Supporting Information

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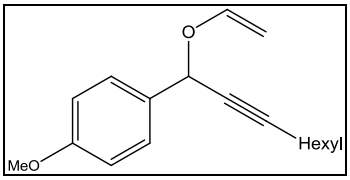
General Consideration. All commercially procured chemicals were used as received. Dichloromethane (DCM), tetrahydrofuran (THF), triethylamine (Et_3N), diethyl ether (Et_2O) were distilled from calcium hydride (CaH_2). Tetrahydrofuran (THF) was distilled from lithium aluminum hydride (LAH). Reagent grade solvents were used for solvent extraction and organic extracts were dried over anhydrous sodium sulfate (Na_2SO_4). Silica gel 60 (230-400 mesh ASTM) was used for Flash Chromatography with dry hexane/ethyl acetate eluent system. ^1H NMR spectra were recorded on 700 MHz Bruker, 500 MHz Varian, 500 MHz Bruker, 400 MHz Varian, or 300 MHz Varian spectrometers. ^{13}C spectra were recorded on 75 MHz Varian spectrometers. The proton chemical shifts (δ) are reported as parts per million relative to 7.26 ppm for $CDCl_3$, 7.14 ppm for C_6D_6, 5.32 for CD_2Cl_2. The carbon chemical shifts (δ) were reported as the centerline of triplet at 77.0 ppm for $CDCl_3$, quintet at 54.00 ppm for CD_2Cl_2 and triplet at 128.0 for C_6D_6. Infrared spectra were recorded on sodium chloride plates using a Perkin-Elmer FT-IR Paragon 1000 spectrometer and frequencies were reported as reciprocal of centimeters (cm^{-1}). Mass spectra were recorded using a Jeol JMS-600 instrument. The computations were performed using Gaussian03 on High Performance Computing facility (HPC) at Florida State University.

General Procedure for Vinylation of Alcohols:

To a 0.1M solution of 1-(4-methoxyphenyl)non-2-yn-1-ol (1mmol) in ethyl vinyl ether was added 0.6 mmol of mercuric acetate. The reaction mixture was refluxed at 45 ^oC for 12 hours before quenching with a saturated aqueous sodium carbonate solution. The organic phase was extracted using diethyl ether and dried over anhydrous potassium carbonate. The solvent was removed under vacuum and the crude vinyl ether was purified on alumina gel column using hexane as an eluent. Vinyl ether **11** was obtained in 45% yield (0.12g).

Vinyl Ether **1**



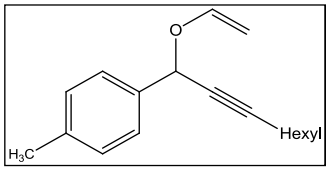
^{1}H NMR (300 MHz, C_6D_6) δ: 7.42 (d, *J* = 8.8 Hz, 2H), 6.93 (dd, *J* = 19.4, 8.8 Hz, 2H), 6.49 (dd, *J* = 14.1, 6.6 Hz, 1H), 5.45 (s, 1H), 4.43 (dd, *J* = 14.1, 1.5 Hz, 1H), 4.12 (dd, *J* = 6.6, 1.5 Hz, 1H), 3.80 (s, 3H), 2.28 (td, *J* = 7.0, 1.9 Hz, 2H), 1.61 – 1.47 (m, 2H), 1.47 – 1.20 (m, 6H), 0.89 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 160.07, 149.77, 130.75, 128.96, 113.92, 89.93, 89.56, 77.36, 71.04, 55.47, 31.51, 28.72, 22.77, 18.90, 14.03.

FTIR (neat): 3115, 3069, 3038, 3001, 2955, 2932, 2858, 2281, 2226, 2056, 2026, 1892, 1727, 1636, 1611, 1587, 1513, 1464, 1304, 1250, 1171, 1140, 1108, 1033.

HRMS (EI+) Calcd. For $C_{18}H_{24}O_2$ (M^+): 272.17763, Found: 272.17747.

Vinyl Ether **2**



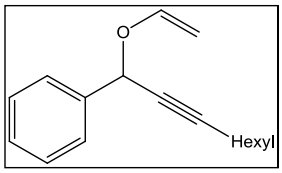
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.57 – 7.08 (m, 4H), 6.50 (dd, *J* = 14.1, 6.6 Hz, 1H), 5.48 (s, 1H), 4.44 (dd, *J* = 14.1, 1.7 Hz, 1H), 4.14 (dd, *J* = 6.6, 1.7 Hz, 1H), 2.37 (s, 1H), 2.29 (td, *J* = 7.0, 2.0 Hz, 1H), 1.61 – 1.48 (m, 1H), 1.47 – 1.24 (m, 2H), 0.90 (t, *J* = 6.8 Hz, 1H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 149.82, 138.69, 135.73, 129.32, 127.49, 89.99, 89.55, 77.41, 71.27, 31.54, 28.75, 22.81, 21.13, 18.94, 14.07.

FTIR (neat): 3116, 3028, 2956, 2930, 2859, 2237, 2200, 1727, 1637, 1612, 1513, 1457, 1378, 1270, 1177, 1140, 1109, 1019.

HRMS (EI+) Calcd. For $C_{18}H_{24}O$ (M^+): 256.18272, Found: 256.18139.

Vinyl Ether **3**



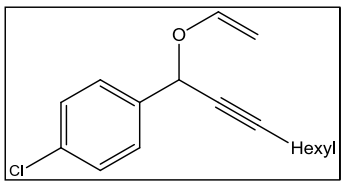
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.67 – 7.53 (m, 2H), 7.50 – 7.36 (m, 3H), 6.59 (dd, *J* = 14.1, 6.6 Hz, 1H), 5.58(s, 1H), 4.55 (dd, *J* = 14.1, 1.7 Hz, 1H), 4.23 (dd, *J* = 6.6, 1.8 Hz, 1H), 2.36 (td, *J* = 7.0, 2.0 Hz, 2H), 1.72 – 1.56 (m, 2H), 1.56 – 1.31 (m, 6H), 0.98 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 149.84, 138.74, 128.70, 127.55, 90.15, 89.79, 77.33, 71.37, 31.58, 28.77, 22.84, 18.98, 14.12.

FTIR (neat): 3436, 3033, 3064, 2956, 2931, 2859, 2236, 2202, 1727, 1645, 1598, 1582, 1493, 1451, 1315, 1266, 1175, 1108, 1068, 1024, 1001.

HRMS (EI+) Calcd. For $C_{17}H_{22}O$ (M^+): 242.16677, Found: 242.16707.

Vinyl Ether **4**



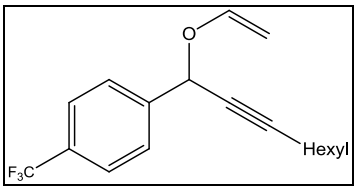
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.42 (dd, *J* = 30.4, 8.5 Hz, 2H), 6.50 (dd, *J* = 14.1, 6.6 Hz, 2H), 5.50 (s, 1H), 4.47 (dd, *J* = 14.1, 1.8 Hz, 1H), 4.17 (dd, *J* = 6.6, 1.8 Hz, 1H), 2.29 (td, *J* = 7.0, 1.9 Hz, 2H), 1.54 (m, 2H), 1.47 – 1.24 (m, 6H), 0.90 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ 149.60, 137.33, 134.40, 128.94, 128.78, 90.39, 90.20, 76.78, 70.51, 31.49, 28.71, 28.64, 22.77, 18.89, 14.03.

FTIR (neat): 3115, 3030, 2956, 2930, 2858, 2237, 2201, 1727, 1638, 1617, 1595, 1490, 1466, 1402, 1267, 1171, 1139, 1091, 1015.

HRMS (EI+) Calcd. For $C_{17}H_{21}OCl$ (M^+): 276.12810 Found: 276.12679.

Vinyl Ether **5**



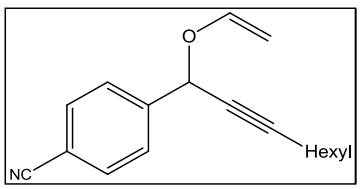
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.67 (s, 4H), 6.53 (dd, *J* = 14.2, 6.6 Hz, 1H), 5.59 (s, 1H), 4.49 (dd, *J* = 14.2, 2.0 Hz, 1H), 4.20 (dd, *J* = 6.6, 2.0 Hz, 1H), 2.29 (td, *J* = 7.04, 1.98 Hz, 2H), 1.61-1.22 (m, 8H), 0.89 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 149.53, 142.73, 130.73, 130.30, 127.75, 126.17, 125.67, 125.62, 125.57, 125.52, 118.96, 100.34, 90.58, 90.53, 76.55, 70.45, 31.47, 28.69, 28.59, 22.74, 18.87, 13.98.

FTIR (neat): 3118, 3052, 2959, 2933, 2860, 2283, 2227, 1925, 1638, 1618, 1467, 1417, 1326, 1261, 1167, 1130, 1108, 1067, 1019.

HRMS (EI+) Calcd. for $C_{18}H_{21}OF_3$ (M^+): 310.15446, Found: 310.15528.

Vinyl Ether **6**



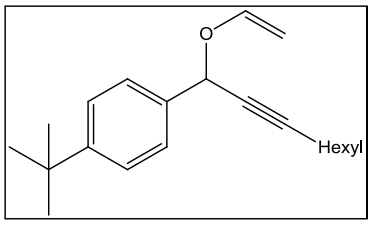
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.75 – 7.60 (m, 4H), 6.52 (dd, *J* = 14.1, 6.6 Hz, 1H), 5.57 (s, 1H), 4.49 (dd, *J* = 14.1, 2.0 Hz, 1H), 4.22 (dd, *J* = 6.6, 2.0 Hz, 1H), 2.29 (td, *J* = 7.0, 2.0 Hz, 1H), 1.53 (m, 2H), 1.47 – 1.22 (m, 6H), 0.90 (t, *J* = 6.7 Hz, 1H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 149.43, 143.64, 132.54, 127.97, 118.70, 112.46, 90.86, 90.76, 76.18, 70.29, 31.44, 28.68, 28.54, 22.74, 18.86, 14.00.

FTIR (neat): 3117, 3059, 2956, 2931, 2859, 2282, 2230, 1926, 1638, 1620, 1504, 1466, 1411, 1328, 1297, 1181, 1138, 1109, 1035, 1020.

HRMS (EI+) Calcd. For $C_{18}H_{21}ON$ (M^+): 267.16232, Found: 267.16235.

Vinyl Ether **13**



^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.44 (m, 4H), 6.54 (dd, *J* = 13.8, 6.6 Hz, 2H), 5.50 (m, 1H), 4.48 (dd, *J* = 14.2, 1.7 Hz, 1H), 4.16 (dd, *J* = 6.7, 1.9 Hz, 1H), 2.31 (td, *J* = 6.9, 1.9 Hz, 2H), 1.64-1.51 (m, 2H), 1.50 – 1.29 (m, 15H), 0.93 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 151.89, 149.89, 135.72, 127.29, 125.65, 89.94, 89.54, 77.43, 71.22, 34.73, 31.54, 31.30, 28.76, 22.80, 18.95, 14.07.

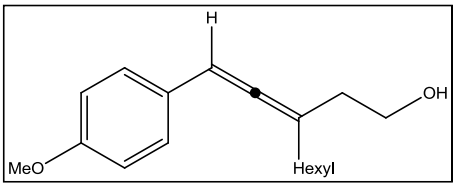
FTIR (neat): 3031, 2960, 2932, 2861, 2226, 1911, 1636, 1615, 1511, 1464, 1364, 1269, 1179, 1141, 1030.

HRMS (EI+) Calcd. For $C_{21}H_{30}O$ (M^+): 298.22967 Found: 298.22874.

General Procedure for Propargyl Claisen Rearrangement:

A solution of Ph_3PAuCl (5mg, 0.01 mmol) was prepared in 10mL methylene chloride. A separate solution of $AgSbF_6$ (3.4mg, 0.01 mmol) was prepared in 10mL of methylene chloride. To a solution of vinyl ether **11** (0.2 mmol) in 0.05M methylene chloride was added 0.1mL of a standard solution of Ph_3PAuCl and 0.1mL of $AgSbF_6$. The reaction time was recorded at the moment of addition of $AgSbF_6$. The reaction was allowed to run for exactly five minutes before quenching with 2 mL of methanol and sodium borohydride (10 mg). The reaction mixture was stirred for another 30 minutes before extracting the organic phase with the methylene chloride. The organic phase was dried over anhydrous potassium carbonate. Products were isolated using silica column chromatography. Yields given represent average of three runs.

Allene **7**



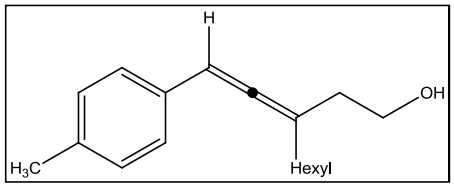
Using the general procedure described above, vinyl ether **1** gave 21% of allene **8** in five minutes. **^{1}H NMR** (300 MHz, CD_2Cl_2) δ: 7.23 (m, 2H), 6.88 (m, 2H), 6.18 (dd, *J* = 5.9, 2.9 Hz, 1H), 3.80 (s, 3H), 3.75 (t, *J* = 6.1 Hz, 2H), 2.36 (m, 2H), 2.13 (td, *J* = 7.4, 2.8 Hz, 2H), 1.90 (s, 1H), 1.51 (m, 2H), 1.45 – 1.23 (m, 6H), 0.90 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 201.39, 158.90, 128.00, 127.65, 114.26, 105.90, 95.38, 61.00, 55.43, 36.26, 33.27, 31.93, 29.30, 27.82, 22.88, 14.12.

FTIR (neat): 3383, 3064, 3001, 2955, 2928, 2856, 2872, 1946, 1735, 1608, 1580, 1510, 1465, 1442, 1297, 1248, 1171, 1107, 1036.

HRMS (EI+) Calcd. For $C_{18}H_{26}O_2$ (M^+): 274.19328, Found: 274.19323.

Allene **8**



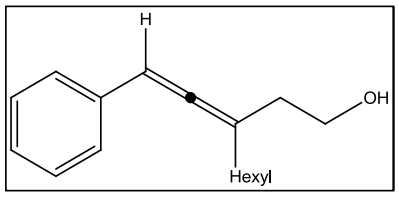
Using the general procedure described above, vinyl ether **2** gave 28% of allene **9** in five minutes. **^{1}H NMR** (300 MHz, CD_2Cl_2) δ: 7.39 – 6.96 (m, 5H), 6.20 (m, 1H), 3.75 (t, *J* = 6.4 Hz, 2H), 2.35 (s, 3H), 2.13 (m, 2H), 1.60 – 1.24 (m, 8H), 0.91 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 201.85, 136.70, 132.80, 129.51, 126.53, 105.85, 95.80, 61.01, 36.18, 33.25, 31.98, 29.35, 27.84, 22.93, 21.11, 14.13.

FTIR (neat): 3446, 3088, 3019, 2955, 2926, 2856, 2871, 1948, 1513, 1465, 1457, 1377, 1046, 1019.

HRMS (EI+) Calcd. For $C_{18}H_{26}O$ (M^+): 258.19837, Found: 258.19716.

Allene **9**



Using the general procedure described above, vinyl ether **4** gave 100% of allene **11** in five minutes.

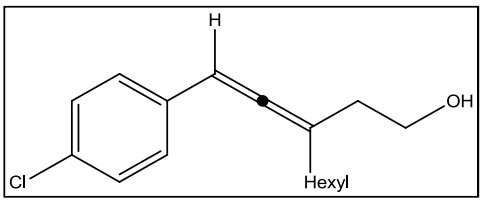
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.39 – 7.11 (m, 5H), 6.30 – 6.12 (m, 1H), 3.75 (t, *J* = 6.3 Hz, 2H), 2.41 – 2.32 (m, 2H), 2.14 (dd, *J* = 10.9, 3.8 Hz, 2H), 1.61 – 1.45 (m, 2H), 1.43 – 1.22 (m, 6H), 0.89 (t, *J* = 6.6 Hz, 1H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 202.21, 135.83, 128.77, 126.83, 126.61, 106.04, 95.92, 60.97, 36.16, 33.14, 31.92, 29.29, 27.79, 22.87, 14.06.

FTIR (neat): 3333, 3083, 3063, 3031, 2954, 2926, 2871, 2856, 1947, 1598, 1496, 1461, 1377, 1046, 1028.

HRMS (EI+) Calcd. For $C_{17}H_{24}O$ (M^+): 244.18272, Found: 244.18242.

Allene **10**



Using the general procedure described above, vinyl ether **5** gave 60% of allene **12** in five minutes.

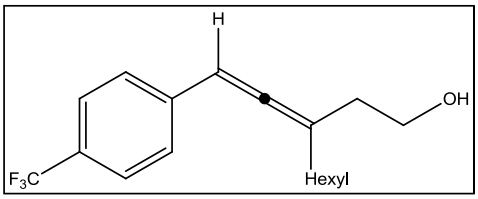
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.32 – 7.20 (m, 4H), 6.17 (s, 1H), 3.73 (t, *J* = 6.3 Hz, 2H), 2.35 (ddd, *J* = 10.0, 6.3, 3.7 Hz, 2H), 2.12 (td, *J* = 7.4, 2.8 Hz, 2H), 1.63 – 1.20 (m, 8H), 0.87 (t, *J* = 6.6 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ 202.57, 134.65, 132.21, 128.88, 127.94, 106.41, 95.03, 60.86, 36.02, 33.11, 31.98, 29.36, 27.81, 22.95, 14.17.

FTIR (neat): 3345, 3081, 3045, 2955, 2927, 2871, 2856, 1948, 1707, 1490, 1466, 1458, 1387, 1091, 1046, 1013.

HRMS (EI+) Calcd. For $C_{17}H_{23}OCl$ (M^+): 278.14375, Found: 258.14266.

Allene **11**



Using the general procedure described above, vinyl ether **6** gave 5% of allene **13** in five minutes.

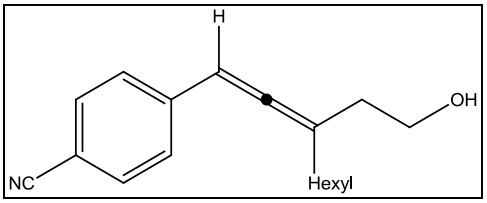
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.54 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 6.23 (m, 1H), 3.74 (q, *J* = 6.2 Hz, 2H), 2.36 (ddd, *J* = 9.4, 6.2, 3.1 Hz, 1H), 2.13 (td, *J* = 7.5, 2.9 Hz, 1H), 1.47 (m, 2H), 1.39 – 1.21 (m, 6H), 0.85 (t, *J* = 6.6 Hz, 2H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 203.47, 140.08, 128.59, 128.16, 126.79, 126.46, 125.70, 125.65, 125.59, 125.54, 122.86, 106.73, 95.04, 60.82, 35.97, 32.92, 31.88, 29.26, 27.71, 22.84, 14.01.

FTIR (neat): 3343, 3069, 3044, 2957, 2929, 2858, 2873, 1948, 1616, 1516, 1467, 1394, 1330, 1231, 1202, 1164, 1126, 1066, 1016.

HRMS (EI+) Calcd. For $C_{18}H_{23}OF_3$ (M^+): 312.17011, Found: 312.17023.

Allene **12**



Using the general procedure described above, vinyl ether **7** gave trace of allene **14** in five minutes.

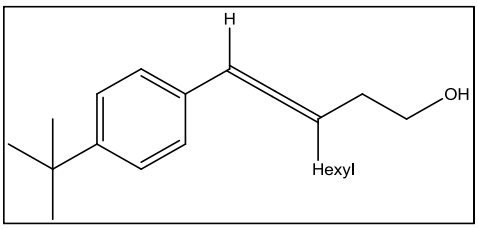
^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.58 (m, 2H), 7.40 (m, 2H), 6.22 (quin., *J* = 2.7 Hz, 1H), 3.74 (m, 2H), 2.37 (ddd, *J* = 9.3, 6.4, 3.0 Hz, 2H), 2.13 (td, *J* = 7.6, 3.2 Hz, 2H), 1.67 (m, 2H), 1.55 – 1.20 (m, 6H), 0.86 (t, *J* = 6.87 Hz, 3H).

^{13}C NMR (75 MHz, CD_2Cl_2) δ: 204, 141.24, 132.57, 127.10, 119.29, 109.87, 107.08, 95.14, 60.76, 35.93, 32.82, 31.84, 29.22, 27.66, 22.82, 14.01.

FTIR (neat): 3426, 3063, 3038, 2955, 2928, 2857, 2227, 1964, 1604, 1502, 1458, 1395, 1379, 1340, 1205, 1173, 1107, 1047.

HRMS (EI+) Calcd. For $C_{18}H_{23}ON$ (M^+): 269.17797, Found: 269.17791.

Allene **14**



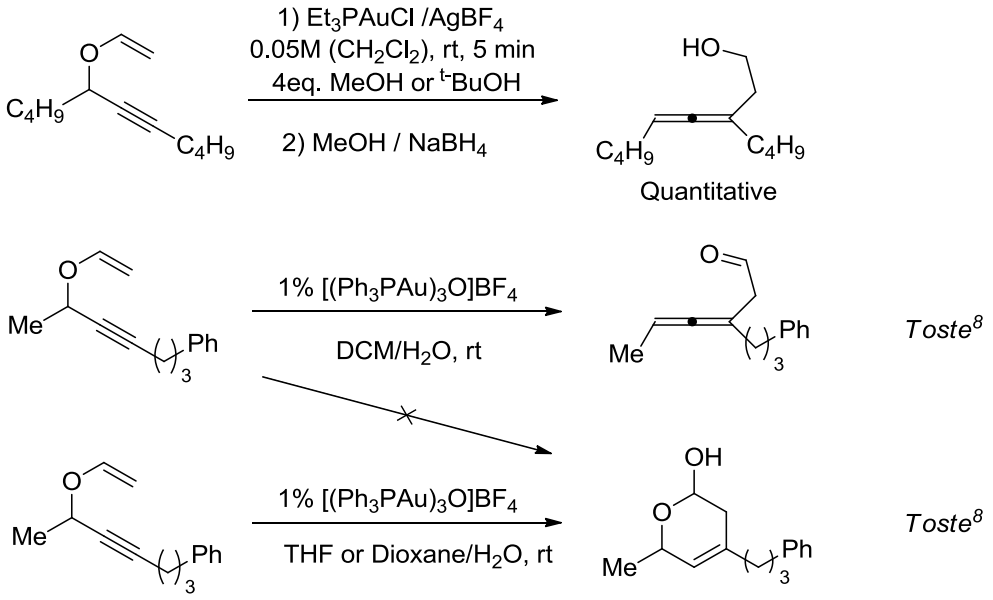
Using the general procedure described above, vinyl ether **3** gave 100% of allene **10** in five minutes.

^{1}H NMR (300 MHz, CD_2Cl_2) δ: 7.27 (m, 4H), 6.19 (m, 1H), 3.62 (q, *J* = 6.3 Hz, 2H), 2.17 (m, 2H), 1.97 (m, 2H), 1.53 – 1.40 (m, 2H), 1.39-1.11(m, 15H), 083 (t, *J* = 6.9 Hz, 3H).

