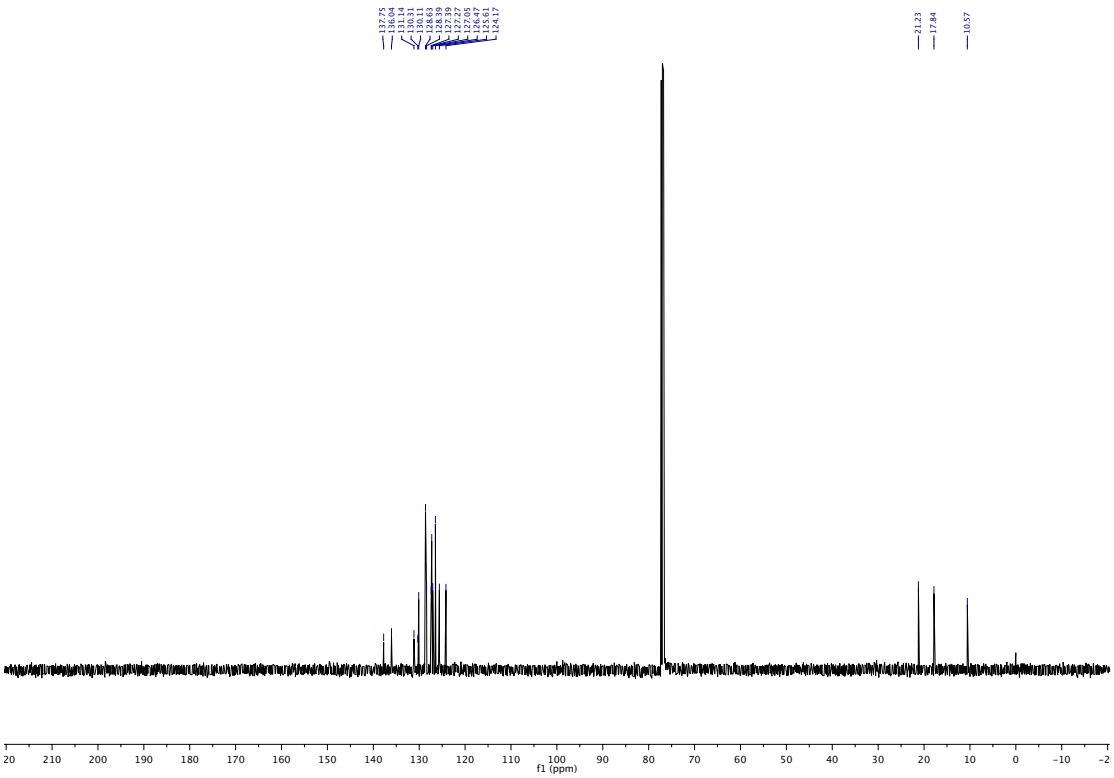

7.51
7.50
7.49
7.49
7.33
7.32
7.31
7.30
7.29
7.23
7.22
7.20
7.20
7.19
7.17
7.15
7.14
7.12
7.12
6.53
6.49
5.54
5.53
5.51
5.49
3.31
2.73
2.71
2.70
2.68
2.21
2.20
2.20
2.19
2.18
2.17
2.16
2.15
1.46
1.44
1.44
1.43
1.42
1.41
1.26
1.25
1.24
1.23
1.22
1.01
1.12
3.75
2.97
1.00
0.98
1.00
1.02
1.11
1.22
f1 (ppm)

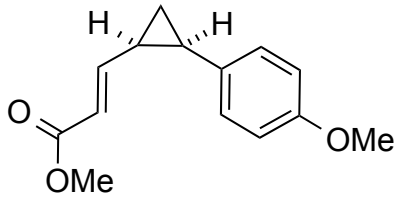

141.39
132.88
132.68
129.96
129.39
128.37
128.33
127.72
126.54
125.91
125.66
123.95
82.60
81.15
23.16
22.93
17.71
12.51
12.30
f1 (ppm)