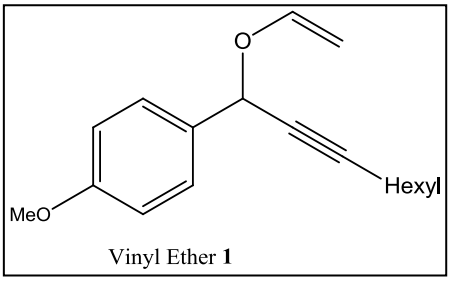
^{13}C NMR (75 MHz, CD_2Cl_2) δ: 201.98, 150.04, 132.76, 126.30, 125.77, 105.86, 95.68, 60.99, 36.23, 34.61, 33.22, 31.95, 31.29, 29.32, 27.82, 22.89, 14.08.

FTIR (neat): 3346, 3054, 3025, 2958, 2927, 2858, 1947, 1514, 1463, 1393, 1379, 1362, 1269, 1201, 1108, 1047, 1018.

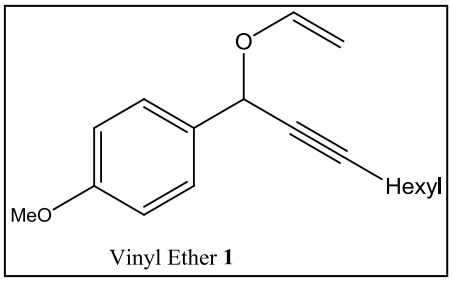
HRMS (EI+) Calcd. For $C_{21}H_{32}O$ (M^+): 300.24532, Found: 300.24586.



Scheme 1 The intermediacy of the six-membered intermediate in Au-catalyzed propargyl Claisen rearrangements depends on the reaction conditions.



Vinyl Ether **1**



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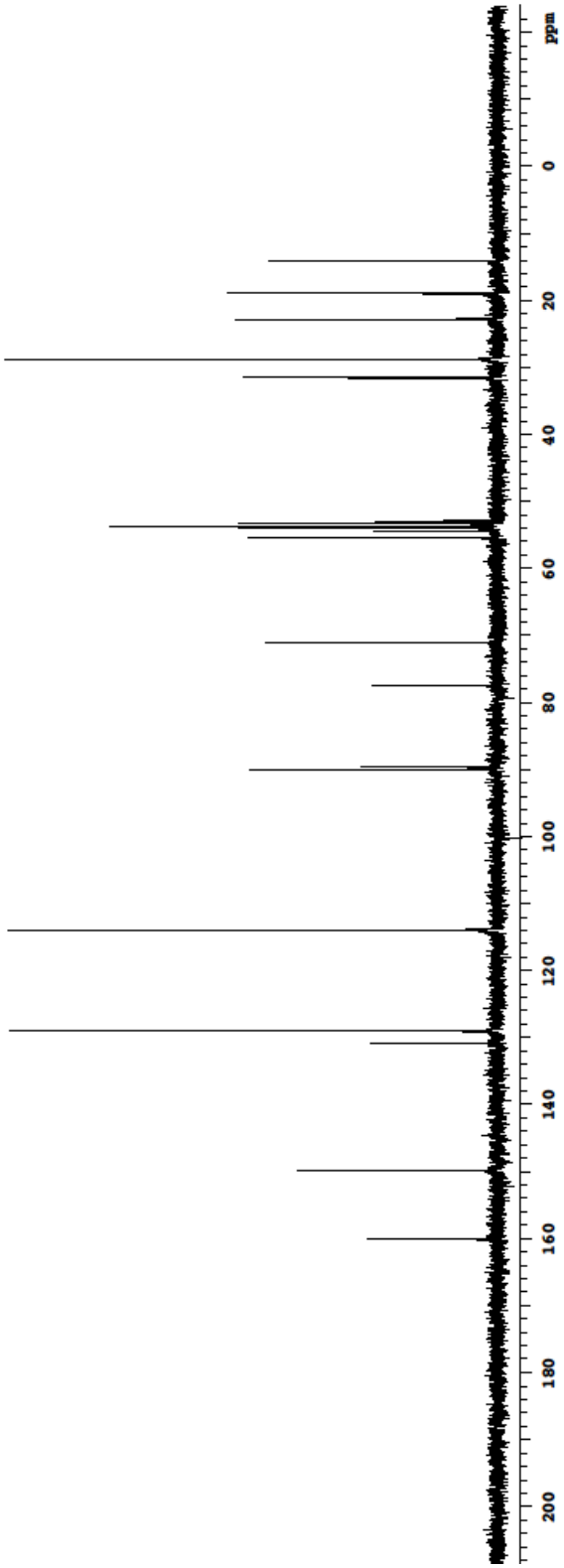

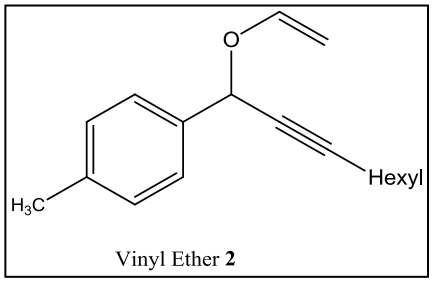

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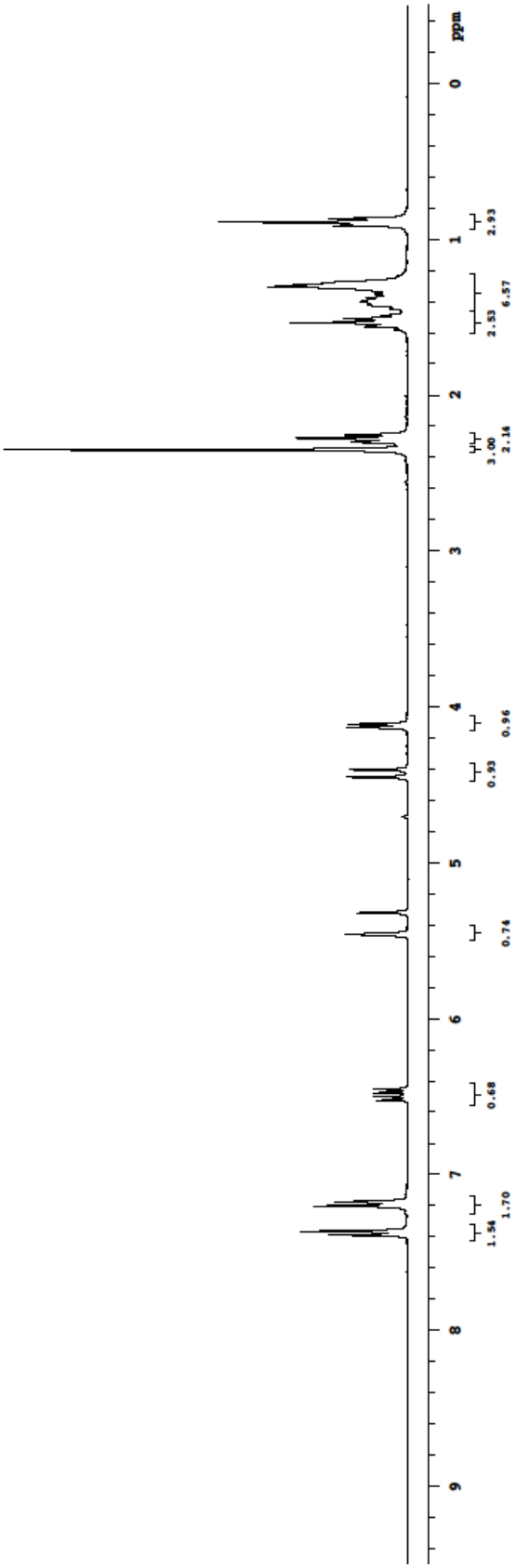

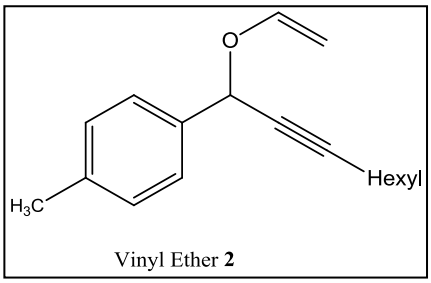

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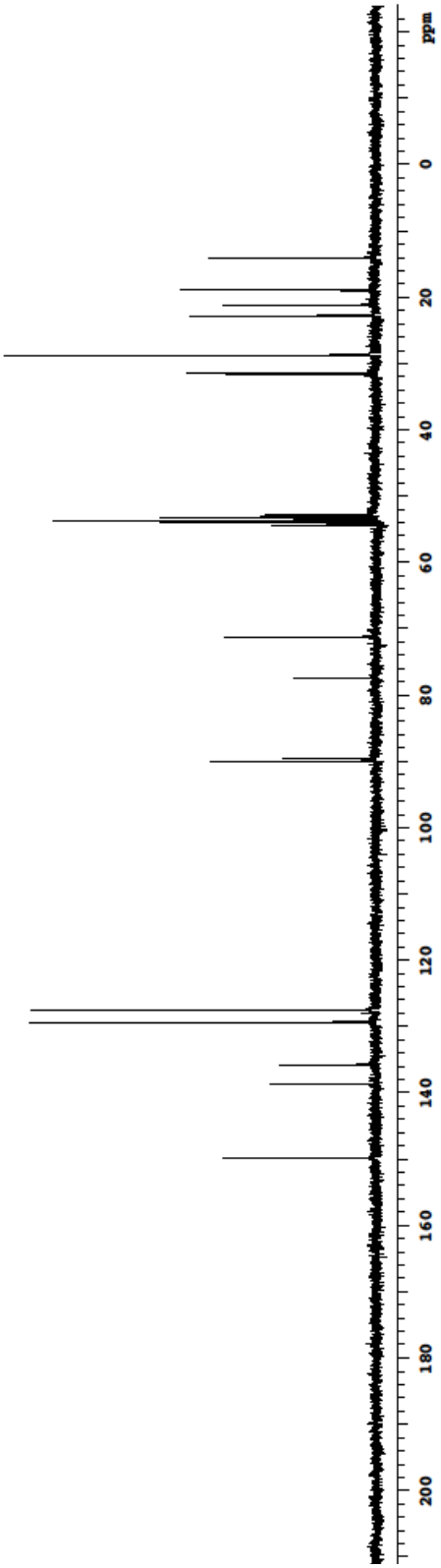

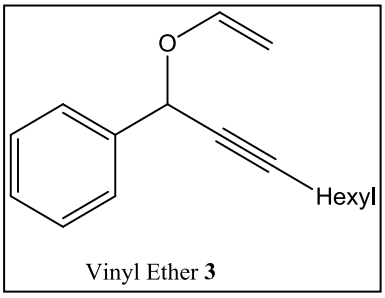

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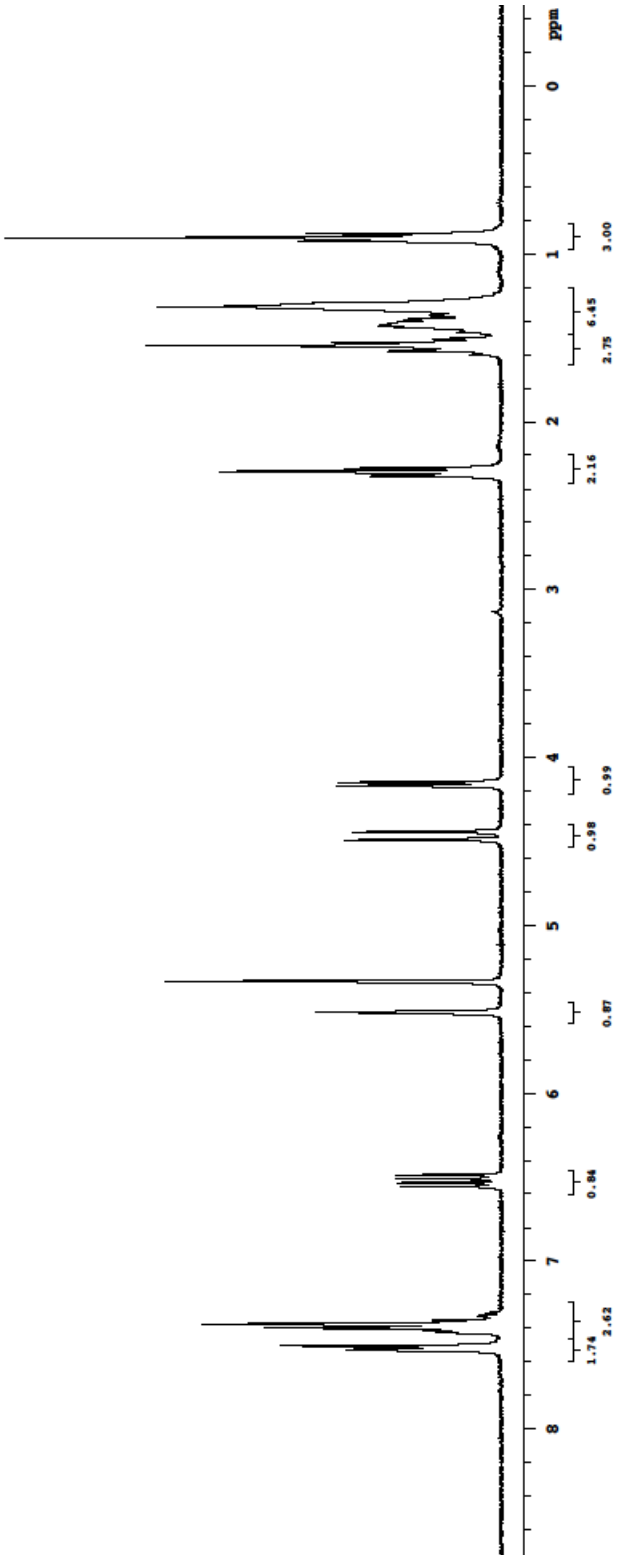

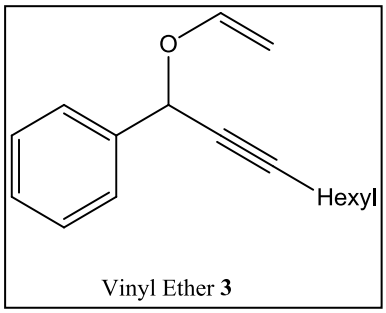

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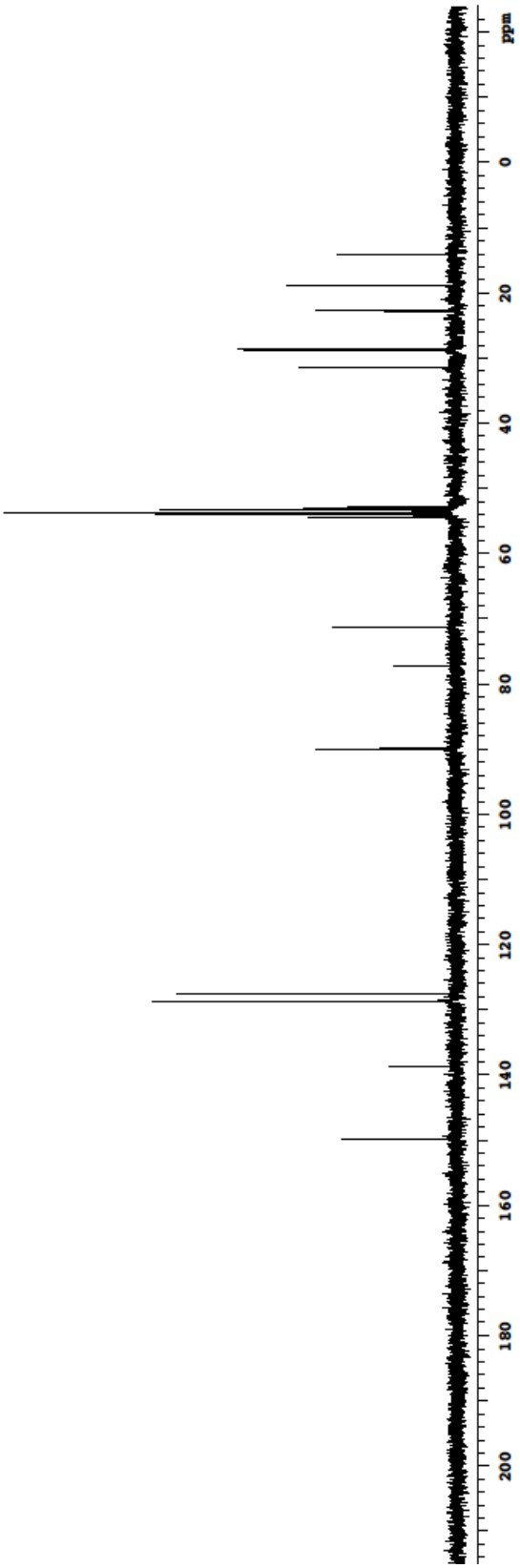

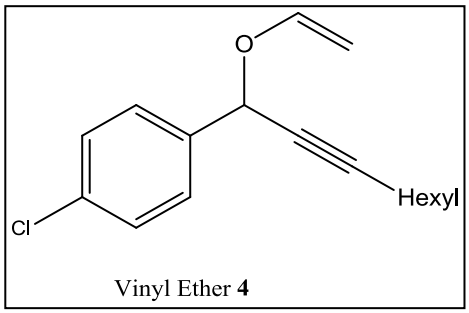

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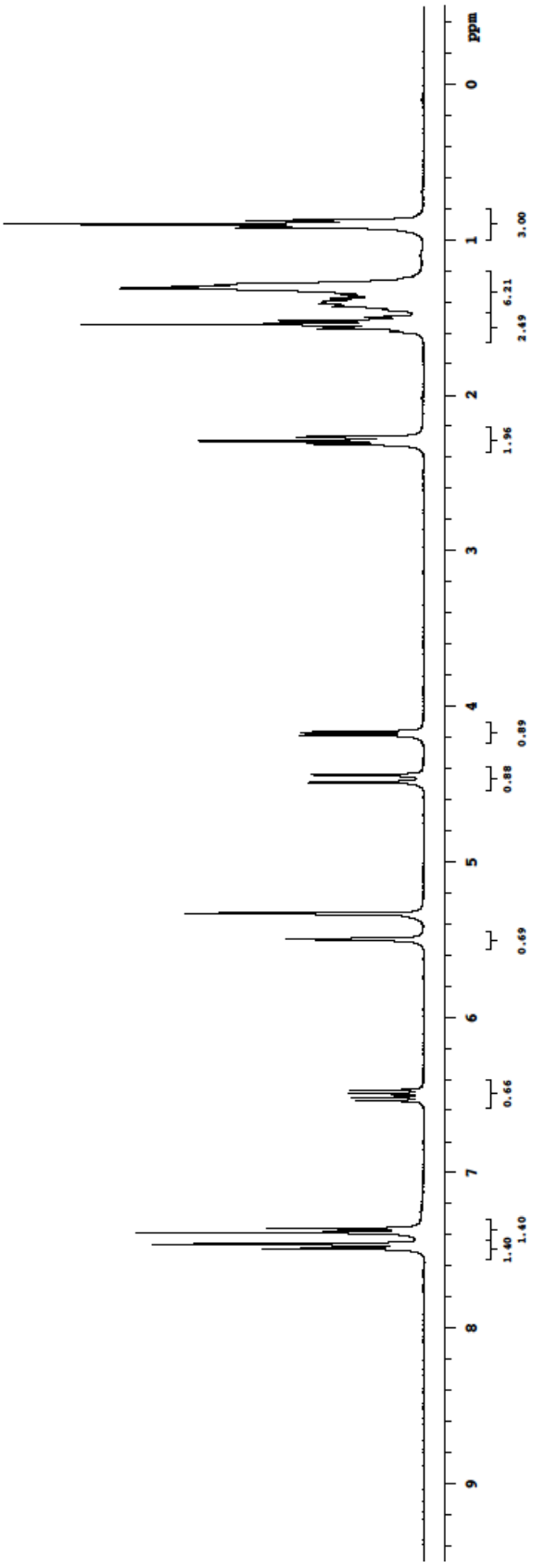

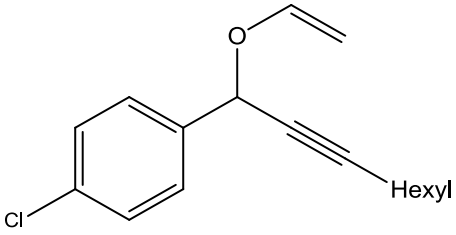

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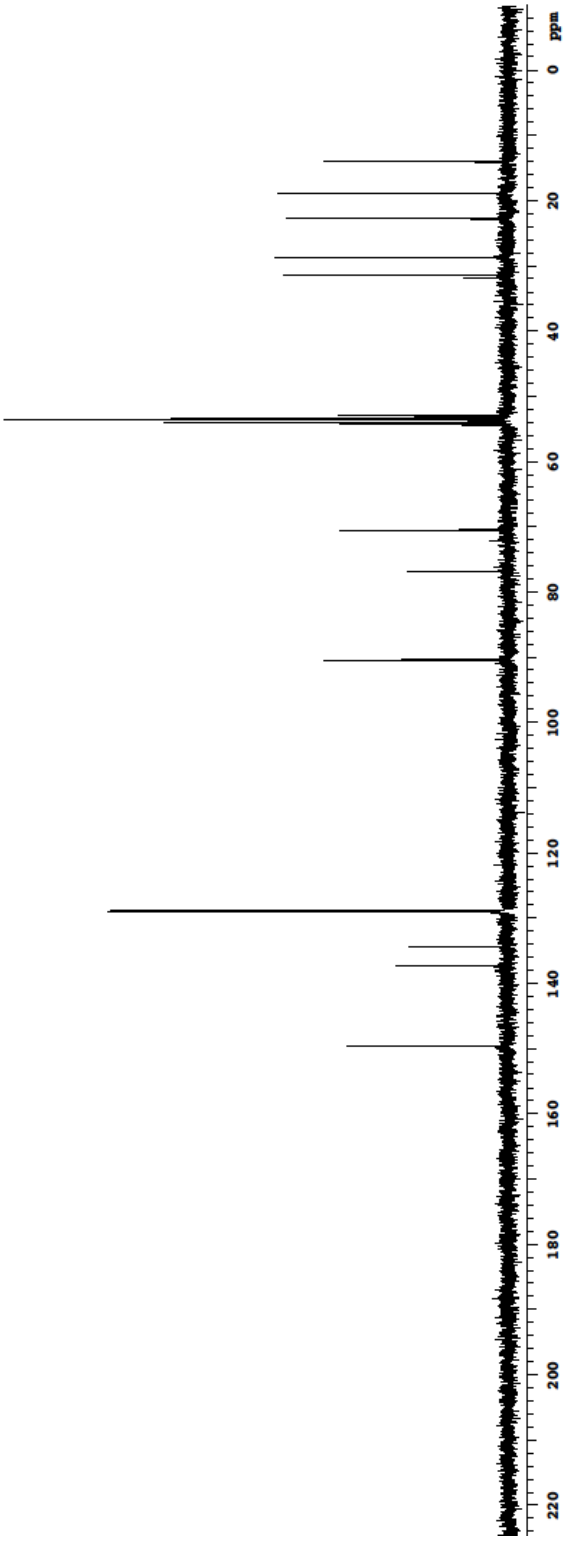

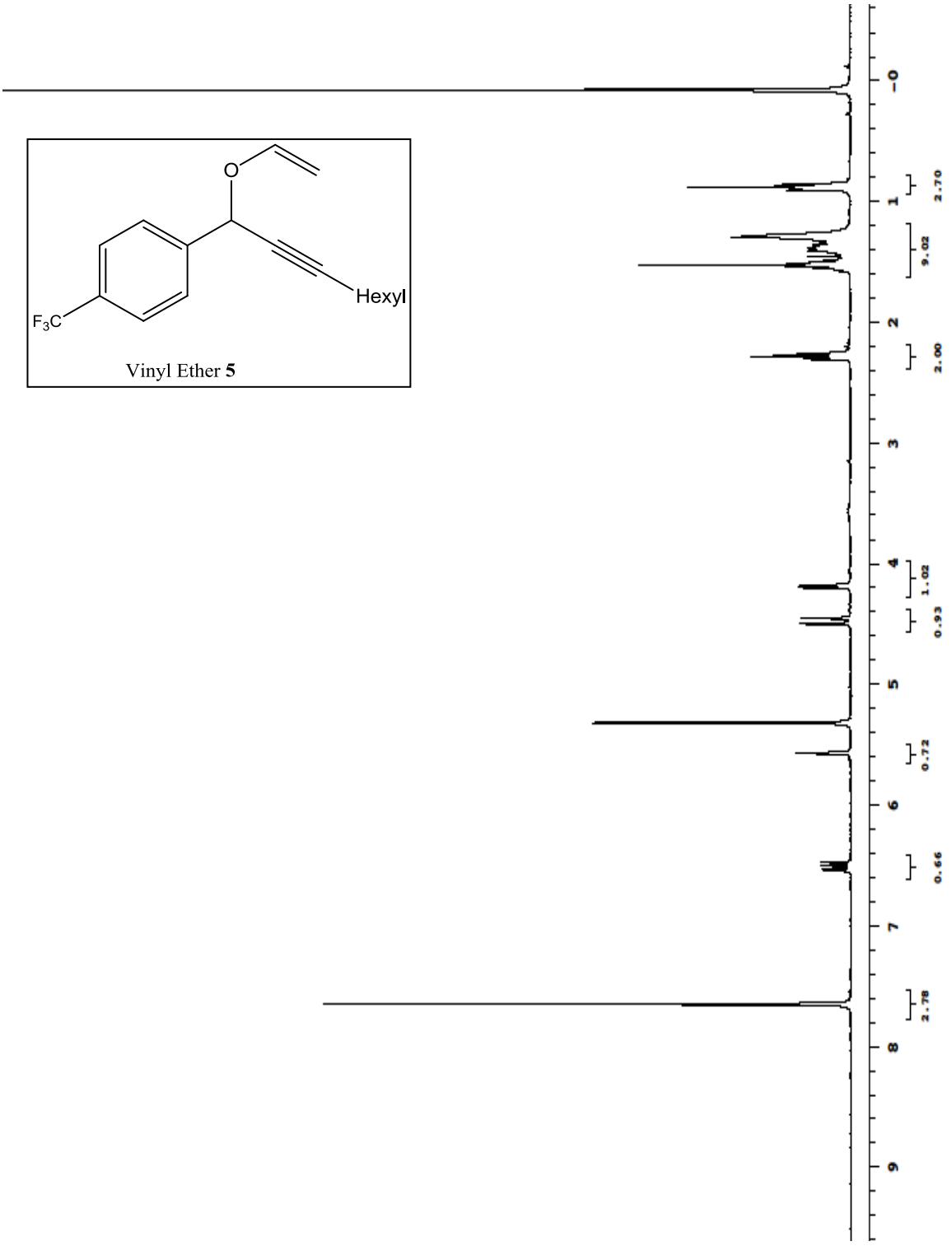

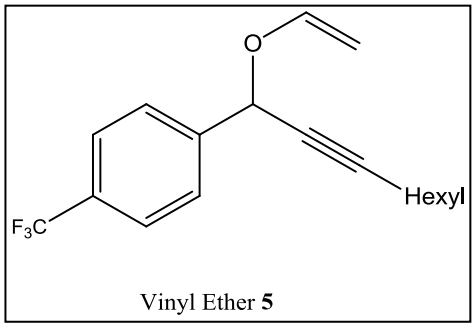

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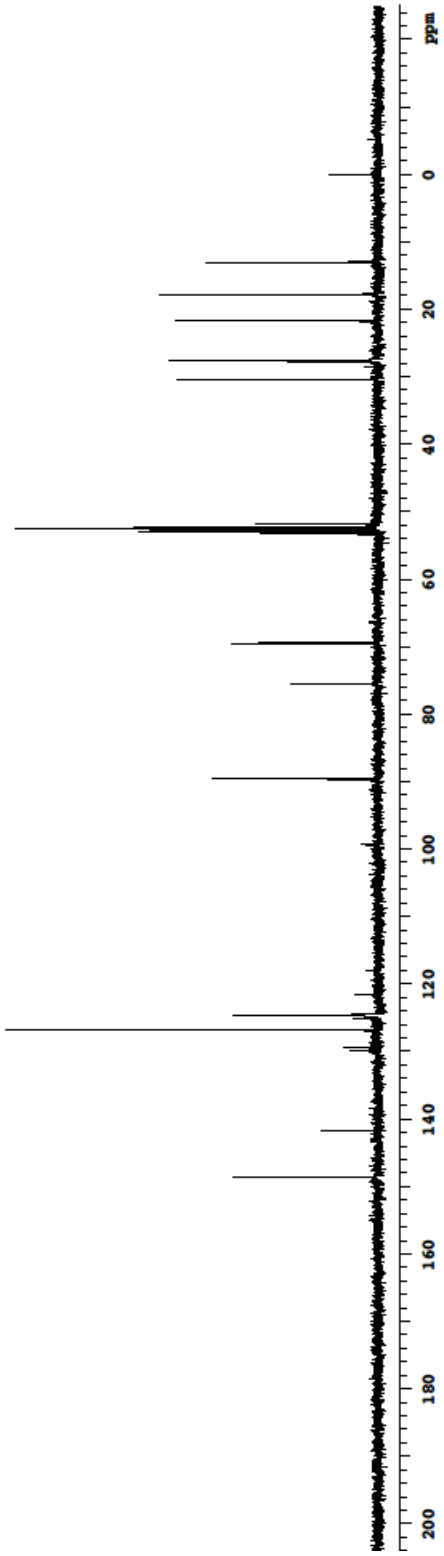

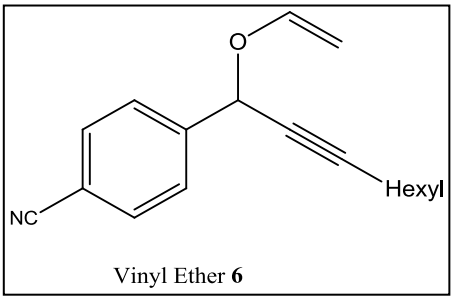

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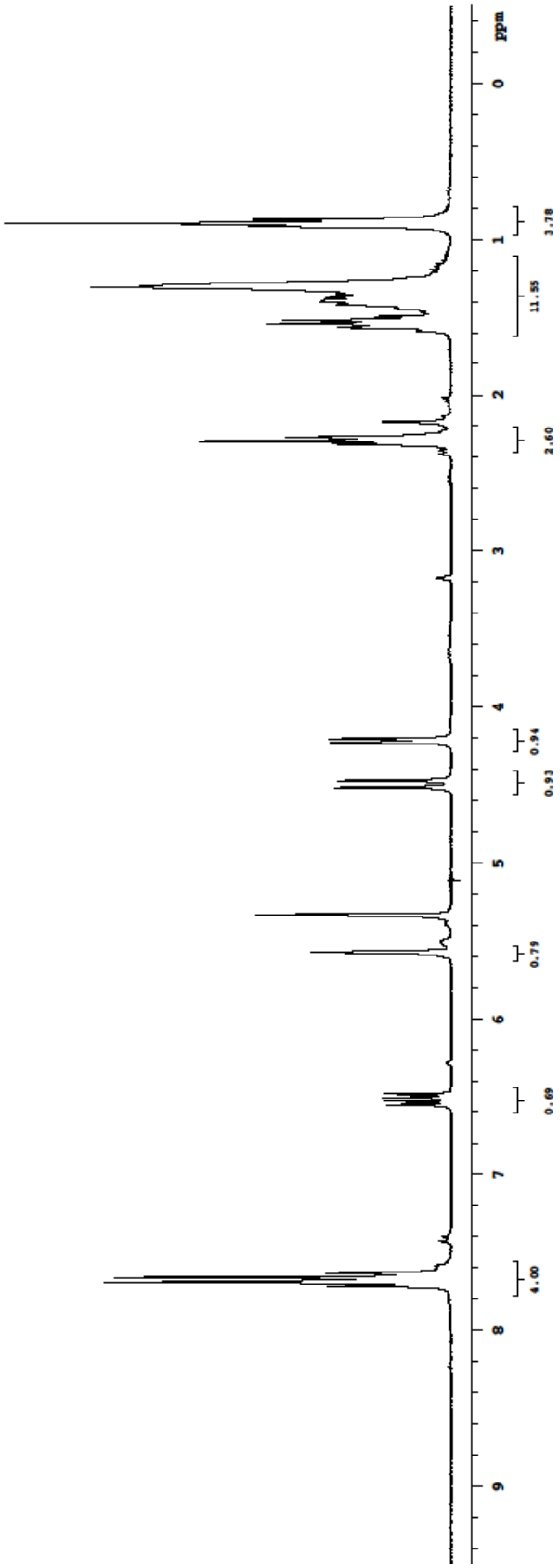

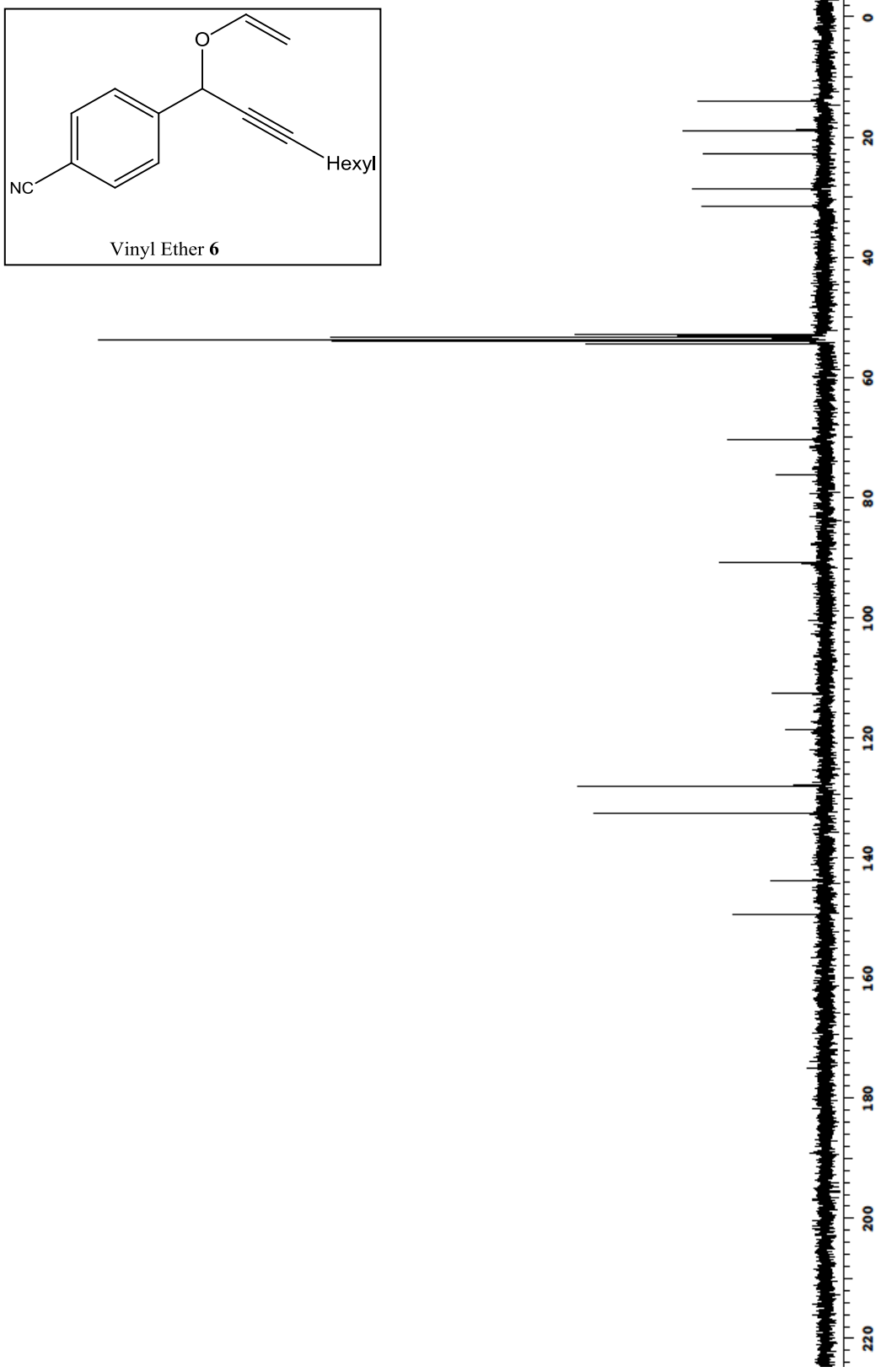

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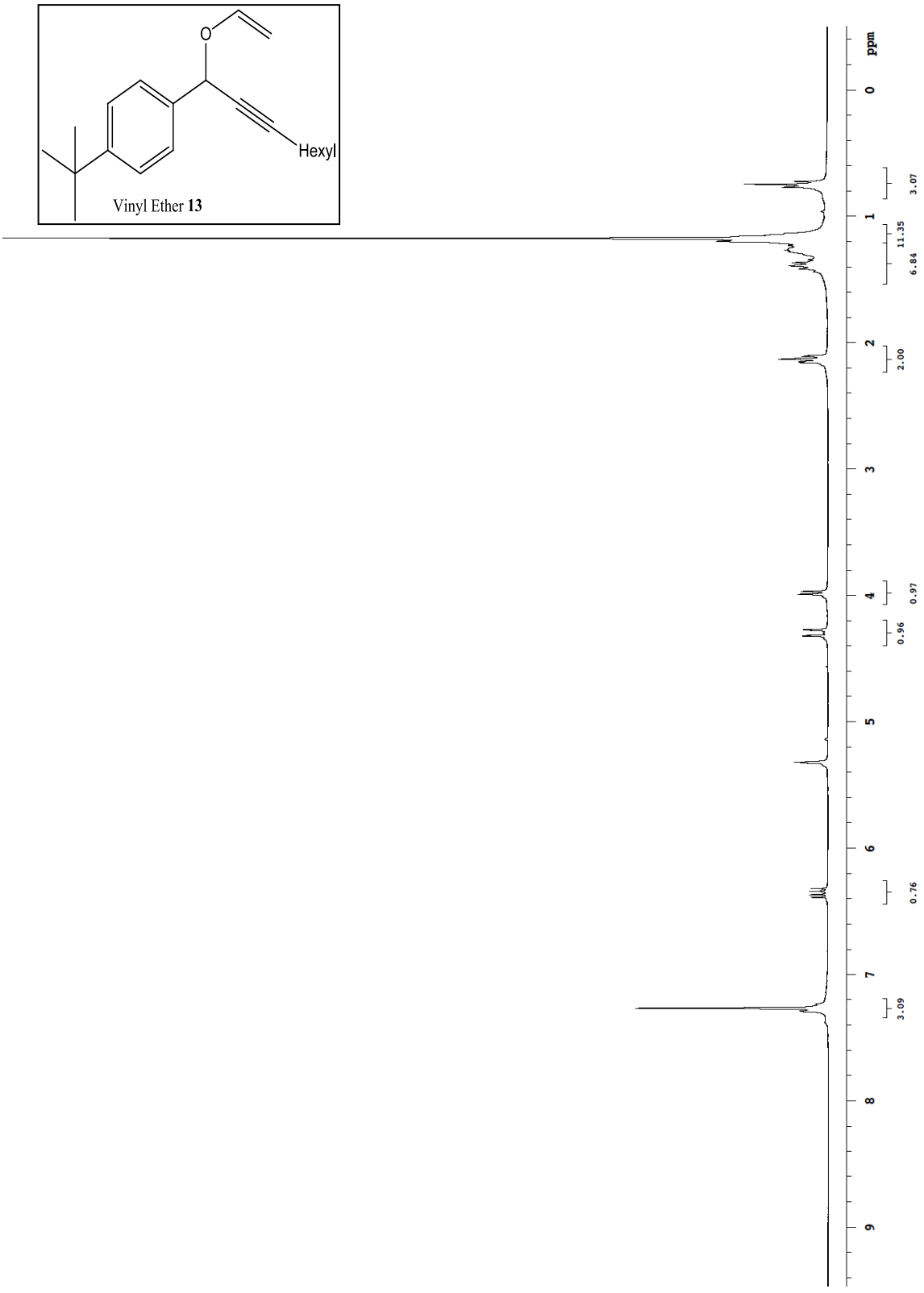
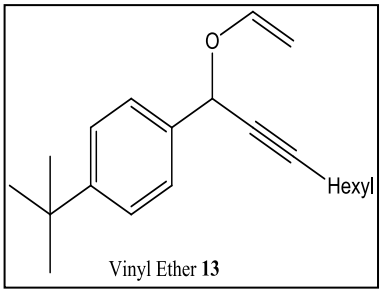
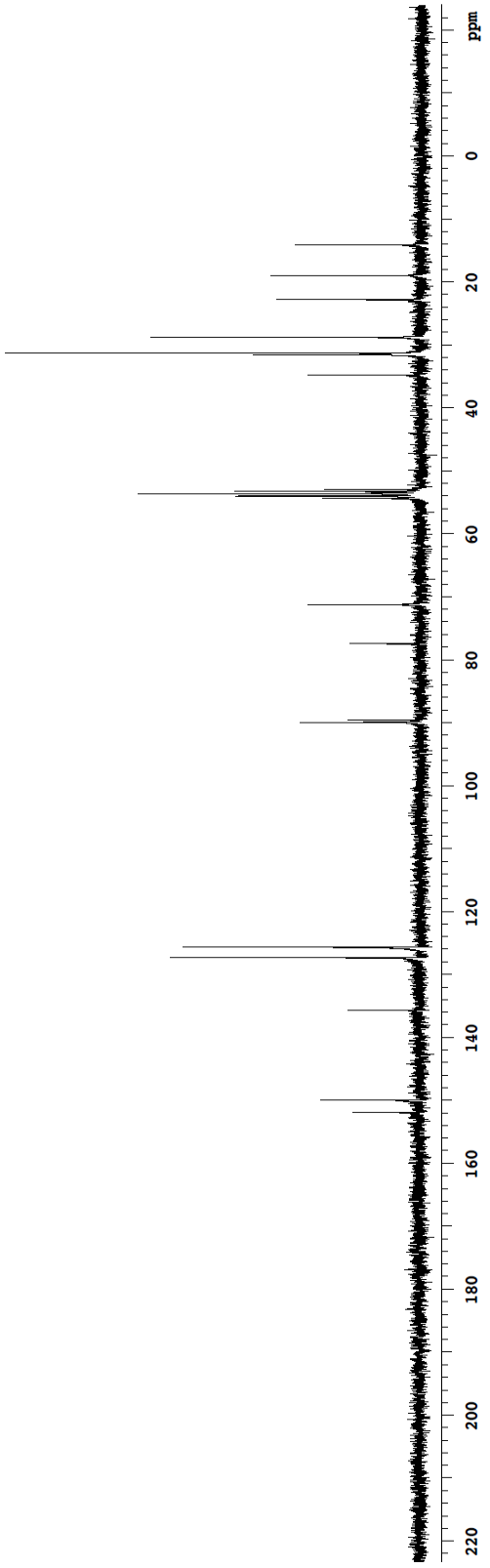
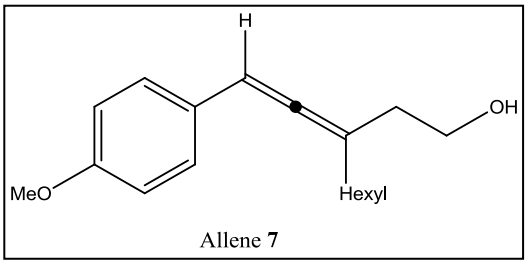




Vinyl Ether **13**





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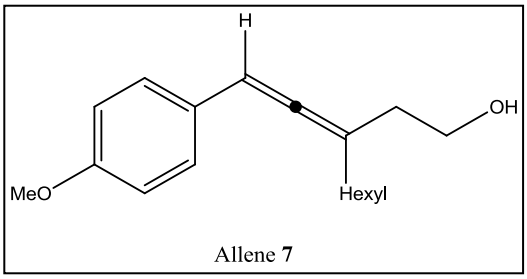

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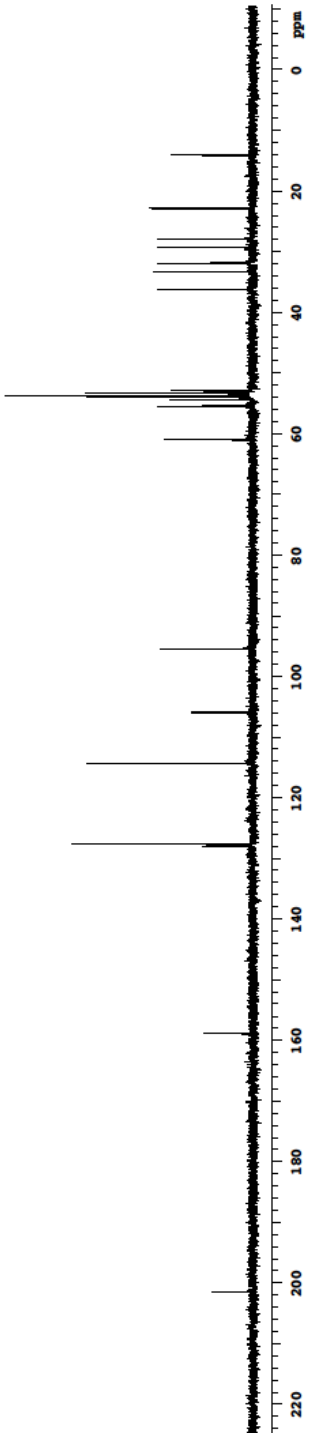