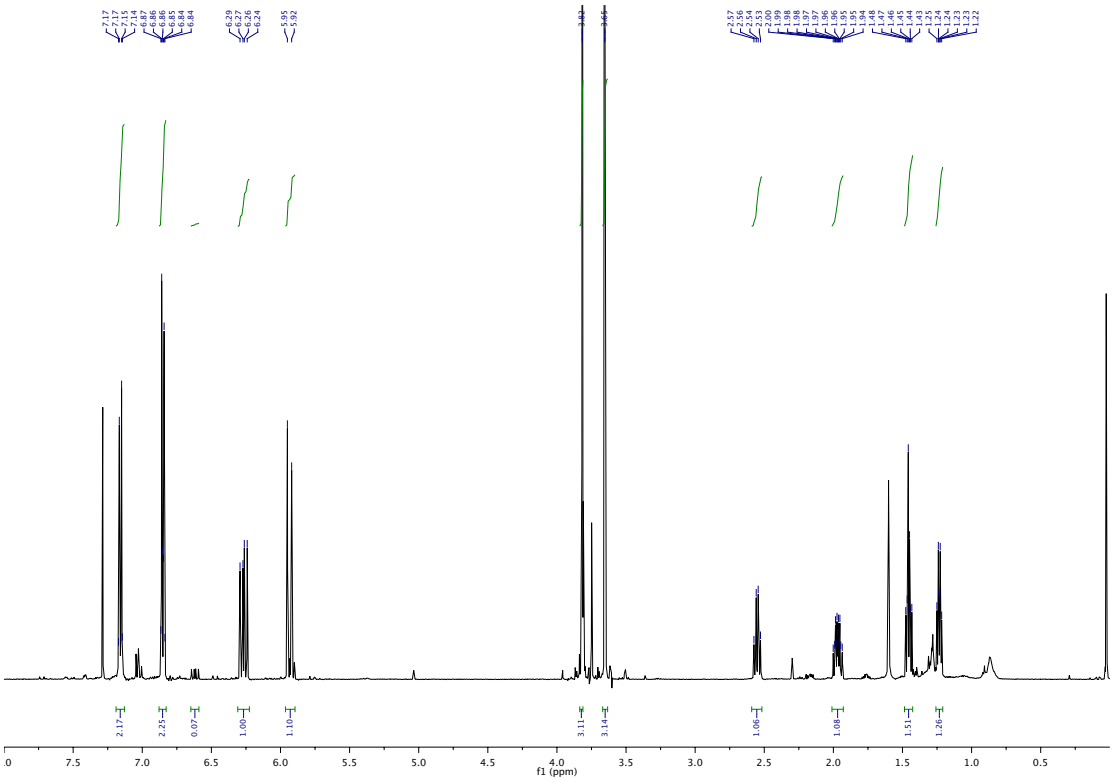
13

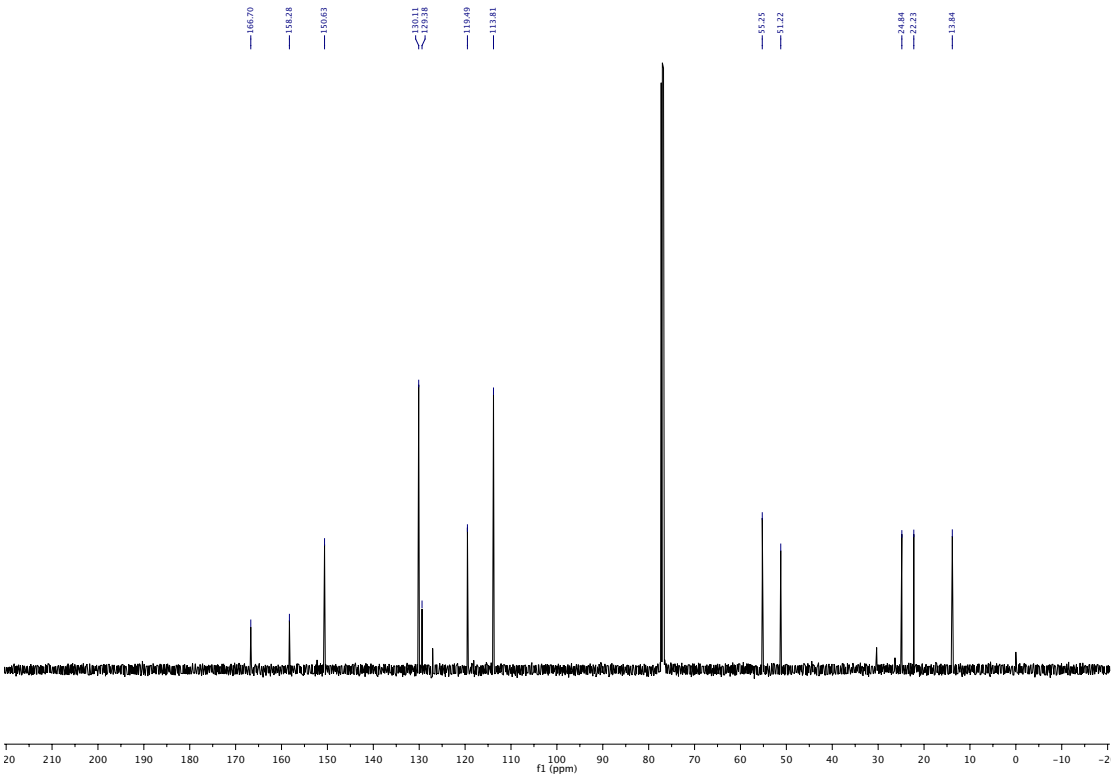






14





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8. This substrate was obtained by formation of the ester: Anciaux, A. J.; Demonceau, A.; Noels, A. F.; Hubert, A. J.; Warin, R.; Teyssi, P. *J. Org. Chem.* **1981**, *46*, 873–876, followed by reduction to the alcohol: Kerber, R.C.; Ehntholt, D.J. *J. Am. Chem. Soc.* **1973**, *95*, 2927–2934.

9. In a separate experiment, the thioether intermediate was isolated in 80% yield. The quality of the hydrogen peroxide was found to be crucial in the oxidation step: when H_2O_2 of inferior quality was used, predominantly sulfoxide was formed, which could be isolated and resubmitted to the reaction conditions to give the sulfone.

10. This compound was obtained following a literature procedure: Zhu, L.; Ni, C.; Zhao, Y.; Hu, J. *Tetrahedron*, **2010**, *66*, 5089–5100.

11. Lower yields were obtained for this compound due to the poor solubility of the thiol under the Mitsunobu conditions, which led to significant amount of homo-coupled alcohol product. In a separate experiment, this was overcome by adding a small amount of CH_2Cl_2 to the reaction mixture. Again, the quality of H_2O_2 proved to be crucial.

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14. Compound **12** is not UV active, nor can be made visible using TLC stains ($KMnO_4$, vanillin, I_2, bromocresol green, ninhydrin, phosphomolybdic acid, 2,4-DNP). The compound was poorly detected electrophoretic light scattering (ELS). We had to resort to GC-FID in order to detect the desired compound.

15. Yeh, M.-C. P.; Liang, C.-J.; Chen, H.-F.; Weng, Y.-T. *Adv. Synth. Catal.* **2015**, *357*, 3242–3254.

16. This compound was obtained following a literature procedure: Madhushaw, R. J.; Lin, M.-Y.; Sohel, S. M. A.; Liu, R.-S. *J. Am. Chem. Soc.* **2004**, *126*, 6895–6899.

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