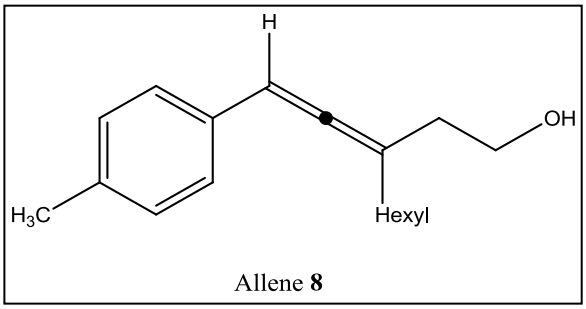

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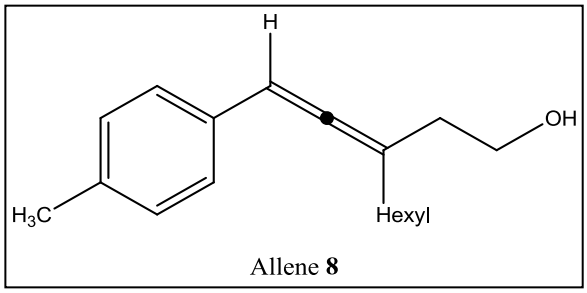

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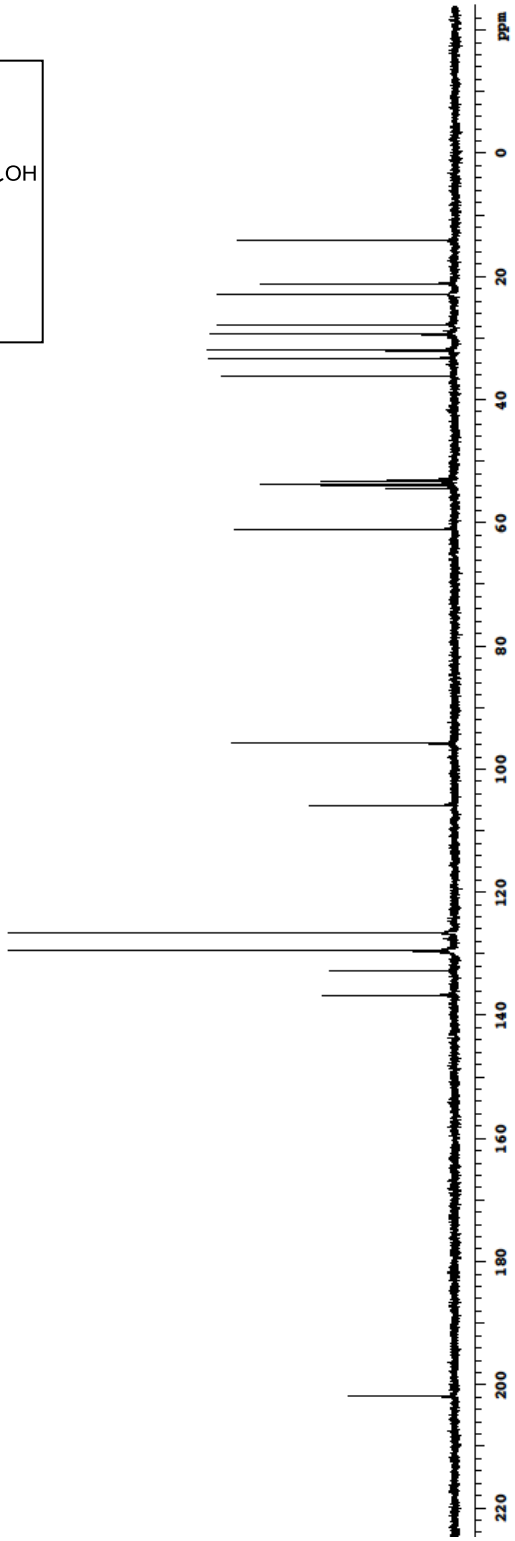

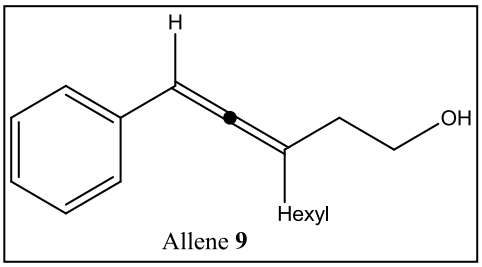

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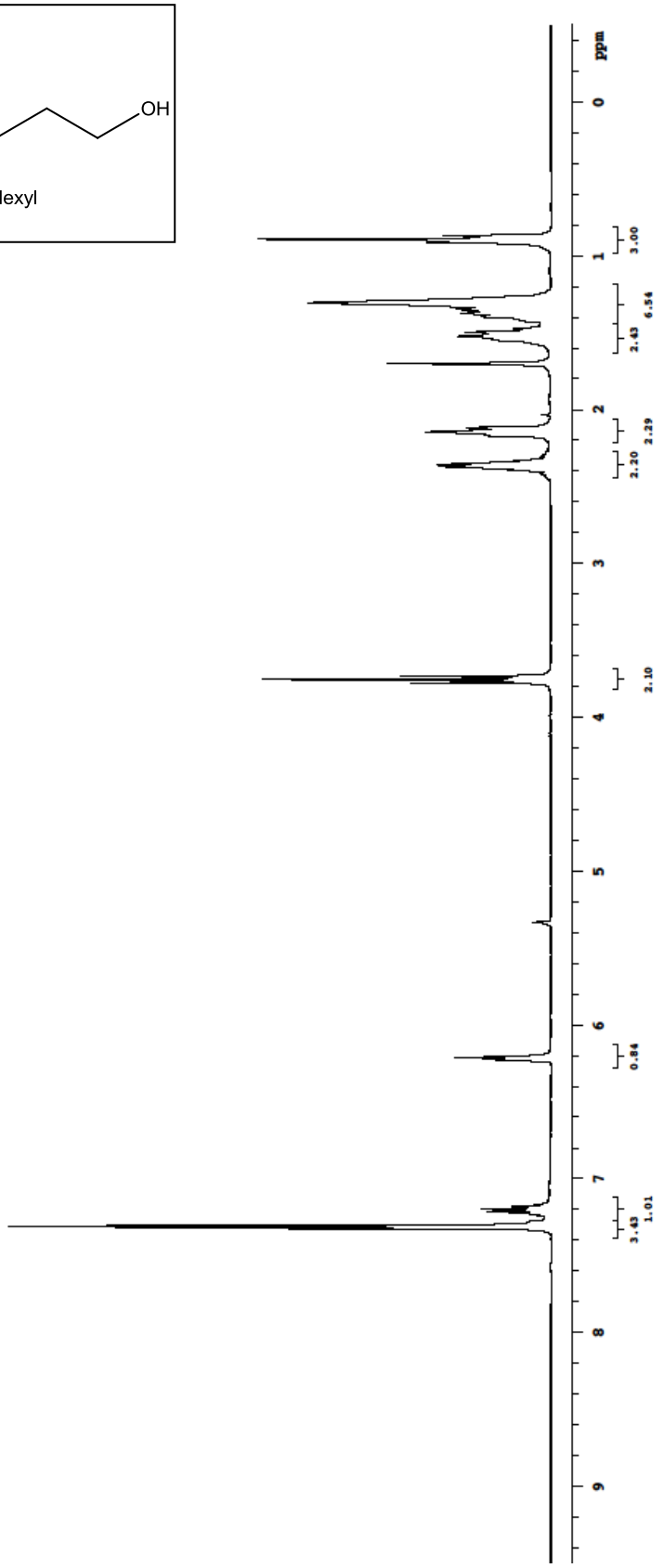

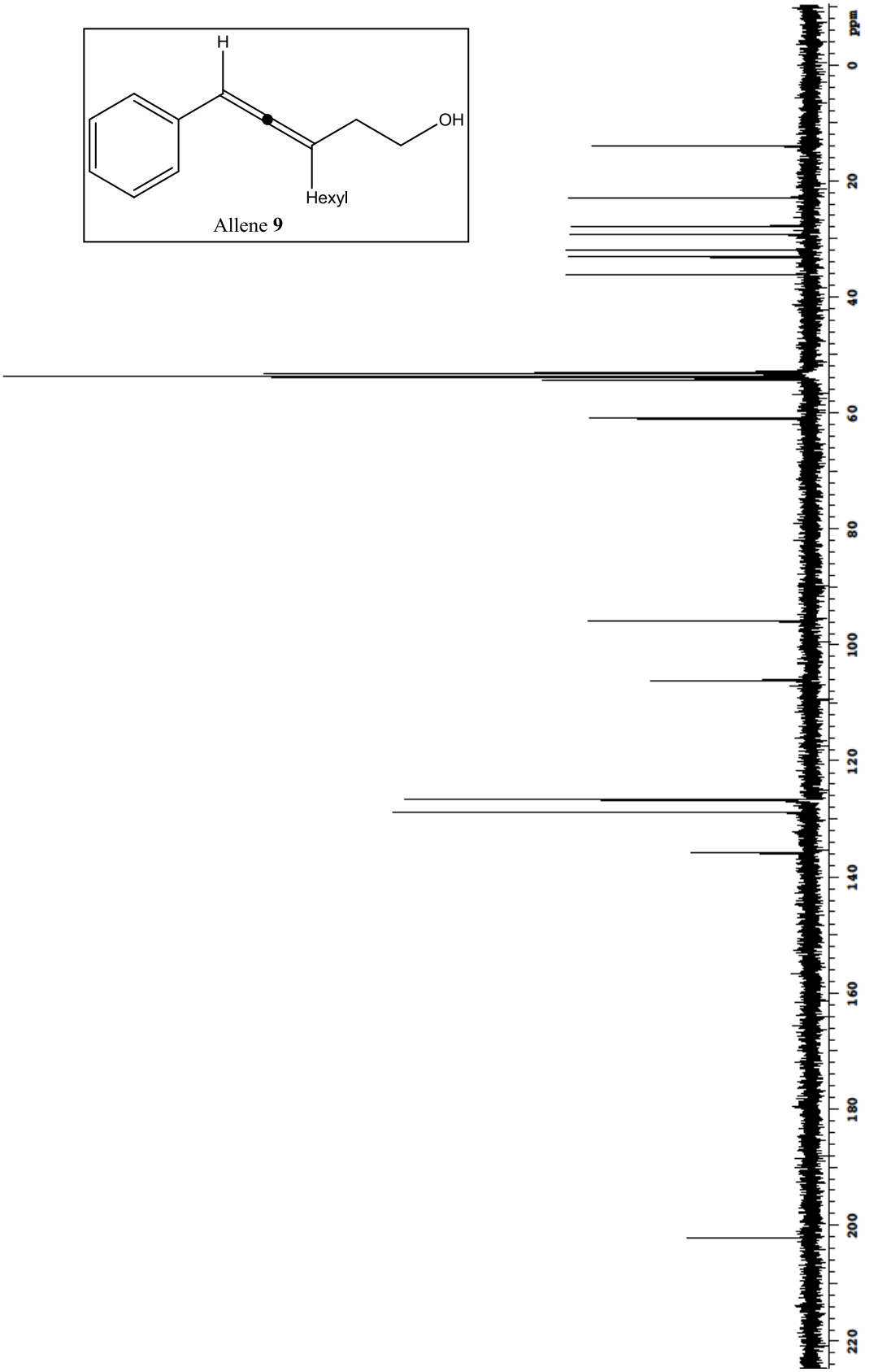

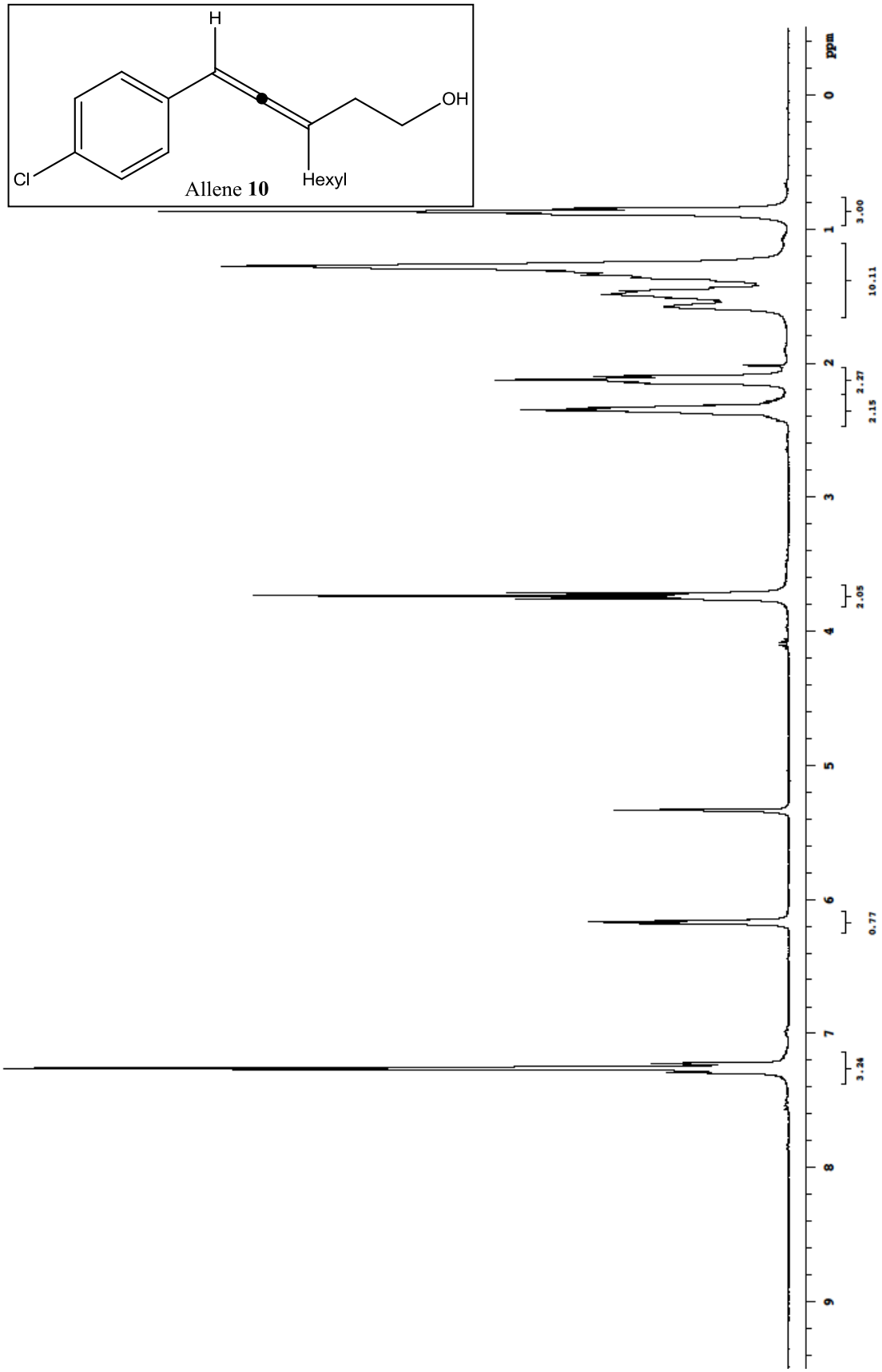

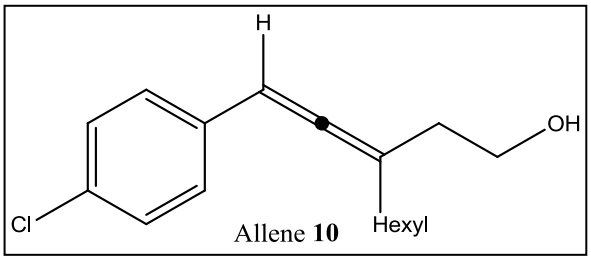

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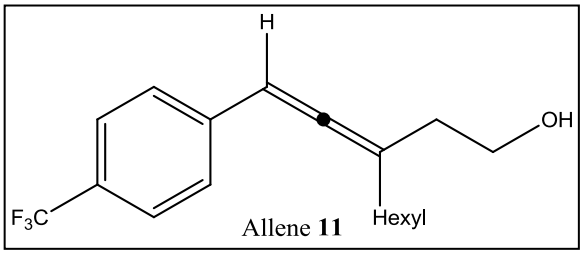

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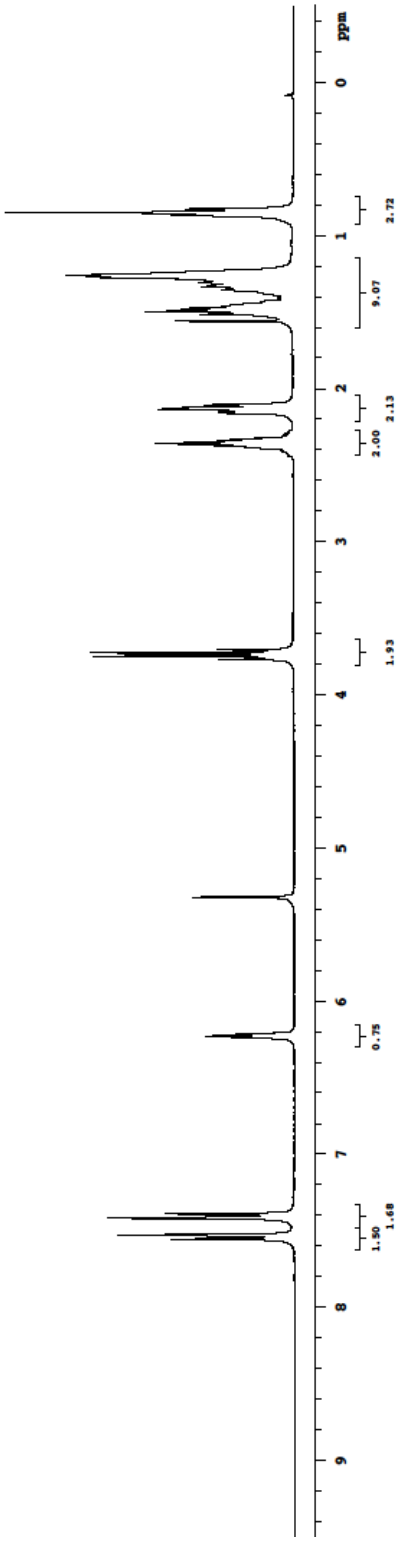

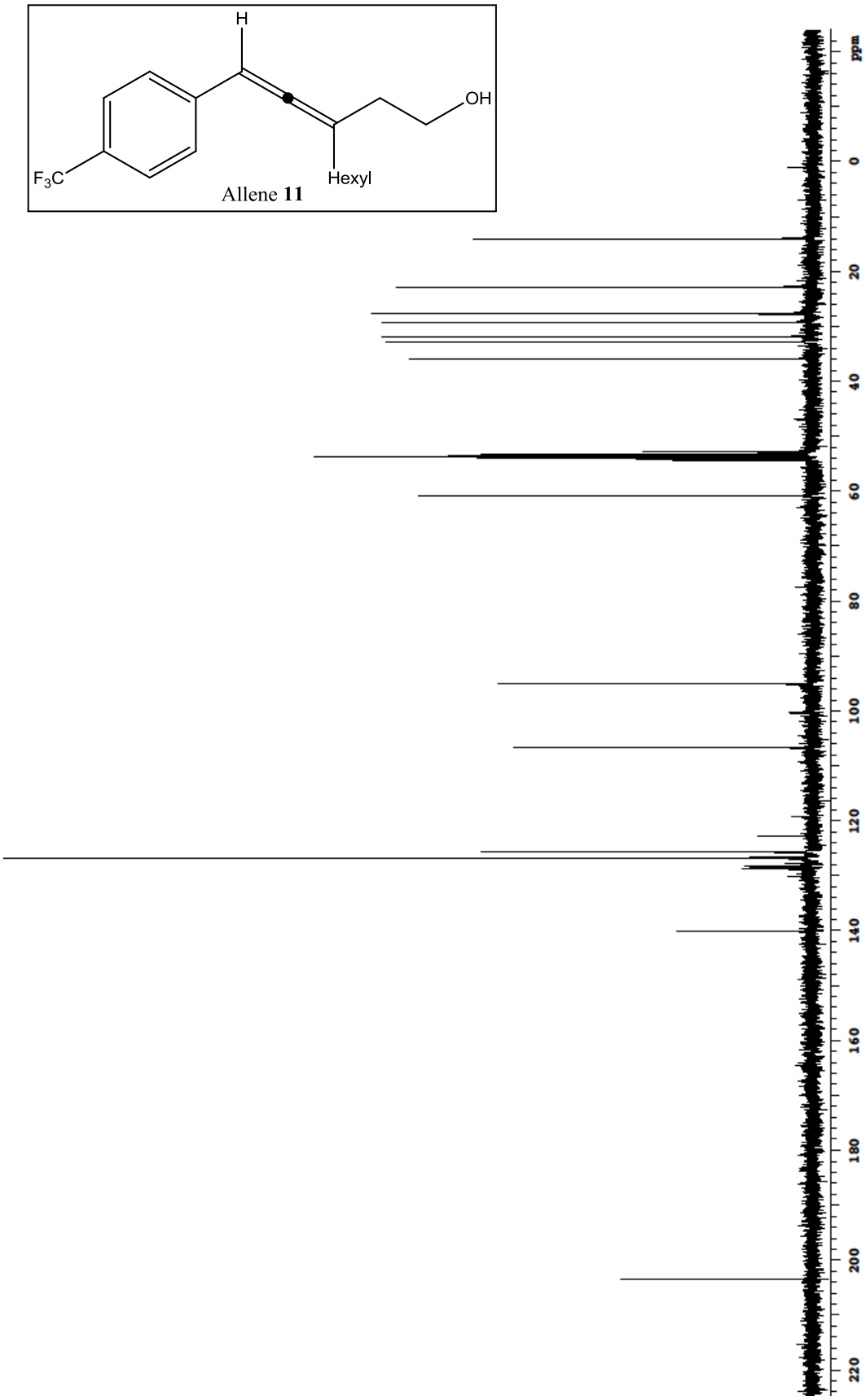

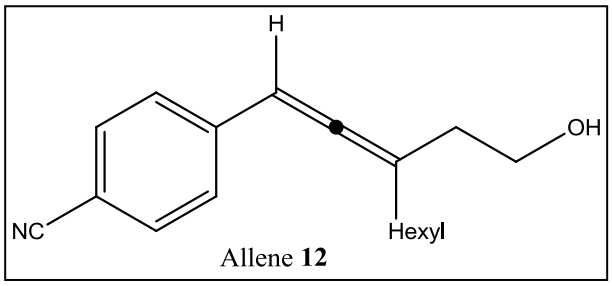

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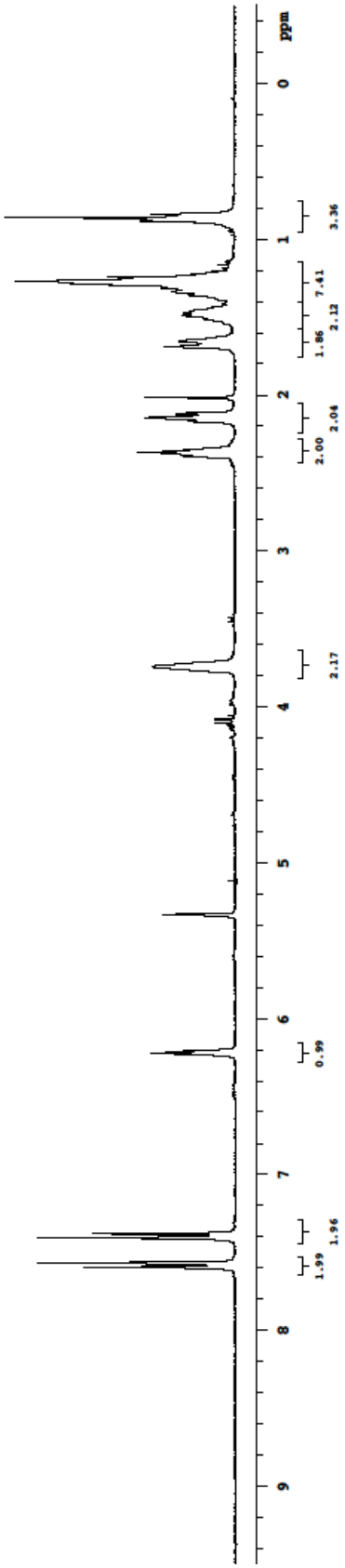

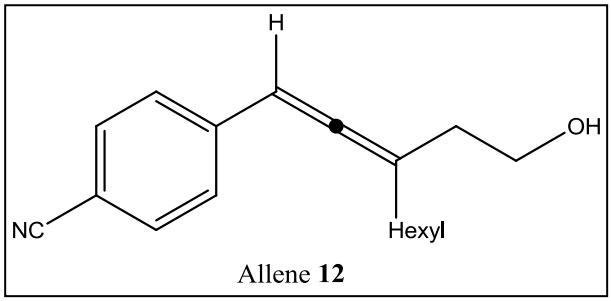

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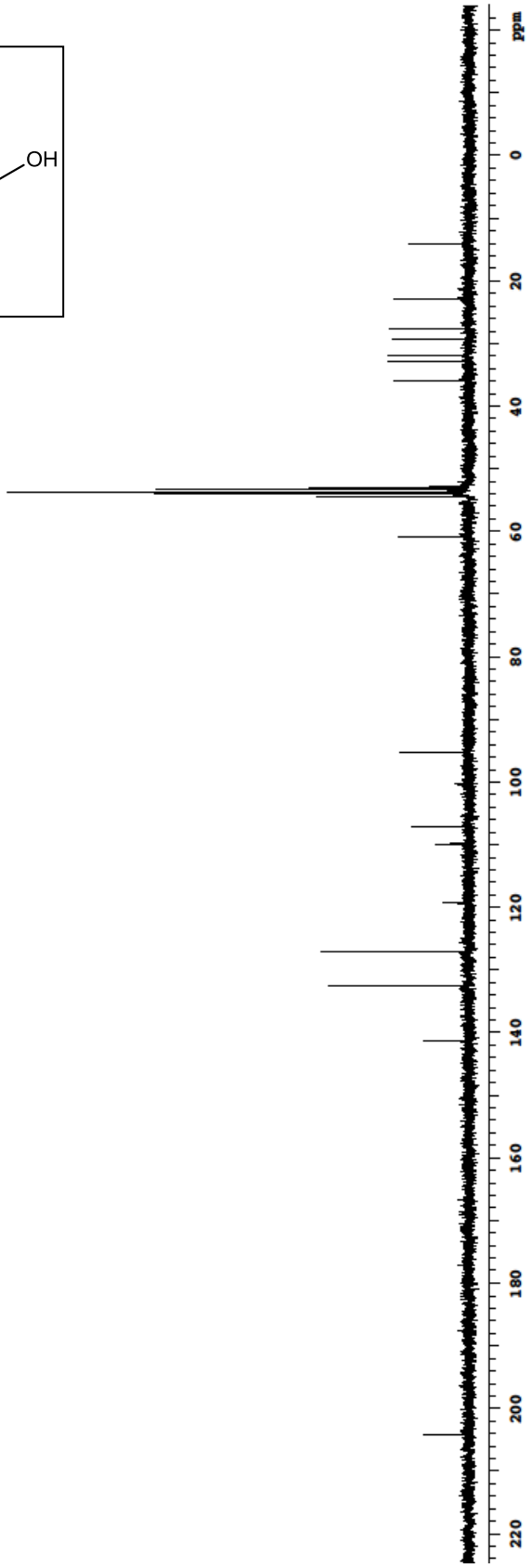

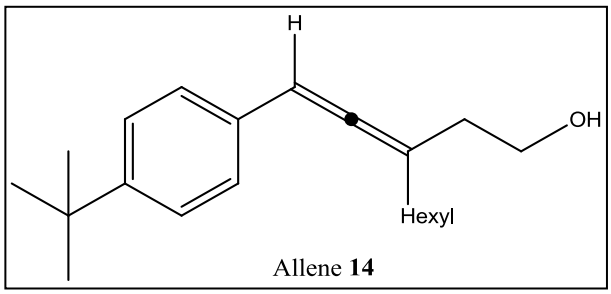

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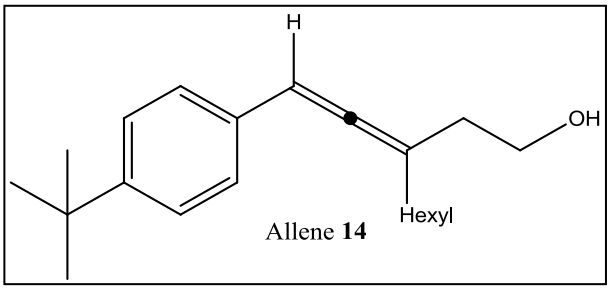

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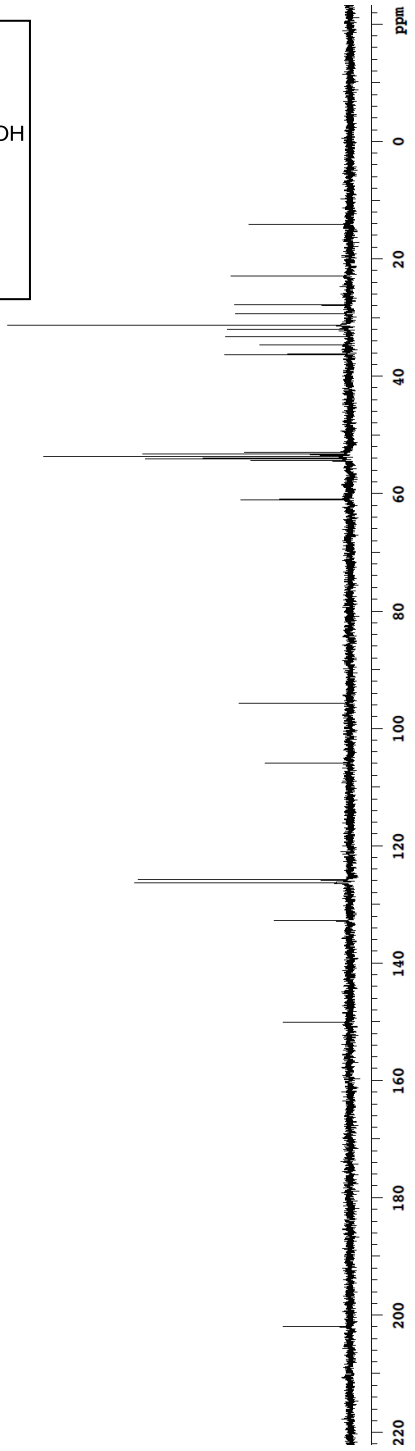

Computational Study

All geometries were optimized by DFT computations at the B3LYP level with the LANL2DZ basis set which frequently performs well for the transition metal compounds (e.g. Xia, Y.; Dudnik, A. S.; Gevorgyan, V.; Li, Y. *J Am Chem Soc.* **2008**, *130*, 6940–6941 and Soriano, E.; Marco-Contelles, J. *Acc. Chem. Res.* **2009**, *42*, 1026–1036) using Gaussian 03 program (see reference). Force Field calculation indicated that optimized structures were found to be true minima with no imaginary frequency.

Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford, CT, 2003.

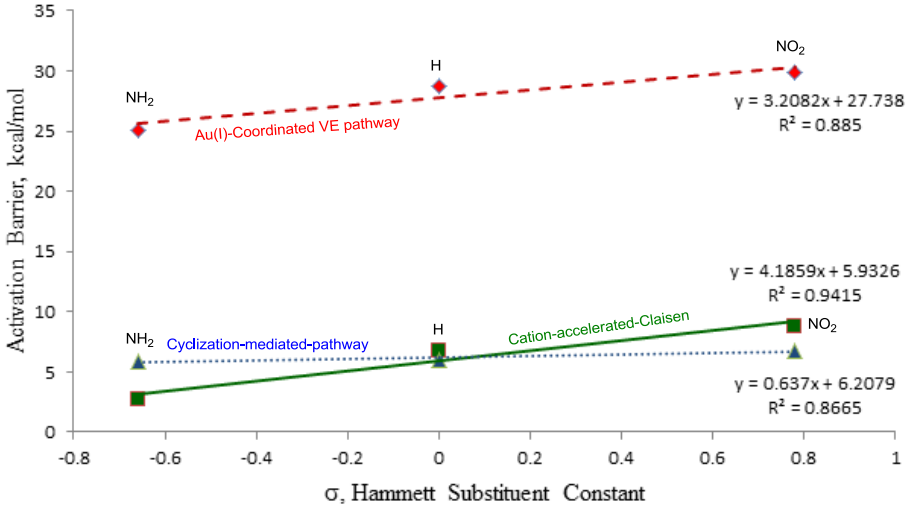

Figure 1 Correlation of Hammett constants and the activation energies

	Coordination of PMe3Au(I) to the terminal carbon of vinyl ether
Reactant_Ph	**Total Energy** = -801.0922963 C 1.03070700 -0.01349800 -0.88540600 H 1.16025700 1.03539700 -1.16703300 C 0.08416500 -0.82824800 -1.54167300 H -0.19164900 -0.49467000 -2.54426000 H 0.18771100 -1.90655400 -1.41324300 O 1.79003100 -0.47741000 0.08892600 C 2.88679900 0.40775100 0.83062800 H 2.57485800 0.22699600 1.86353500 C 2.75511700 1.81178900 0.47299400 C 2.67190600 3.00899400 0.23136200 Au -1.76215200 -0.34023200 -0.46559000 P -3.91552000 0.00483200 0.59084300 C -5.33645500 0.03359000 -0.63618000 H -5.19136800 0.85007000 -1.34938900 H -5.36775800 -0.91095500 -1.18691400 H -6.28707800 0.17675900 -0.11087600 C -4.05418400 1.61807700 1.54156200 H -3.88261500 2.46068200 0.86557900 H -5.05145500 1.70886800 1.98589500 H -3.30184900 1.64487300 2.33502100 C -4.35880200 -1.33619400 1.82746500 H -4.37624300 -2.30849000 1.32673300 H -3.60977000 -1.36644800 2.62387800 H -5.34372800 -1.13691500 2.26372500 C 4.21234500 -0.25501100 0.54213200 C 4.58671900 -1.37675500 1.31331700 C 5.79855100 -2.03884100 1.05494100 C 6.64344900 -1.58153500 0.02437800 C 6.27433800 -0.45944600 -0.74386900 C 5.06279100 0.20396500 -0.48619000 H 3.93511000 -1.73224300 2.10913600 H 6.08551400 -2.89945900 1.65253700 H 6.93089900 -0.10241500 -1.53257700 H 4.78974700 1.08018700 -1.06878700 H 7.58310700 -2.09037800 -0.17363700 C 2.60702100 4.45193600 -0.03808500 H 1.64989100 4.87596900 0.28761600 H 3.40769300 4.97138500 0.50295800 H 2.73445600 4.66302700 -1.10657400
Reactant_PhNH2	**Total Energy** =-856.4516862 C 0.74491600 0.11375900 -0.83090600 H 0.81885600 1.17149400 -1.10740700 C -0.17761600 -0.73210900 -1.50209600 H -0.43749800 -0.40122300 -2.51094300 H -0.01204300 -1.80570900 -1.39523100 O 1.52457000 -0.31453600 0.12861200 C 2.66147500 0.67226800 0.89453700 H 2.31527100 0.45367000 1.90752800 C 2.42371900 2.04628100 0.50463200 C 2.23561200 3.22324000 0.22208900 Au -2.05802700 -0.36932400 -0.46865100 P -4.23793700 -0.14386600 0.57403100 C -5.65377300 -0.13768800 -0.65997500

	H -5.53719900 0.70288500 -1.35011600 H -5.64389400 -1.06718000 -1.23663000 H -6.61247400 -0.04687000 -0.13761200 C -4.45684400 1.43290000 1.57092200 H -4.31774900 2.30182600 0.92119700 H -5.46013800 1.46687800 2.00966700 H -3.71147500 1.46965700 2.37061600 C -4.64110200 -1.53472400 1.76952400 H -4.61205800 -2.49295100 1.24274400 H -3.89997800 -1.55605500 2.57368500 H -5.63819400 -1.38869300 2.19931100 C 3.98241600 0.07013000 0.59881300 C 4.42343000 -1.03853400 1.36379100 C 5.64765500 -1.65353700 1.10535100 C 6.48485300 -1.17342300 0.05724800 C 6.04414400 -0.05770300 -0.71236800 C 4.81723800 0.54705000 -0.44216300 H 3.79680300 -1.42118800 2.16726500 H 5.97192400 -2.49979100 1.70619500 H 6.67707700 0.32543600 -1.50952400 H 4.50622100 1.40625400 -1.03146400 N 7.70070700 -1.77220700 -0.20362800 C 2.04806400 4.64655300 -0.09034400 H 1.04417700 4.98775800 0.18882600 H 2.77609500 5.25244600 0.46358200 H 2.19602600 4.84191000 -1.15925700 H 8.30352100 -1.43258000 -0.93915800 H 8.02329700 -2.55844100 0.34188900
Reactant_PhOMe	**Total Energy** = -915.6028562 C 0.66429700 -0.42405100 -0.26774000 H 0.87947800 0.29264200 -1.06557200 C -0.18618000 -1.52324500 -0.50844900 H -0.26904800 -1.82046300 -1.55599500 H -0.14952500 -2.33965000 0.21434200 O 1.22180200 -0.21133700 0.90822500 C 2.26303300 1.00315500 1.10559700 H 2.22580400 1.03161300 2.19723600 C 1.70265700 2.20896200 0.51488500 C 1.25766900 3.25685300 0.06625900 Au -2.17695900 -0.66264500 -0.20001000 P -4.47263500 0.03452400 0.13302400 C -5.59833100 -0.42140300 -1.29854700 H -5.24009700 0.05298600 -2.21666000 H -5.59239100 -1.50608400 -1.44000300 H -6.62244200 -0.08977400 -1.09537400 C -4.68842600 1.88597300 0.36036300 H -4.32433000 2.41150400 -0.52714800 H -5.74618300 2.12652300 0.51392600 H -4.11267500 2.21974500 1.22838700 C -5.26535800 -0.74213000 1.64741200 H -5.25152200 -1.83172700 1.55207100 H -4.70403400 -0.46245600 2.54352800 H -6.30177800 -0.40186200 1.74846200 C 3.60322500 0.54804100 0.60388400 C 4.38271000 -0.30466100 1.41364100

	C 5.62526500 -0.78556200 0.97526400 C 6.10365100 -0.40643900 -0.30073800 C 5.33372600 0.45532300 -1.11828600 C 4.09883500 0.92621100 -0.66813300 H 4.01785700 -0.59966800 2.39557100 H 6.20622400 -1.43605000 1.62009900 H 5.73454000 0.74170800 -2.08531800 H 3.52951500 1.61027200 -1.29232600 O 7.30824300 -0.81362300 -0.83971700 C 0.75255900 4.53254000 -0.45972900 H -0.17323700 4.83190500 0.04564900 H 1.49370200 5.32610300 -0.30301000 H 0.55517000 4.46902800 -1.53672100 C 8.18766500 -1.69047800 -0.06532100 H 7.69612700 -2.64815200 0.14970900 H 9.05572000 -1.85570300 -0.70444400 H 8.50007200 -1.20620900 0.86880600
Reactant_PhCN	**Total Energy** = -893.304841 C 0.50158600 0.44173600 -0.95607700 H 0.49668200 1.53179500 -1.04046200 C -0.37133700 -0.35240700 -1.72313000 H -0.74620600 0.11831500 -2.63412500 H -0.14450800 -1.41672300 -1.79458000 O 1.36668900 -0.09791800 -0.11092600 C 2.34203500 0.75899800 0.78491100 H 1.96365000 0.50278300 1.77994000 C 2.20557400 2.18325500 0.52026200 C 2.11701900 3.39407300 0.36234400 Au -2.20376300 -0.27989000 -0.50825400 P -4.33342900 -0.38573000 0.64056000 C -5.79157500 -0.40313700 -0.54211000 H -5.78554500 0.50575600 -1.15053700 H -5.71808900 -1.26958900 -1.20562100 H -6.73113500 -0.45675700 0.01866800 C -4.65366700 1.05666000 1.79891100 H -4.62711100 1.99464400 1.23700100 H -5.63571700 0.94728100 2.27203600 H -3.88195700 1.08795700 2.57333200 C -4.53388800 -1.92489900 1.69588700 H -4.43959500 -2.81674100 1.06970700 H -3.75523500 -1.95195600 2.46346400 H -5.51760000 -1.92493000 2.17790200 C 3.71105700 0.15251300 0.56305500 C 4.06644700 -1.00019600 1.29476000 C 5.31121500 -1.61248600 1.09491500 C 6.21730600 -1.07054500 0.15308200 C 5.86478500 0.08864300 -0.57833300 C 4.61839900 0.69496800 -0.37045000 H 3.37320600 -1.42260800 2.01842400 H 5.58720600 -2.49785000 1.65901900 H 6.56642500 0.50451200 -1.29482300 H 4.35865400 1.59263800 -0.92422900 C 7.49791200 -1.69446400 -0.05828200 C 2.04269600 4.85136300 0.19193700 H 1.10107000 5.25112500 0.58594500

	H 2.86709000 5.33551700 0.72997100 H 2.12343600 5.13163800 -0.86515300 N 8.54815200 -2.20723100 -0.23355900
Reactant_PhNO2	**Total Energy** = -1005.554239 C 0.12514500 0.68917500 -0.95571000 H 0.06412100 1.77979000 -0.91371500 C -0.72131800 -0.05747500 -1.79394600 H -1.14691700 0.49336900 -2.63484900 H -0.44492000 -1.09379400 -1.99047500 O 1.04013900 0.10148500 -0.19599000 C 1.96908300 0.89676100 0.78856900 H 1.56982400 0.57103300 1.75510800 C 1.83147300 2.33606300 0.62337600 C 1.74107700 3.55479300 0.55008400 Au -2.52139700 -0.21984000 -0.53341300 P -4.60717900 -0.58847300 0.64067900 C -6.05559200 0.33088100 -0.12115000 H -5.86433400 1.40753900 -0.09939800 H -6.18500200 0.01844500 -1.16133600 H -6.97340800 0.11542500 0.43682100 C -4.57762800 -0.06543900 2.44369700 H -4.35123900 1.00207500 2.51651000 H -5.55135500 -0.26018400 2.90639700 H -3.80621400 -0.62700400 2.97839600 C -5.11835900 -2.39442000 0.65551400 H -5.22846100 -2.75510000 -0.37123800 H -4.35179500 -2.99237100 1.15654000 H -6.07116200 -2.51187700 1.18316000 C 3.35187100 0.31716400 0.56337000 C 3.70073100 -0.87422000 1.23366800 C 4.95717100 -1.46277100 1.03001800 C 5.85037500 -0.83665400 0.14586200 C 5.53116500 0.35162300 -0.53133500 C 4.27148800 0.92812800 -0.31409600 H 2.99441700 -1.34536100 1.91279300 H 5.25118900 -2.37626800 1.53426000 H 6.25766400 0.79980300 -1.19975800 H 4.01040500 1.85380300 -0.81822000 N 7.18264100 -1.45122000 -0.07884000 C 1.66325000 5.02004400 0.47925500 H 0.71394900 5.38870000 0.88494500 H 2.47720400 5.46863800 1.06209800 H 1.75917400 5.37203300 -0.55482100 O 7.97878900 -0.86590400 -0.88716900 O 7.45317100 -2.53028700 0.54754500
Product_Ph	**Total Energy** = -801.1196886 C 2.27134900 -2.58296600 -0.27249000 H 2.97384500 -3.18854500 -0.86075200 C 2.78890500 -1.86166300 0.93029000 H 3.50835600 -2.49233300 1.46314100 H 1.97023600 -1.59419700 1.60791400 O 1.09257700 -2.49329400 -0.71671700 C 2.16041600 1.18649100 -1.03565100 C 2.84042500 0.30175400 -0.31398700

	C 3.51871400 -0.58698200 0.39663000 C 4.99351100 -0.45518100 0.74558800 H 5.41091500 0.47767000 0.35703900 H 5.13436600 -0.47237600 1.83509600 H 5.57183700 -1.29030000 0.32590300 H 2.17294400 1.07085500 -2.12296800 C 1.39192200 2.34699200 -0.52535400 C 0.72768300 3.18685100 -1.45119700 C -0.00138100 4.30647400 -1.01012300 C -0.07814600 4.60262100 0.36461300 C 0.58138800 3.77118100 1.29552300 C 1.30845600 2.65301800 0.85602600 H 0.80034500 2.97577300 -2.51668700 H -0.48962100 4.95403900 -1.73370600 H 0.54387300 4.01087600 2.35546800 H 1.83372200 2.02936800 1.57621500 Au -0.61515200 -1.30286500 -0.17690300 P -2.54903100 -0.03586300 0.30262700 C -4.08330500 -1.09842300 0.47600100 H -4.25738600 -1.65098200 -0.45153700 H -3.94820100 -1.81389700 1.29186000 H -4.95189600 -0.46576700 0.68887300 C -2.39971500 0.93775000 1.89586700 H -3.32598300 1.49351300 2.07871900 H -2.21574400 0.25724800 2.73187200 H -1.56549400 1.64000400 1.81435300 C -2.92766900 1.22237600 -1.03319700 H -3.83378600 1.77943900 -0.77058100 H -2.08895700 1.91782300 -1.12837300 H -3.08087400 0.71353700 -1.98902200 H -0.62596900 5.47708900 0.70560100
Product_PhNH2	**Total Energy** = -856.477033 C 3.20795600 1.75321400 -0.13767300 H 3.96238200 2.34460900 -0.67320600 C 2.49339300 2.38074900 1.01286900 H 3.18483400 2.99551400 1.59836000 H 2.04759200 1.61695400 1.65950700 O 2.95236800 0.60610200 -0.60629600 C -0.54967500 2.21103000 -1.06935700 C 0.41680600 2.75152800 -0.32992400 C 1.39288400 3.29841300 0.37888300 C 1.54135500 4.79197500 0.63056100 H 0.73322200 5.35426600 0.15492800 H 1.52639400 5.00594300 1.70835400 H 2.49681800 5.16528400 0.23516900 H -0.37069900 2.14638200 -2.14701600 C -1.85882600 1.70372300 -0.61749100 C -2.76686600 1.18002500 -1.57092300 C -4.03102600 0.70786400 -1.19812700 C -4.44247800 0.74925600 0.16172600 C -3.53107900 1.26636100 1.12691800 C -2.27175900 1.73341400 0.73934900 H -2.48628000 1.16223700 -2.62305600 H -3.83401400 1.32222500 2.17080200 H -1.60473700 2.14992600 1.49153200

	Au 1.43521700 -0.82962000 -0.13598500 P -0.20675100 -2.47969200 0.25632800 C 0.52077200 -4.19055700 0.49526700 H 1.08640100 -4.47968300 -0.39494100 H 1.19606000 -4.18866900 1.35550200 H -0.28160100 -4.91654500 0.66620900 C -1.23883500 -2.13181600 1.78017800 H -1.98385200 -2.92430200 1.91195600 H -0.59517200 -2.09062900 2.66339700 H -1.74774900 -1.17115000 1.66093900 C -1.42397900 -2.62061200 -1.16135700 H -2.15005600 -3.41297100 -0.94823800 H -1.94970800 -1.66948800 -1.28556900 H -0.89011400 -2.85833000 -2.08574900 H -4.71536600 0.33103900 -1.95527900 N -5.69781300 0.29926600 0.54193900 H -6.01945000 0.40147100 1.49362600 H -6.37188400 0.00023000 -0.14794400
Product_PhOMe	**Total Energy** = -915.6296023 C 3.44774900 1.64900400 -0.27472500 H 4.17795300 2.22335700 -0.86016900 C 2.86476700 2.27590000 0.94898300 H 3.63759400 2.83159600 1.49051100 H 2.43546400 1.51482900 1.61061800 O 3.10576300 0.52569300 -0.74229500 C -0.24761400 2.39022500 -1.03396400 C 0.75782900 2.82670500 -0.28086100 C 1.76902800 3.27399400 0.44888800 C 1.95202900 4.72879600 0.85571600 H 1.13378000 5.34993100 0.48149200 H 1.98734000 4.82193800 1.95009700 H 2.89590400 5.13094000 0.46117400 H -0.11753000 2.43545300 -2.11906700 C -1.54762200 1.85879100 -0.57286400 C -2.51079000 1.46555900 -1.52801900 C -3.76836400 0.96572700 -1.14336900 C -4.07887400 0.85262400 0.22897700 C -3.12377800 1.24154200 1.20100400 C -1.88055100 1.73778000 0.80317900 H -2.28562500 1.56484000 -2.58837600 H -4.49094800 0.69163500 -1.90503700 H -3.39971900 1.16956300 2.24896700 H -1.16624800 2.05949600 1.55787000 Au 1.59770100 -0.88711600 -0.18173500 P -0.05992300 -2.49867600 0.29881900 C 0.62287700 -4.24190100 0.38821300 H 1.09418600 -4.50398900 -0.56316000 H 1.37262400 -4.30588900 1.18180400 H -0.18746800 -4.94862400 0.59787700 C -0.93298700 -2.19344400 1.92785900 H -1.66767500 -2.98588500 2.10854800 H -0.20555800 -2.18279800 2.74426900 H -1.44562400 -1.22822600 1.88987000 C -1.40392600 -2.52673800 -1.00650000 H -2.16189200 -3.27241400 -0.74238200

	H -1.87007900 -1.53961300 -1.07186500 H -0.96972700 -2.78033200 -1.97777500 O -5.27936900 0.37750800 0.73312100 C -6.37466200 0.07759800 -0.18900300 H -6.65144400 0.96644500 -0.77033000 H -6.10865600 -0.74600500 -0.86528800 H -7.20801500 -0.22254600 0.44743800
Product_PhCN	**Total Energy** = -893.3338111 C 3.32559200 1.51130700 -0.29203500 H 4.06566200 2.05029100 -0.89887000 C 2.84778500 2.15239100 0.97224700 H 3.69755500 2.60111400 1.49926700 H 2.36975300 1.41546600 1.62869700 O 2.89579100 0.42170000 -0.76053500 C -0.16705300 2.70083300 -1.05755900 C 0.83699600 2.99882800 -0.24019600 C 1.84574400 3.27885400 0.57122100 C 2.10041200 4.65470600 1.16796800 H 1.32123300 5.36484300 0.87816900 H 2.13058200 4.59915200 2.26489800 H 3.06824200 5.05163200 0.83161700 H -0.01604800 2.84606100 -2.13006900 C -1.49254900 2.17411900 -0.66033400 C -2.42230800 1.82507500 -1.66902900 C -3.67955600 1.29841600 -1.33936500 C -4.03385900 1.11283700 0.01771100 C -3.11627600 1.47800500 1.03576300 C -1.86281100 1.99989200 0.69718800 H -2.16169900 1.97071600 -2.71490400 H -3.40262100 1.36424300 2.07763600 H -1.17111500 2.29237500 1.48320700 Au 1.38049700 -0.98670700 -0.19271100 P -0.28232500 -2.59437800 0.29458300 C 0.37757700 -4.34790600 0.25527600 H 0.79169000 -4.56549000 -0.73317700 H 1.16794200 -4.46377000 1.00210800 H -0.43165000 -5.05381200 0.47176200 C -1.04967200 -2.35968200 1.98779500 H -1.80900600 -3.13005600 2.16120300 H -0.27828100 -2.43363100 2.75935100 H -1.51854700 -1.37346100 2.04466100 C -1.69912100 -2.53712800 -0.93063900 H -2.45000100 -3.28925100 -0.66489800 H -2.15968600 -1.54551400 -0.91755200 H -1.32445700 -2.74077300 -1.93772900 H -4.38903600 1.03988500 -2.11979100 C -5.31215400 0.55220700 0.36689700 N -6.35481400 0.07647800 0.65809400
Product_PhNO2	**Total Energy** = -1005.584553 C 2.87882100 1.91603900 -0.88043000 H 3.22338500 2.59117000 -1.67601600 C 2.97719700 2.39702500 0.53641000 H 3.98194400 2.81513100 0.69577200 H 2.84011100 1.56287000 1.23787500

	O 2.40527400 0.80774600 -1.24502200 C -0.31020800 3.52854100 -0.61559700 C 0.80869400 3.54829400 0.10225500 C 1.92472000 3.49928300 0.81391500 C 2.24287400 4.44104300 1.96531600 H 1.40388500 5.11011800 2.17419800 H 2.47302100 3.87545300 2.87906000 H 3.12049300 5.05790400 1.72847000 H -0.38000900 4.15956800 -1.50361000 C -1.47937500 2.66640600 -0.33002800 C -2.56057300 2.63583200 -1.24293700 C -3.63135900 1.74780200 -1.06122200 C -3.60351800 0.88177200 0.04409500 C -2.57073400 0.92619800 1.00035700 C -1.51730800 1.82227500 0.80993500 H -2.55485800 3.29505000 -2.10741200 H -2.61875500 0.27571300 1.86706000 H -0.71541800 1.87661700 1.54136800 Au 1.42571200 -0.90206100 -0.37360300 P 0.32999300 -2.86288300 0.37337200 C 1.03703300 -4.39359300 -0.44561400 H 0.91314900 -4.32387800 -1.52998700 H 2.10293300 -4.48003400 -0.21702600 H 0.51400100 -5.28367900 -0.07904700 C 0.50941200 -3.13247600 2.21916800 H 0.00143700 -4.05863500 2.50954100 H 1.56823500 -3.20395700 2.48259300 H 0.06402400 -2.29458100 2.76258800 C -1.50753000 -2.87970600 0.01061600 H -1.94077500 -3.82077400 0.36692600 H -2.00986200 -2.05022600 0.51417700 H -1.67230400 -2.79439100 -1.06729000 H -4.45956300 1.70390700 -1.76017100 N -4.66040600 -0.13190400 0.19841000 O -5.70219300 -0.04452900 -0.53142600 O -4.45335800 -1.07725900 1.04503200
TS_Ph	**Total Energy** =-801.0466061, **Frequency** -396.5274 cm^{-1} C -0.93725000 -0.23394500 -0.26518000 H -1.04113400 -0.56326900 -1.31505900 C -0.33165400 1.09678600 -0.07538500 H -0.03914800 1.67898100 -0.95094400 H -0.10388800 1.45035100 0.93387200 O -1.40656100 -0.92238800 0.67669200 C -3.84004400 0.62460600 1.16636600 C -2.99502700 1.54864900 0.64476200 C -2.04697900 2.26532300 0.18856500 C -1.62504800 3.64067700 -0.19725800 H -2.43180300 4.34297300 0.04678100 H -0.72575900 3.95483500 0.34589200 H -1.42361800 3.71537600 -1.27270600 H -3.77518600 0.45298400 2.24298600 C -4.85665600 -0.12993400 0.45518300 C -5.62769900 -1.07932200 1.18050300 C -6.61314100 -1.83592900 0.53248100 C -6.84581300 -1.65242900 -0.84622400

	C -6.08968700 -0.70758600 -1.57701000 C -5.10360100 0.04877000 -0.93497200 H -5.44277600 -1.22159900 2.24306100 H -7.19783200 -2.56168100 1.08996200 H -6.28145300 -0.56726400 -2.63710400 H -4.52954900 0.78542900 -1.49165100 Au 1.82221300 0.18757100 -0.06293300 P 4.04801800 -0.71612100 -0.01119700 C 4.27352700 -2.14574800 -1.20485700 H 3.56757700 -2.94438600 -0.96039000 H 4.08174400 -1.80773300 -2.22711100 H 5.29621500 -2.53294000 -1.13743500 C 5.37434600 0.53423000 -0.45416800 H 6.36147200 0.06022800 -0.41970700 H 5.19545300 0.92313800 -1.46051300 H 5.34855900 1.36647600 0.25490500 C 4.51673100 -1.38272600 1.67855500 H 5.53323800 -1.79052300 1.65188200 H 4.46855400 -0.57953900 2.41925300 H 3.81729000 -2.17108000 1.97042800 H -7.61258800 -2.23646300 -1.34841500
TS_PhNH2	**Total Energy** = -856.4117518, **Frequency =** -440.0879 cm^{-1} C -0.60748800 -0.18787000 -0.18123800 H -0.76390900 -0.59631500 -1.19704200 C 0.00378000 1.15851500 -0.13045000 H 0.33619000 1.62151500 -1.06208700 H 0.31952400 1.56875000 0.83357500 O -1.03328000 -0.79418800 0.83208300 C -3.53661300 1.01312700 1.21038500 C -2.60092400 1.76149200 0.56867400 C -1.59817300 2.33576700 0.02418800 C -1.16306300 3.66410000 -0.51129200 H -1.94911000 4.40563600 -0.32809900 H -0.24469800 4.01252600 -0.02229100 H -0.97900400 3.62189400 -1.59233700 H -3.47412000 0.99291700 2.30089300 C -4.62563800 0.27721300 0.62343300 C -5.50525200 -0.45932100 1.47174000 C -6.56752700 -1.19115000 0.95487700 C -6.80382400 -1.21601500 -0.45221900 C -5.93094800 -0.47774600 -1.31191200 C -4.87209000 0.24715700 -0.78277200 H -5.33611900 -0.45134600 2.54652400 H -7.22480700 -1.74782400 1.61828000 H -6.10941300 -0.48574300 -2.38482400 H -4.22306700 0.81272600 -1.44696900 Au 2.15526800 0.15168100 -0.08921000 P 4.35324000 -0.81717600 0.01042300 C 4.57197100 -2.24596700 -1.18582700 H 3.83974500 -3.02719500 -0.96325800 H 4.41388100 -1.89747000 -2.21033700 H 5.58236000 -2.66007400 -1.09597500 C 5.72699600 0.39630000 -0.38985200 H 6.69904500 -0.10581600 -0.33197300 H 5.58563600 0.79542500 -1.39819100

	H 5.70570400 1.22539000 0.32306800 C 4.75990600 -1.50753000 1.70687700 H 5.76384400 -1.94621400 1.70343900 H 4.71690200 -0.70734300 2.45114100 H 4.02904000 -2.27517900 1.97613600 N -7.85423500 -1.93297600 -0.97511000 H -8.03213900 -1.95191900 -1.96969100 H -8.48107000 -2.45360800 -0.37728600
TS_PhOMe	**Total Energy** = -915.5606879, **Frequency** = -426.604 cm^{-1} C -0.33470400 -0.07527300 -0.15287200 H -0.51720800 -0.50965700 -1.15314600 C 0.37945500 1.21776000 -0.14602500 H 0.70979600 1.64641400 -1.09425000 H 0.70176600 1.65135800 0.80508500 O -0.80678400 -0.61150400 0.88007100 C -3.14905400 1.30885400 1.21564700 C -2.19173300 2.01210100 0.55802400 C -1.17276200 2.53370700 -0.00394700 C -0.64432200 3.80997000 -0.57173500 H -1.37224300 4.61119800 -0.39710900 H 0.30150900 4.09994800 -0.09798500 H -0.47715600 3.73174300 -1.65314900 H -3.08154300 1.29593600 2.30580300 C -4.27246200 0.61070600 0.63603400 C -5.17117800 -0.08056900 1.49369800 C -6.27008300 -0.77868600 0.98636500 C -6.49360400 -0.79389700 -0.41288800 C -5.60883400 -0.10485800 -1.28741000 C -4.52001300 0.58400500 -0.77059300 H -4.99647700 -0.07116000 2.56745300 H -6.93808500 -1.29926500 1.66373000 H -5.81770700 -0.13312400 -2.35197600 H -3.85248000 1.11964400 -1.44055300 Au 2.45684700 0.11193300 -0.08926200 P 4.60429600 -0.96262900 0.00985500 C 4.92028200 -2.11099200 -1.43956600 H 4.15781600 -2.89466900 -1.46176700 H 4.87293700 -1.54746700 -2.37561500 H 5.90989100 -2.57126900 -1.34358500 C 6.03786900 0.24813600 0.02046900 H 6.98758300 -0.29603600 0.06849700 H 6.01506800 0.85584200 -0.88851800 H 5.95612400 0.90891100 0.88807300 C 4.81399300 -2.01570100 1.54809100 H 5.80096700 -2.49129800 1.54485400 H 4.71612500 -1.39057900 2.44007700 H 4.03925000 -2.78704000 1.57474400 O -7.53706200 -1.44025700 -1.02908900 C -8.52351500 -2.17377900 -0.22901400 H -8.04495900 -2.99308700 0.32159400 H -9.04129700 -1.49849300 0.46321800 H -9.23029000 -2.57599100 -0.95512600
TS_PhCN	**Total Energy** = -893.258332, **Frequency** = -381.6414 cm^{-1} C -0.52879700 -0.02793700 -0.16654300

	H -0.70245600 -0.51245400 -1.14412800 C 0.22022000 1.23773800 -0.20805900 H 0.51945300 1.65060700 -1.17278700 H 0.51235100 1.72851800 0.72378200 O -1.03931600 -0.49730600 0.88500100 C -3.20374000 1.28526700 1.24612000 C -2.35109300 2.07044500 0.54114700 C -1.38720400 2.63174600 -0.06849700 C -0.85456200 3.87221300 -0.69104400 H -1.56986500 4.68813700 -0.52643600 H 0.10368600 4.16727100 -0.24776300 H -0.71625300 3.75540400 -1.77242100 H -3.07081600 1.25997500 2.32938300 C -4.31475400 0.51266500 0.71397000 C -5.07861000 -0.28354000 1.60886400 C -6.14921900 -1.05253400 1.14283300 C -6.47993200 -1.03445800 -0.23420300 C -5.72825100 -0.23609700 -1.13617400 C -4.65929900 0.52774100 -0.66573600 H -4.82234000 -0.30206700 2.66527800 H -6.72993300 -1.66336200 1.82655300 H -5.99676300 -0.22357700 -2.18796600 H -4.09264800 1.14801800 -1.35480000 Au 2.26777500 0.12158700 -0.10877100 P 4.40645700 -0.96559800 0.02076200 C 4.27864800 -2.83080600 -0.13380700 H 3.63791500 -3.22409600 0.66031600 H 3.84013900 -3.09291200 -1.10076600 H 5.27403800 -3.28142200 -0.05373400 C 5.59615300 -0.41870400 -1.32224600 H 6.55089900 -0.94482200 -1.21300500 H 5.17207200 -0.64172700 -2.30531300 H 5.76739600 0.65892400 -1.24863400 C 5.28450200 -0.64441800 1.64700000 H 6.24914100 -1.16372100 1.66057500 H 5.45079200 0.42919600 1.77228700 H 4.66893400 -1.00457800 2.47600200 C -7.57954900 -1.82243300 -0.72246800 N -8.48134000 -2.47079600 -1.12741200
TS_PhNO2	**Total Energy** = -1005.506778, **Frequency** = -367.4761 cm^{-1} C -0.21764700 0.11534800 -0.12995200 H -0.42237700 -0.38695400 -1.09202100 C 0.59268500 1.33867000 -0.20951500 H 0.89643200 1.71660400 -1.18695300 H 0.91398400 1.84211300 0.70543700 O -0.74719800 -0.29791900 0.93758000 C -2.77716500 1.53638600 1.29314900 C -1.92929200 2.30069500 0.55998300 C -0.96473800 2.82172100 -0.08141400 C -0.38920500 4.01793100 -0.74688900 H -1.06832700 4.86744200 -0.59812600 H 0.58572700 4.28629900 -0.32374100 H -0.27085800 3.86366700 -1.82579400 H -2.62456200 1.52129900 2.37370200 C -3.91312700 0.77606700 0.78853200

C	-4.66718600	-0.00217100	1.70623300
C	-5.75759400	-0.76311200	1.26914200
C	-6.08683200	-0.73255900	-0.09640300
C	-5.36778500	0.03453100	-1.03327600
C	-4.28118000	0.78888900	-0.58463900
H	-4.38901900	-0.01570500	2.75685900
H	-6.34533000	-1.36770900	1.95036700
H	-5.67214200	0.02750100	-2.07379300
H	-3.71973800	1.39840200	-1.28700500
Au	2.57427300	0.10956300	-0.10693400
P	4.64684600	-1.10071000	0.00772600
C	4.65630700	-2.37417200	1.38488100
H	4.50811800	-1.87825500	2.34823000
H	3.84447900	-3.09034900	1.23077200
H	5.61374400	-2.90661700	1.39446300
C	5.02814400	-2.04315300	-1.56853600
H	5.97561800	-2.58265900	-1.46096400
H	4.22708600	-2.75840000	-1.77489700
H	5.10298500	-1.34602300	-2.40784400
C	6.13072800	0.00423000	0.31636800
H	7.04348900	-0.60023200	0.35823900
H	6.22019800	0.73790900	-0.48969400
H	6.00593700	0.53493800	1.26440100
N	-7.23895700	-1.53786200	-0.57262700
O	-7.51122600	-1.50378400	-1.82003100
O	-7.88653900	-2.21815500	0.29153700

	Coordination of PMe3Au(I) to the Alkyne (Cyclization-Mediated Pathway)					
	B3LYP/LANL2DZ			M05-2X/LANL2DZ		
Reactant_Ph	**Total Energy** = -801.0745515			**Total Energy** = -800.83386033		
C	4.18917500	-1.22832100	0.05228000	4.25549900	-0.21189300	0.34301000
H	4.12262800	-0.46819500	0.82827600	3.89394600	0.55555600	1.01819400
C	5.03479700	-2.27058300	0.09749200	5.28881900	-1.01573500	0.60410300
H	5.70933700	-2.38618800	0.93954200	5.82403800	-0.92459000	1.53930200
H	5.09344400	-2.99042200	-0.71367900	5.62861700	-1.74087800	-0.12433100
O	3.38578500	-1.01487600	-1.08799100	3.62412100	-0.26096200	-0.91761400
C	2.11028700	-0.29968800	-0.91936100	2.18652500	-0.04607500	-0.96246100
C	1.14028500	-1.20844600	-0.21186600	1.48691200	-1.22761800	-0.36960400
C	0.77195000	-2.26971900	0.33652600	1.16157600	-2.33635400	0.07241700
C	0.45334500	-3.56190900	0.96031900	0.94571800	-3.70493300	0.57090200
H	-0.27851000	-4.12618500	0.37205900	0.27734300	-4.26049100	-0.08801600
H	1.37843300	-4.15287100	1.00386300	1.90995200	-4.21778700	0.59426500
H	0.08054500	-3.44410600	1.98357700	0.53335200	-3.70094800	1.58014200
Au	-0.99647600	-0.54235900	-0.03243600	Au-0.76318100	-0.80417200	-0.07127900
P	-3.12503000	0.57857900	-0.08824300	P -2.82568600	0.34414700	-0.00032300
H	1.77567600	-0.19173500	-1.95696000	H 1.97588100	-0.03356100	-2.03259500
C	2.25958300	1.08222300	-0.28921800	C 1.74153300	1.27360900	-0.34995600
C	2.78354400	2.11805200	-1.09283000	C 1.78845000	2.42464700	-1.15076000
C	2.98294700	3.40117800	-0.55634700	C 1.40826500	3.66652500	-0.62515900
C	2.65916100	3.66158700	0.79088100	C 0.97989400	3.76408500	0.70756100
C	2.13815500	2.63214100	1.59735100	C 0.93984000	2.61684600	1.51526800
C	1.94105200	1.34591400	1.06000700	C 1.32163700	1.37538500	0.98838900
H	3.04920300	1.91583400	-2.12835000	H 2.13599900	2.35193700	-2.17526900

	H 3.39158200 4.19137800 -1.18008900 H 1.90006200 2.82617800 2.63996300 H 1.55412000 0.55231200 1.69623800 C -3.31860200 1.66747300 -1.60319000 H -4.29706100 2.15947600 -1.58596800 H -2.53243700 2.42765800 -1.61534500 H -3.23632800 1.06039100 -2.50914800 C -3.40420900 1.70195600 1.38730300 H -3.36891300 1.11720900 2.31080400 H -2.62067700 2.46411200 1.42295000 H -4.38118700 2.19052700 1.30588800 C -4.58168000 -0.60411400 -0.11866600 H -4.57119200 -1.22886100 0.77894400 H -5.51968700 -0.03946800 -0.15470300 H -4.51524300 -1.24958200 -0.99904400 H 2.81825700 4.65274400 1.20713400	H 1.45543300 4.55245000 -1.24515400 H 0.63864300 2.69388200 2.55255700 H 1.31814800 0.49625800 1.62675900 C -2.64765500 1.99710100 -0.84131200 H -3.57354700 2.56763100 -0.74497000 H -1.82625400 2.55054400 -0.38340800 H -2.42315100 1.84875400 -1.89762600 C -3.39021900 0.72045200 1.73377600 H -3.55756000 -0.20689200 2.28091800 H -2.62211600 1.29996400 2.24656800 H -4.31792900 1.29524500 1.70483900 C -4.24926300 -0.51765800 -0.83455600 H -4.44712600 -1.46825800 -0.33972100 H -5.14157900 0.10921700 -0.78354800 H -4.00223700 -0.70929900 -1.87854600 H 0.69856100 4.72604100 1.11677500
Reactant_PhNH2	**Total Energy** = -856.4321889 C -3.84442500 -1.99604000 -0.06738600 H -3.89546100 -1.15444800 -0.75539100 C -4.55406000 -3.12669900 -0.21863000 H -5.23058200 -3.23465600 -1.06014800 H -4.49999600 -3.93329800 0.50669500 O -3.04268400 -1.80512900 1.07495600 C -1.87684500 -0.90033800 0.97132600 C -0.80167300 -1.61040100 0.19460300 C -0.25801700 -2.54503600 -0.43172100 C 0.26298400 -3.72264300 -1.14207800 H 1.07894900 -4.19994100 -0.58840600 H -0.55361800 -4.45131200 -1.23523100 H 0.61012800 -3.47395400 -2.15076400 Au 1.18453200 -0.56733100 0.01112800 P 3.06650500 0.92695300 0.10196600 H -1.55381900 -0.84406300 2.01677900 C -2.20061000 0.49200700 0.45957000 C -2.79369900 1.41635400 1.35035300 C -3.17002400 2.69378800 0.92718900 C -2.96931200 3.09472800 -0.42382900 C -2.37114200 2.16837200 -1.32111300 C -2.00093400 0.89116800 -0.88135200 H -2.97635900 1.12465100 2.38294500 H -3.62930200 3.38518400 1.62997000 H -2.21798300 2.45048800 -2.36063500 H -1.56483700 0.19608300 -1.59701900 C 3.39044900 1.57263400 1.83316000 H 4.25567600 2.24432700 1.82604100 H 2.51360000 2.11731600 2.19456700 H 3.58845000 0.73611400 2.50928200 C 2.83978000 2.44682500 -0.97379000 H 2.72505700 2.14617800 -2.01905300 H 1.94058700 2.98610600 -0.66280300 H 3.71001400 3.10534000 -0.87971800 C 4.67546600 0.13847200 -0.45533200 H 4.58108200 -0.20761900 -1.48844400 H 5.49023200 0.86788700 -0.39152700 H 4.90748600 -0.71788300 0.18417600	**Total Energy** = -856.18551085 C -4.28950000 -0.30510000 -0.23608500 H -3.97151300 0.56713700 -0.79588200 C -5.30858700 -1.09165200 -0.59182100 H -5.87199300 -0.87627800 -1.48947800 H -5.60888200 -1.92855600 0.02567100 O -3.62327700 -0.51801500 0.98625900 C -2.17907400 -0.32022500 1.02163400 C -1.50771400 -1.46120500 0.32481300 C -1.16993000 -2.50946300 -0.23756900 C -0.93707800 -3.81813600 -0.87144300 H -0.24508200 -4.42004600 -0.28105100 H -1.89039800 -4.34820600 -0.92886600 H -0.54282100 -3.70727100 -1.88185700 Au 0.73825300 -0.95837100 0.03560300 P 2.82695200 0.14175700 0.04850500 H -1.95342600 -0.39570900 2.08609700 C -1.69702800 1.01919800 0.50042400 C -1.55121400 2.09295200 1.39388600 C -1.11419000 3.34294300 0.95504800 C -0.81872900 3.55916700 -0.41111000 C -0.97351900 2.48136300 -1.31503900 C -1.40404600 1.23533200 -0.86023600 H -1.79223100 1.95328700 2.44223600 H -1.01446700 4.15938900 1.66042900 H -0.76973400 2.63199100 -2.36902500 H -1.52807700 0.42756400 -1.57623900 C 3.39122000 0.56518000 1.77255800 H 4.34551000 1.09393600 1.73138400 H 2.64633000 1.20000300 2.25274600 H 3.50780600 -0.34632900 2.35833900 C 2.74726900 1.76213600 -0.86587000 H 2.51667700 1.57781300 -1.91533600 H 1.95691100 2.38285300 -0.44185600 H 3.70516700 2.28076300 -0.78902900 C 4.22481900 -0.81755800 -0.72303600 H 3.98871800 -1.04191300 -1.76315600 H 5.14271800 -0.22801600 -0.68012600 H 4.37147100 -1.75362600 -0.18474900

	N -3.34588100 4.35743800 -0.85046900 H -3.25295200 4.63074500 -1.81782400 H -3.80695400 5.00140400 -0.22431100	N -0.37526800 4.79144500 -0.85269800 H -0.25427100 4.97464100 -1.83517300 H -0.32775500 5.57592200 -0.22342200
Reactant_PhNO2	**Total Energy** = -1005.536344 C 2.37540300 3.54991900 -0.03224000 H 2.78587000 2.82836300 -0.73665300 C 2.52134900 4.87880000 -0.15270300 H 3.08375600 5.29011700 -0.98459100 H 2.12321600 5.56385300 0.59015500 O 1.73764900 3.00639400 1.10651400 C 1.05564500 1.71458800 0.96550200 C -0.15275600 1.88298100 0.08326000 C -0.91959700 2.54024700 -0.65423800 C -1.75817600 3.39013700 -1.50975600 H -2.72670100 3.60347600 -1.04462500 H -1.23502500 4.34577100 -1.65217200 H -1.92070200 2.94543300 -2.49764300 Au -1.65776000 0.22122400 -0.01333100 P -2.96521500 -1.79243500 0.17420800 H 0.70809300 1.52678600 1.98738500 C 1.99952200 0.58765300 0.54319800 C 2.95537200 0.14919200 1.48617000 C 3.86198600 -0.86989900 1.16306500 C 3.79568800 -1.44266900 -0.11873100 C 2.86692700 -1.01917000 -1.08121400 C 1.96792300 0.00418800 -0.74058600 H 2.99653600 0.61324400 2.46819100 H 4.60350300 -1.22082400 1.87209400 H 2.86439900 -1.48089200 -2.06234300 H 1.25110400 0.34921600 -1.48091100 C -2.93034400 -2.51347900 1.90548400 H -3.54360900 -3.42031400 1.94287000 H -1.90260600 -2.76315600 2.18390300 H -3.32248900 -1.78374100 2.61945100 C -2.36648900 -3.15546500 -0.96609100 H -2.42296700 -2.82083000 -2.00570700 H -1.32749000 -3.40424300 -0.73226800 H -2.98830700 -4.04825400 -0.83964200 C -4.77708200 -1.52978300 -0.23563800 H -4.87838900 -1.17452400 -1.26493200 H -5.32298400 -2.47292600 -0.12416000 H -5.20524600 -0.78403400 0.44007400 N 4.73724800 -2.53456900 -0.46862800 O 4.63684200 -3.05562900 -1.63094600 O 5.58655200 -2.89378100 0.41306900	**Total Energy** = -1005.25417681 C 2.06279300 3.76025500 -0.28101800 H 2.52100700 2.98517000 -0.88579800 C 2.04538900 5.05456400 -0.60598400 H 2.50929400 5.39014200 -1.52340000 H 1.60532900 5.78892000 0.05665200 O 1.54916800 3.33966100 0.96650100 C 0.85077000 2.06651100 1.00579400 C -0.42216900 2.16515300 0.22929900 C -1.40006900 2.58517900 -0.40215500 C -2.50056500 3.22759900 -1.13750600 H -3.43074500 3.18196400 -0.56997100 H -2.24134000 4.27834600 -1.28852700 H -2.65066600 2.76770200 -2.11472900 Au-1.54220100 0.15507300 0.03532800 P -2.18255100 -2.12247000 0.11359700 H 0.59914300 1.95522400 2.06134400 C 1.72232000 0.89592400 0.57396500 C 2.62475200 0.36805700 1.51032000 C 3.45039700 -0.70756600 1.16977200 C 3.34679500 -1.23615900 -0.11920700 C 2.48111900 -0.71496500 -1.08321800 C 1.66615800 0.36279700 -0.72526600 H 2.68791200 0.80255500 2.50074700 H 4.15377900 -1.13247800 1.87221100 H 2.46282700 -1.14074100 -2.07654300 H 1.00357400 0.79837300 -1.46537600 C -2.18220600 -2.80346300 1.84692800 H -2.46530700 -3.85770800 1.82918600 H -1.18687200 -2.70561800 2.28010600 H -2.89100100 -2.25012800 2.46252700 C -1.01887300 -3.20151200 -0.86127300 H -1.02928300 -2.90373200 -1.90981300 H -0.00463100 -3.09347400 -0.47594700 H -1.32600100 -4.24598300 -0.78067400 C -3.88426500 -2.44774200 -0.56996300 H -3.93212200 -2.12747000 -1.61051600 H -4.10520100 -3.51523300 -0.51161300 H -4.62626000 -1.89456400 0.00529900 N 4.18477800 -2.39280600 -0.48190400 O 4.00897900 -2.90568800 -1.62176200 O 5.01325300 -2.80811800 0.37030700
Product_Ph	**Total Energy** = -801.1171399 C -3.52259600 2.50767100 -0.83341900 H -4.38242100 3.18354900 -0.99446700 C -2.62494400 2.89493000 0.32838000 H -3.22978100 2.74907600 1.24270300 H -2.49057100 3.98630300 0.26695400 O -3.37375100 1.52065100 -1.57846600 C -1.64491600 0.04572800 -0.77357400 C -0.93921700 1.03666400 -0.05276100	

	C -1.26037000 2.22911700 0.49833300 C -0.28679500 3.06273200 1.31133300 H 0.62657000 2.50592900 1.54304500 H -0.00142500 3.97497100 0.76729100 H -0.74377700 3.38426000 2.25815200 Au 1.01718600 0.21003700 -0.06102700 P 3.29842600 -0.66097000 -0.04133400 H -1.43245300 -0.04115600 -1.83989800 C -2.48394500 -0.99637200 -0.20862400 C -3.08418200 -1.93777400 -1.09010200 C -3.94849300 -2.92185800 -0.59280800 C -4.21545400 -2.98425300 0.79096300 C -3.61681400 -2.06075300 1.67874400 C -2.75591800 -1.07431500 1.18617400 H -2.88439200 -1.87488700 -2.15755500 H -4.41367200 -3.63343600 -1.26833600 H -3.82359300 -2.12444500 2.74320800 H -2.27645800 -0.37335700 1.86432800 C 3.50405100 -2.25793100 -1.00998000 H 3.22801200 -2.09354700 -2.05562300 H 4.54419900 -2.59836700 -0.96013900 H 2.85110400 -3.02930300 -0.59146100 C 3.95003000 -1.05499300 1.67613800 H 3.30478100 -1.79775300 2.15412200 H 4.96963800 -1.45036000 1.61133700 H 3.95363700 -0.14829900 2.28821900 C 4.56371300 0.51633000 -0.77716400 H 4.56826800 1.45316100 -0.21230100 H 5.56302400 0.06882600 -0.74225200 H 4.30279100 0.73587900 -1.81656000 H -4.88241700 -3.75013300 1.17828500	
Product_PhNH2	**Total Energy** =-856.4862384 C -2.64498500 3.12611300 -0.97622700 H -3.30726200 3.99610900 -1.14549400 C -2.05338600 3.04757400 0.42691400 H -2.87169300 2.67371200 1.06994700 H -1.88594400 4.08047400 0.76105600 O -2.46340600 2.29986400 -1.88721400 C -1.40409100 0.24909400 -0.80088600 C -0.53796000 1.04268800 0.01376700 C -0.78201200 2.22370900 0.64583900 C 0.21552200 2.89130300 1.57421500 H 1.05266300 2.22750500 1.81140700 H 0.62413100 3.80736800 1.12194700 H -0.26868100 3.18985700 2.51553200 Au 1.34078000 0.10119600 0.00268100 P 3.54367300 -0.96187400 -0.04397800 H -1.10293700 0.10467600 -1.83860200 C -2.54425100 -0.48795800 -0.36956300 C -3.31089000 -1.22414100 -1.33170500 C -4.46022500 -1.90814500 -0.97133900 C -4.89730800 -1.90604000 0.39159700 C -4.12677800 -1.19390200 1.36961200 C -2.98479600 -0.50724200 0.99468300 H -2.99120400 -1.22201200 -2.37143400	

	H -5.03772800 -2.44829600 -1.71715600 H -4.44300600 -1.21183700 2.40984800 H -2.38964500 0.00557300 1.74566700 C 3.57929300 -2.60593200 -0.95476200 H 3.25589000 -2.45873400 -1.98946900 H 4.59225400 -3.02340100 -0.94931800 H 2.89582900 -3.30999200 -0.47101000 C 4.25765000 -1.34678600 1.65171400 H 3.58179300 -2.01546000 2.19287000 H 5.23792200 -1.82579400 1.55242200 H 4.36586400 -0.42108000 2.22470900 C 4.86903600 0.07006500 -0.88740000 H 4.98365800 1.02293200 -0.36217200 H 5.82671100 -0.46206700 -0.88361200 H 4.57349000 0.27518300 -1.92054100 N -6.02696800 -2.58351100 0.76082800 H -6.34578000 -2.59106700 1.72066800 H -6.57593700 -3.09676100 0.08378700	
Product_PhNO2	**Total Energy** = -1005.575049 C -1.66635800 4.06801700 -0.55494200 H -2.25195200 5.00539800 -0.57953100 C -0.59958100 4.02939900 0.52534600 H -1.12497300 4.17401800 1.48640700 H -0.01094300 4.95448600 0.40360200 O -1.92059800 3.16785300 -1.37777900 C -0.74280400 1.08958600 -0.89671000 C 0.17185600 1.68839700 -0.02290700 C 0.35864100 2.84559300 0.63860100 C 1.54221300 3.11171000 1.54987400 H 2.15357700 2.21568200 1.69488100 H 2.18522000 3.90007000 1.13309000 H 1.20526100 3.46059000 2.53611700 Au 1.56003100 0.04750700 -0.07327800 P 3.24865300 -1.71300800 -0.01589500 H -0.52119100 1.12904400 -1.96429300 C -1.90927300 0.28733900 -0.51667000 C -2.71680000 -0.25773700 -1.54714300 C -3.87342600 -0.98497100 -1.23742000 C -4.20316800 -1.16284500 0.11590200 C -3.42404600 -0.63710800 1.16424600 C -2.27423000 0.08865700 0.84087400 H -2.44632000 -0.09460500 -2.58724000 H -4.51082800 -1.40611200 -2.00655400 H -3.72733700 -0.80656600 2.19126700 H -1.64951600 0.49546200 1.63074500 C 2.91287300 -3.10563800 -1.23068100 H 2.88024900 -2.70834500 -2.24923500 H 3.70355100 -3.86097200 -1.16356800 H 1.94966800 -3.57100700 -1.00277200 C 3.40542700 -2.54631900 1.65930600 H 2.44638200 -2.98944900 1.94252400 H 4.16815600 -3.33160000 1.61943700 H 3.68805200 -1.80854700 2.41583900 C 4.97561000 -1.10365800 -0.42981700 H 5.27964200 -0.33494800 0.28657000	

	H 5.68785500 -1.93495400 -0.39016000 H 4.98322600 -0.67006600 -1.43401800 N -5.42127800 -1.94325700 0.45841700 O -6.11284600 -2.41520100 -0.50396900 O -5.69813800 -2.09455800 1.69527300	
TS_Ph	**Total Energy** = -801.0648663, **Frequency** = -202.7327 cm^{-1} C 3.60487300 -1.91712500 -0.25912900 H 4.18256900 -1.44137600 0.53525900 C 3.18995400 -3.22350000 -0.20359400 H 3.52651000 -3.87379100 0.59949100 H 2.71007200 -3.67854000 -1.06586700 O 3.18062200 -1.13648200 -1.29345200 C 1.97043900 -0.24282400 -0.96038500 C 1.01626100 -1.09748200 -0.16517200 C 1.20208200 -2.22511700 0.44782800 C 0.74134500 -3.29213200 1.37220400 H -0.25876500 -3.03735800 1.74533400 H 0.68728800 -4.26801400 0.87822800 H 1.40517800 -3.37784700 2.24042300 Au -0.96747000 -0.35267900 -0.05847400 P -3.18496500 0.61310500 -0.04213700 H 1.58383800 -0.04020500 -1.96231100 C 2.42437700 1.04466600 -0.29390400 C 2.91820200 2.07970600 -1.11841000 C 3.40347600 3.27003100 -0.55104600 C 3.39696300 3.43743100 0.84814700 C 2.90114100 2.41080500 1.67483300 C 2.41592200 1.21868600 1.10702600 H 2.93613100 1.94877600 -2.19857400 H 3.78536200 4.05984300 -1.19200200 H 3.77267200 4.35743300 1.28798300 H 2.89263400 2.53977100 2.75395800 H 2.02291300 0.43739900 1.75293100 C -3.68333700 1.33257700 1.61882400 H -3.67563300 0.54715100 2.38007400 H -2.97299000 2.11122700 1.91116200 H -4.68804500 1.76454900 1.55590400 C -4.54837900 -0.60016000 -0.48265200 H -4.56570000 -1.41705400 0.24458100 H -5.51913400 -0.09256200 -0.47859700 H -4.36391700 -1.01829000 -1.47639800 C -3.36911600 2.02500800 -1.26546500 H -4.38333400 2.43624700 -1.21754600 H -2.64838400 2.81343400 -1.03044800 H -3.17489000 1.66269300 -2.27911800	**Total Energy** = -800.82148920, **Frequency** = -255.0172 cm^{-1} C 3.64843700 -1.77094700 -0.18576900 H 4.16048900 -1.20252600 0.58497400 C 3.34751100 -3.09217400 -0.08526500 H 3.70459500 -3.67462500 0.75512200 H 2.91163200 -3.60884000 -0.93278400 O 3.19080100 -1.07693900 -1.27638600 C 1.97338400 -0.23908000 -0.99520800 C 1.03639300 -1.09940400 -0.19945600 C 1.21843600 -2.17897300 0.46326400 C 0.84068900 -3.26891300 1.38845400 H -0.18507200 -3.10238800 1.72904000 H 0.89160700 -4.24231600 0.90038600 H 1.49001200 -3.27523600 2.26537200 Au -0.96378100 -0.37880000 -0.07533500 P -3.14567300 0.57619800 -0.05099000 H 1.58852800 -0.04721800 -1.99491300 C 2.36284300 1.05436100 -0.30795600 C 3.02564200 2.02467400 -1.07838200 C 3.45350100 3.21898200 -0.48967500 C 3.21949400 3.45146800 0.87516000 C 2.55945900 2.48533300 1.64617200 C 2.13239900 1.28663000 1.05655800 H 3.21800000 1.83590200 -2.12875700 H 3.96720300 3.96197300 -1.08568300 H 3.55073000 4.37554000 1.33138300 H 2.38212900 2.66241000 2.69937000 H 1.62261500 0.54258500 1.65837700 C -3.63283600 1.30401600 1.59484700 H -3.62467400 0.52785200 2.35998100 H -2.92426400 2.08282700 1.87636900 H -4.63427800 1.73367300 1.52712100 C -4.50864600 -0.62257200 -0.47659500 H -4.52691000 -1.43480800 0.24989000 H -5.47076000 -0.10661600 -0.46592800 H -4.33509600 -1.04136700 -1.46780100 C -3.32746400 1.97346600 -1.27147200 H -4.33664300 2.38636700 -1.21539700 H -2.60379800 2.75646300 -1.04533500 H -3.14410400 1.60686500 -2.28144100
TS_PhNH2	**Total Energy** =-856.4227526, **Frequency** = -204.7950 cm^{-1} C -2.92321200 2.78051400 -0.28039600 H -3.63068200 2.35519700 0.43398100 C -2.27192000 3.96816300 -0.06478600 H -2.53255900 4.59322000 0.78533300 H -1.64915100 4.39634700 -0.84560000 O -2.58616800 2.02976600 -1.36486400	**Total Energy** = -856.17259521, **Frequency** = -260.8318 cm^{-1} C -3.03638600 2.63617000 -0.18671700 H -3.68942000 2.11015600 0.50370400 C -2.49110700 3.85565300 0.06246600 H -2.77452400 4.41572700 0.94520300 H -1.91413200 4.35146700 -0.70986500 O -2.66137800 1.97083500 -1.32321900

	C -1.63551300 0.84466300 -1.03466800 C -0.56957100 1.42351600 -0.13588700 C -0.54607200 2.50687900 0.57372100 C 0.06621300 3.38122700 1.60492000 H 0.96722800 2.89538900 2.00098100 H 0.34977200 4.35798300 1.19890300 H -0.61886200 3.53980100 2.44583300 Au 1.21164700 0.27657900 -0.03577000 P 3.18138700 -1.12654800 -0.04002000 H -1.24496500 0.63074700 -2.03261600 C -2.39320200 -0.33740500 -0.48517300 C -3.04951300 -1.20182800 -1.39334200 C -3.82383300 -2.27460600 -0.94538200 C -3.97094700 -2.52403900 0.44796500 C -3.30562500 -1.66216200 1.36317600 C -2.53520000 -0.59052400 0.89858800 H -2.96375200 -1.02159900 -2.46349100 H -4.32239500 -2.92226600 -1.66289900 H -3.39875300 -1.84143500 2.43216300 H -2.03011600 0.04524500 1.62229500 C 3.15916200 -2.40997200 -1.40993500 H 3.10217300 -1.91176400 -2.38205800 H 4.06780300 -3.02048400 -1.36949600 H 2.28390800 -3.05582700 -1.29501800 C 3.41604000 -2.10673900 1.54405900 H 2.54499600 -2.74646800 1.71270000 H 4.31442200 -2.72958100 1.47280300 H 3.51752400 -1.42234700 2.39127200 C 4.78758800 -0.18348500 -0.27737000 H 4.91855800 0.53435400 0.53754600 H 5.63513000 -0.87752900 -0.28700900 H 4.75754900 0.36263000 -1.22463800 N -4.73733000 -3.58448800 0.90005800 H -4.86099100 -3.75640500 1.88702600 H -5.22351100 -4.18861400 0.25369200	C -1.66074000 0.86579000 -1.07385700 C -0.61036200 1.45492500 -0.17636200 C -0.60146000 2.48379500 0.58300200 C -0.06235900 3.39161500 1.61772300 H 0.89445500 2.99641100 1.97038300 H 0.09953400 4.39493100 1.22343200 H -0.73881300 3.44936000 2.47190400 Au 1.18862900 0.32474000 -0.05442600 P 3.12238900 -1.06427700 -0.04851500 H -1.27575500 0.68431800 -2.07548300 C -2.32352200 -0.36531400 -0.50951800 C -3.08006100 -1.17351300 -1.37807700 C -3.76492600 -2.29010000 -0.90827800 C -3.71345100 -2.63692600 0.46356400 C -2.95077400 -1.82785100 1.33635900 C -2.27120000 -0.70939800 0.85134100 H -3.14420900 -0.91357500 -2.42933600 H -4.34633600 -2.89723000 -1.59201400 H -2.89920200 -2.07890100 2.38946300 H -1.69283400 -0.10453200 1.54166700 C 3.10400400 -2.32368100 -1.42321600 H 3.06172600 -1.81623400 -2.38692600 H 4.00575300 -2.93745600 -1.37741400 H 2.22600200 -2.96191000 -1.32411900 C 3.32917500 -2.05848100 1.51507300 H 2.45663100 -2.69502400 1.66169100 H 4.22349100 -2.68078400 1.44446700 H 3.42247300 -1.38826700 2.36948300 C 4.72820500 -0.13992200 -0.25575400 H 4.85643700 0.56600400 0.56469300 H 5.56330000 -0.84316000 -0.26108900 H 4.71576500 0.41239500 -1.19529400 N -4.39190500 -3.74312900 0.93480000 H -4.37582600 -3.98481100 1.91120400 H -4.94790500 -4.31051500 0.31728800
TS_PhNO2	**Total Energy** =-1005.526999, **Frequency** = -206.8975 cm^{-1} C -1.56622700 3.74202400 -0.14663500 H -2.37715800 3.57099800 0.56347900 C -0.54606700 4.63091600 0.08029100 H -0.57145600 5.28365200 0.94875700 H 0.16892200 4.85412800 -0.70705100 O -1.51914500 2.95465300 -1.26142700 C -0.91160600 1.56088100 -1.04631500 C 0.24963800 1.71833300 -0.10226100 C 0.58338300 2.71535400 0.65870000 C 1.41935300 3.29018200 1.74344600 H 2.10459100 2.51826200 2.11604700 H 2.01381400 4.14171400 1.39591200 H 0.80230700 3.61802300 2.58812700 Au 1.58201200 0.06437700 -0.03505200 P 3.01213900 -1.88760900 -0.06238500 H -0.57290900 1.31799600 -2.05676600 C -2.00122300 0.59186200 -0.60637100 C -2.87023900 0.07909600 -1.59469200	**Total Energy** = -1005.24325702, **Frequency** = -249.6983 cm^{-1} C -1.68415800 3.64066700 -0.07269100 H -2.49332400 3.35742900 0.59377300 C -0.75511700 4.58897400 0.21533200 H -0.84049900 5.18548500 1.11530300 H -0.03409700 4.88105900 -0.53964400 O -1.54939300 2.92420700 -1.23723100 C -0.93774400 1.56615300 -1.05837700 C 0.20830700 1.71580800 -0.10456000 C 0.51987300 2.65320900 0.71042300 C 1.28803000 3.27314200 1.81117800 H 2.03397700 2.55707300 2.16732800 H 1.80116500 4.17660900 1.48156600 H 0.63331300 3.52007300 2.64848400 Au 1.58762600 0.08891200 -0.04694800 P 3.01827500 -1.81557400 -0.09695800 H -0.59209800 1.32762400 -2.06260000 C -1.99966200 0.57745900 -0.61009500 C -3.02057000 0.26884100 -1.52571200

	C -3.92322100 -0.77855700 -1.24588600 C -4.09016000 -1.11439900 0.10789100 C -3.24466200 -0.61941900 1.11319600 C -2.19573300 0.23718300 0.74591300 H -2.73141300 0.35924900 -2.63589500 H -4.60224600 -1.18234700 -1.98853100 H -3.41386000 -0.90758500 2.14472300 H -1.52545800 0.61576800 1.51192000 C 2.33849400 -3.26449700 -1.14532400 H 2.23615500 -2.90935800 -2.17478300 H 3.01753800 -4.12381100 -1.12628400 H 1.35497600 -3.57418100 -0.78067100 C 3.25679900 -2.66327700 1.62944300 H 2.28808700 -2.95501300 2.04512400 H 3.89581300 -3.54925300 1.54789500 H 3.72655300 -1.94189200 2.30427100 C 4.74084100 -1.54768300 -0.71027000 H 5.23412700 -0.80370300 -0.07819300 H 5.33059200 -2.47081500 -0.70889400 H 4.68290600 -1.15859700 -1.73089100 N -5.19345700 -2.02990900 0.48998700 O -5.31857400 -2.32644200 1.72616000 O -5.95040100 -2.46990200 -0.43848800	C -4.04447000 -0.61209400 -1.17310300 C -4.02066100 -1.17116400 0.10812300 C -3.02730800 -0.87764500 1.04207000 C -2.00961900 0.00882700 0.67211400 H -3.01755600 0.72781200 -2.50687400 H -4.84164400 -0.86732800 -1.85702800 H -3.06150100 -1.33272900 2.02187500 H -1.22948200 0.25192700 1.38267900 C 2.31441700 -3.21691300 -1.10441100 H 2.16408300 -2.89246700 -2.13398000 H 3.00249800 -4.06437800 -1.09059300 H 1.35500100 -3.52489800 -0.68917400 C 3.35233900 -2.54254700 1.58678500 H 2.41300200 -2.83930900 2.05305900 H 3.99856100 -3.41727900 1.49075900 H 3.84164600 -1.80232000 2.21966300 C 4.69839300 -1.47889200 -0.83066300 H 5.21220600 -0.71599300 -0.24606200 H 5.29164600 -2.39538900 -0.82945700 H 4.58888700 -1.12215600 -1.85467600 N -5.08888800 -2.11124000 0.48976400 O -5.04115300 -2.61374900 1.64564500 O -5.98351300 -2.35865400 -0.36190900

	Cation-Accelerated-Oxonia Claisen (gold(I)-coordinated to oxygen) at B3LYP/LANL2DZ level
Reactant_Ph	**Total Energy** = -801.08155997 C 1.39493200 0.50996200 1.86977000 H 2.41363700 0.16215500 2.00492700 C 0.64244000 1.06154000 2.82997800 H 1.04640100 1.16753300 3.83135000 H -0.37195800 1.41288200 2.65544500 O 0.89846500 0.27327600 0.55525500 C 1.93287000 0.39644400 -0.63299200 C 2.34464000 1.78739600 -0.73534500 C 2.66865100 2.96231500 -0.83831800 C 3.07405300 4.36810200 -0.96941800 H 1.27458300 0.11220500 -1.46174400 C 3.02365200 -0.63613700 -0.44320200 C 2.71652600 -1.99392100 -0.68698900 C 3.69385000 -2.98569500 -0.50918400 C 4.99124200 -2.62696700 -0.08942800 C 5.30468300 -1.27475400 0.14703700 C 4.32513000 -0.28090700 -0.02957500 H 1.71754900 -2.27397300 -1.01750000 H 3.45372900 -4.02758300 -0.70212300 H 6.30715300 -0.99674400 0.46055700 H 4.57389500 0.76434000 0.13318700 H 5.75086700 -3.39273000 0.04317700 H 2.35812900 4.93090700 -1.57991200 H 3.13571800 4.84828000 0.01488900 H 4.06019900 4.44457300 -1.44355500 Au -1.18494200 0.00361400 0.14757400

	P	-3.47139600	-0.34011700	-0.33915900
	C	-4.40467100	1.26154400	-0.61661300
	H	-5.45605900	1.04700400	-0.83692500
	H	-4.34318700	1.88610600	0.27892300
	H	-3.96347700	1.80621200	-1.45603500
	C	-4.37413600	-1.23487700	1.03853700
	H	-5.42513600	-1.37691700	0.76434300
	H	-3.91052500	-2.20982800	1.21269100
	H	-4.31761000	-0.64927900	1.96037800
	C	-3.73980800	-1.36659200	-1.88467700
	H	-3.27040000	-2.34690000	-1.76423400
	H	-4.81255600	-1.49923700	-2.06216500
	H	-3.29165200	-0.86368400	-2.74616500
Reactant_PhNH2	**Total Energy** = -856.44101237			
	C	1.12602900	0.35933500	1.90074800
	H	2.19326000	0.17958100	1.97756300
	C	0.33540800	0.66216700	2.94003200
	H	0.76056300	0.72196200	3.93651400
	H	-0.73103300	0.84953500	2.83604600
	O	0.63626300	0.18921500	0.58047000
	C	1.62940400	0.63297300	-0.63993300
	C	1.63297100	2.08513900	-0.66520800
	C	1.61392700	3.30805300	-0.69916700
	C	1.60856500	4.77644200	-0.74510300
	H	1.03135300	0.20738500	-1.45315300
	C	2.93962400	-0.06530800	-0.49349700
	C	3.03361000	-1.43817200	-0.83263000
	C	4.23209400	-2.13796200	-0.69707500
	C	5.39924300	-1.47786500	-0.21413900
	C	5.30970400	-0.09686700	0.12107900
	C	4.10187700	0.58947300	-0.01828200
	H	2.15514200	-1.96145900	-1.20711100
	H	4.28423400	-3.18981600	-0.96808300
	H	6.19362300	0.42556500	0.47965500
	H	4.05823400	1.64770000	0.22655100
	H	0.77837200	5.15101800	-1.35562100
	H	1.50717200	5.19602700	0.26349000
	H	2.54423500	5.15566400	-1.17397200
	Au	-1.42599100	-0.14617900	0.16069200
	P	-3.69303600	-0.56800200	-0.36416700
	C	-4.82385600	0.85617100	0.09147100
	H	-5.85737200	0.61510200	-0.17998800
	H	-4.76748700	1.04318600	1.16751600
	H	-4.51152800	1.76006400	-0.43891000
	C	-4.38215000	-2.07139100	0.51872500
	H	-5.43065300	-2.22077900	0.23885100
	H	-3.80454600	-2.95854600	0.24438600
	H	-4.31316200	-1.92881700	1.60078800
	C	-3.97173300	-0.87645000	-2.19242900
	H	-3.38481000	-1.74085300	-2.51534900
	H	-5.03337600	-1.06945700	-2.38135000
	H	-3.65568900	-0.00160000	-2.76749400
	N	6.59180800	-2.16109500	-0.08171500
	H	6.66501500	-3.13767500	-0.32774700
	H	7.42618100	-1.69609800	0.24592600

Reactant_PhOMe	**Total Energy** = -915.59159349 C 0.75956600 0.94426000 1.88316300 H 1.83564200 0.88410100 2.00771900 C -0.10090900 1.26089100 2.85967700 H 0.27299000 1.46124600 3.85828000 H -1.17507500 1.32533400 2.70141600 O 0.33557500 0.59827300 0.57066200 C 1.31459800 0.99102400 -0.63531900 C 1.32004900 2.44060800 -0.74130600 C 1.30417300 3.65906600 -0.84860500 C 1.30236300 5.12187400 -0.98294700 H 0.74703600 0.52774700 -1.45003700 C 2.63952700 0.30726200 -0.44214600 C 2.74455800 -1.07266500 -0.71824800 C 3.95320000 -1.76124800 -0.54118300 C 5.08997900 -1.05578300 -0.08079600 C 5.00005500 0.33006800 0.19161900 C 3.78865900 1.00079200 0.01122600 H 1.87474900 -1.61943400 -1.07884900 H 4.00673400 -2.82100200 -0.76630100 H 5.89155200 0.84749900 0.53100700 H 3.73334500 2.06917800 0.20172100 H 0.45761600 5.46251100 -1.59320100 H 1.22912000 5.60227700 0.00052400 H 2.22799300 5.46890300 -1.45828900 Au -1.64055400 -0.11257200 0.15314600 P -3.79843400 -0.93701200 -0.34564500 C -5.01848600 0.41945600 -0.77445400 H -5.99951900 -0.01675700 -0.99182300 H -5.10956800 1.11436200 0.06498100 H -4.66575300 0.97102800 -1.65033200 C -4.55633900 -1.88064400 1.08608300 H -5.55248700 -2.24256200 0.80924600 H -3.92089900 -2.73220400 1.34473400 H -4.63955800 -1.22656700 1.95852000 C -3.80911400 -2.11725500 -1.80233500 H -3.16764700 -2.97628200 -1.58658400 H -4.82970500 -2.46698500 -1.99211600 H -3.43045500 -1.60921200 -2.69365100 O 6.33263800 -1.62071900 0.12724900 C 6.53752100 -3.04334000 -0.14672000 H 6.34850900 -3.27015200 -1.20405400 H 7.58616100 -3.22827000 0.08891100 H 5.89740300 -3.66302300 0.49478400
Reactant_PhCF3	**Total Energy** = -1138.12539466 C 0.21772300 1.16349300 1.87002300 H 1.29379500 1.17033100 2.00768800 C -0.67686000 1.43354100 2.82771600 H -0.33304400 1.66371100 3.83070000 H -1.74987700 1.43181800 2.65064700 O -0.17305100 0.77730600 0.55162400 C 0.75611100 1.23386900 -0.62175500 C 0.72776800 2.68505100 -0.71058700 C 0.67727700 3.90358400 -0.80393200

	C	0.62776800	5.36682200	-0.92036100
	H	0.22656100	0.77449300	-1.46439200
	C	2.11824200	0.58234700	-0.44486500
	C	2.22226200	-0.81632400	-0.61289500
	C	3.45524500	-1.46137600	-0.45583900
	C	4.59732300	-0.70226700	-0.13145500
	C	4.50894500	0.69084800	0.03034700
	C	3.26780100	1.33102000	-0.12530600
	H	1.34164100	-1.40246900	-0.86556000
	H	3.53252900	-2.53718700	-0.57854000
	H	5.39432300	1.26739200	0.27861900
	H	3.19847100	2.40885700	-0.01492400
	H	-0.22931400	5.68591700	-1.52481200
	H	0.54139300	5.83245700	0.06900600
	H	1.54001100	5.74954700	-1.39400400
	Au	-2.07913800	-0.12883400	0.14060500
	P	-4.14885800	-1.16180400	-0.34343800
	C	-5.47864400	0.07403500	-0.81005700
	H	-6.41819300	-0.44992000	-1.01650000
	H	-5.63213200	0.78078700	0.01012600
	H	-5.17124600	0.62927900	-1.70058700
	C	-4.82193900	-2.13060800	1.11273000
	H	-5.77674600	-2.59374900	0.84126800
	H	-4.11050000	-2.90988300	1.39955400
	H	-4.97466400	-1.46252500	1.96487700
	C	-4.04177200	-2.37286400	-1.76988600
	H	-3.31994000	-3.15985400	-1.53466000
	H	-5.02347800	-2.82505700	-1.94790700
	H	-3.71566300	-1.85263500	-2.67479300
	C	5.92848400	-1.39361300	-0.00749200
	F	5.81201800	-2.66435600	0.57428500
	F	6.83934500	-0.66832900	0.76671200
	F	6.54206500	-1.59399800	-1.25915000
Reactant_PhCN	**Total Energy** = -893.29348839			
	C	0.94489000	0.59772500	1.90307100
	H	2.01556100	0.46673500	2.01684900
	C	0.10619400	0.91788400	2.89558900
	H	0.49246300	1.04478600	3.90156100
	H	-0.96216600	1.05576700	2.74554700
	O	0.49140800	0.33452900	0.57477900
	C	1.42254700	0.80315000	-0.59937100
	C	1.41980200	2.25699400	-0.64796400
	C	1.39085700	3.47850100	-0.70658700
	C	1.37003600	4.94525400	-0.78181100
	H	0.87185400	0.37514300	-1.44496300
	C	2.77142400	0.12160800	-0.45813600
	C	2.85143000	-1.27039000	-0.68720800
	C	4.07287700	-1.94344900	-0.56456800
	C	5.24059700	-1.22331100	-0.21288200
	C	5.16664600	0.17115600	0.00878700
	C	3.93711000	0.83641900	-0.11404300
	H	1.95922900	-1.82923900	-0.96092300
	H	4.13469900	-3.01251700	-0.74245300
	H	6.06517800	0.72181100	0.26965000
	H	3.88663100	1.90993100	0.04159500

	H	0.51214900	5.29914600	-1.36548100
	H	1.30721500	5.38500900	0.22106600
	H	2.28367000	5.32203100	-1.25755700
	Au	-1.56338700	-0.15155900	0.14804300
	P	-3.79269800	-0.75019200	-0.36028900
	C	-4.90998000	0.73863100	-0.58063400
	H	-5.93142500	0.40872500	-0.79902800
	H	-4.91213200	1.33895200	0.33337700
	H	-4.54524700	1.35583100	-1.40638600
	C	-4.57671500	-1.79633100	0.98269900
	H	-5.60356100	-2.05376900	0.70118400
	H	-3.99935300	-2.71453400	1.12189000
	H	-4.58916500	-1.24212800	1.92529800
	C	-3.93472100	-1.74550800	-1.94213600
	H	-3.34919300	-2.66494900	-1.85496200
	H	-4.98354000	-2.00182900	-2.12693700
	H	-3.55261500	-1.16156800	-2.78402700
	C	6.50003500	-1.90991900	-0.08703200
	N	7.53262300	-2.47485700	0.01840000
Reactant_PhNO2	**Total Energy** = -1005.54280713			
	C	0.51762100	1.25731700	1.82031600
	H	1.58625400	1.17342900	1.98849500
	C	-0.37309000	1.65165100	2.73764500
	H	-0.03686800	1.89585300	3.73994000
	H	-1.43606200	1.74032300	2.52587700
	O	0.12268000	0.84814300	0.50900100
	C	1.09996400	1.19416200	-0.66108100
	C	1.23661300	2.63824100	-0.75522700
	C	1.32388900	3.85407000	-0.85646700
	C	1.43734300	5.31304300	-0.98023100
	H	0.52788900	0.79401800	-1.50594400
	C	2.38023700	0.39429500	-0.47221300
	C	2.33497100	-1.00339700	-0.67480400
	C	3.48249800	-1.78753500	-0.50298900
	C	4.67695600	-1.14814000	-0.12948100
	C	4.75631100	0.23862600	0.06838500
	C	3.59539300	1.00913100	-0.10671500
	H	1.40322900	-1.48036200	-0.97016400
	H	3.47357300	-2.86091400	-0.65460000
	H	5.70333100	0.68794300	0.34589800
	H	3.63763000	2.08608700	0.02384200
	H	0.93107900	5.67000900	-1.88482100
	H	0.97982000	5.81020800	-0.11600100
	H	2.48789500	5.62290000	-1.03134800
	Au	-1.79055600	-0.05656900	0.12994100
	P	-3.87466600	-1.08464200	-0.29832600
	C	-5.29156800	-0.21212200	0.56434300
	H	-6.23498300	-0.71868200	0.33335300
	H	-5.13152300	-0.22515700	1.64606700
	H	-5.34824700	0.82672300	0.22761400
	C	-3.93300400	-2.86649000	0.27953700
	H	-4.92311600	-3.28993600	0.07882700
	H	-3.17607300	-3.45320000	-0.24829400
	H	-3.73013800	-2.91423500	1.35296700
	C	-4.31246500	-1.10964100	-2.12041600

	H	-3.55296700	-1.66488500	-2.67772200
	H	-5.28662300	-1.59041600	-2.26099400
	H	-4.35612000	-0.08698300	-2.50530900
	N	5.89887900	-1.97071900	0.05505300
	O	5.79951300	-3.23033400	-0.12967600
	O	6.97453100	-1.37135700	0.38979000
Product_Ph	**Total Energy** = -801.1196886			
	C	2.27134900	-2.58296600	-0.27249000
	H	2.97384500	-3.18854500	-0.86075200
	C	2.78890500	-1.86166300	0.93029000
	H	3.50835600	-2.49233300	1.46314100
	H	1.97023600	-1.59419700	1.60791400
	O	1.09257700	-2.49329400	-0.71671700
	C	2.16041600	1.18649100	-1.03565100
	C	2.84042500	0.30175400	-0.31398700
	C	3.51871400	-0.58698200	0.39663000
	C	4.99351100	-0.45518100	0.74558800
	H	5.41091500	0.47767000	0.35703900
	H	5.13436600	-0.47237600	1.83509600
	H	5.57183700	-1.29030000	0.32590300
	H	2.17294400	1.07085500	-2.12296800
	C	1.39192200	2.34699200	-0.52535400
	C	0.72768300	3.18685100	-1.45119700
	C	-0.00138100	4.30647400	-1.01012300
	C	-0.07814600	4.60262100	0.36461300
	C	0.58138800	3.77118100	1.29552300
	C	1.30845600	2.65301800	0.85602600
	H	0.80034500	2.97577300	-2.51668700
	H	-0.48962100	4.95403900	-1.73370600
	H	0.54387300	4.01087600	2.35546800
	H	1.83372200	2.02936800	1.57621500
	Au	-0.61515200	-1.30286500	-0.17690300
	P	-2.54903100	-0.03586300	0.30262700
	C	-4.08330500	-1.09842300	0.47600100
	H	-4.25738600	-1.65098200	-0.45153700
	H	-3.94820100	-1.81389700	1.29186000
	H	-4.95189600	-0.46576700	0.68887300
	C	-2.39971500	0.93775000	1.89586700
	H	-3.32598300	1.49351300	2.07871900
	H	-2.21574400	0.25724800	2.73187200
	H	-1.56549400	1.64000400	1.81435300
	C	-2.92766900	1.22237600	-1.03319700
	H	-3.83378600	1.77943900	-0.77058100
	H	-2.08895700	1.91782300	-1.12837300
	H	-3.08087400	0.71353700	-1.98902200
	H	-0.62596900	5.47708900	0.70560100
Product_PhNH2	**Total Energy** = -856.477033039			
	C	3.20795600	1.75321400	-0.13767300
	H	3.96238200	2.34460900	-0.67320600
	C	2.49339300	2.38074900	1.01286900
	H	3.18483400	2.99551400	1.59836000
	H	2.04759200	1.61695400	1.65950700
	O	2.95236800	0.60610200	-0.60629600
	C	-0.54967500	2.21103000	-1.06935700
	C	0.41680600	2.75152800	-0.32992400
	C	1.39288400	3.29841300	0.37888300

	C	1.54135500	4.79197500	0.63056100
	H	0.73322200	5.35426600	0.15492800
	H	1.52639400	5.00594300	1.70835400
	H	2.49681800	5.16528400	0.23516900
	H	-0.37069900	2.14638200	-2.14701600
	C	-1.85882600	1.70372300	-0.61749100
	C	-2.76686600	1.18002500	-1.57092300
	C	-4.03102600	0.70786400	-1.19812700
	C	-4.44247800	0.74925600	0.16172600
	C	-3.53107900	1.26636100	1.12691800
	C	-2.27175900	1.73341400	0.73934900
	H	-2.48628000	1.16223700	-2.62305600
	H	-3.83401400	1.32222500	2.17080200
	H	-1.60473700	2.14992600	1.49153200
	Au	1.43521700	-0.82962000	-0.13598500
	P	-0.20675100	-2.47969200	0.25632800
	C	0.52077200	-4.19055700	0.49526700
	H	1.08640100	-4.47968300	-0.39494100
	H	1.19606000	-4.18866900	1.35550200
	H	-0.28160100	-4.91654500	0.66620900
	C	-1.23883500	-2.13181600	1.78017800
	H	-1.98385200	-2.92430200	1.91195600
	H	-0.59517200	-2.09062900	2.66339700
	H	-1.74774900	-1.17115000	1.66093900
	C	-1.42397900	-2.62061200	-1.16135700
	H	-2.15005600	-3.41297100	-0.94823800
	H	-1.94970800	-1.66948800	-1.28556900
	H	-0.89011400	-2.85833000	-2.08574900
	H	-4.71536600	0.33103900	-1.95527900
	N	-5.69781300	0.29926600	0.54193900
	H	-6.01945000	0.40147100	1.49362600
	H	-6.37188400	0.00023000	-0.14794400
Product_PhOMe	**Total Energy** = -915.6296023			
	C	3.44774900	1.64900400	-0.27472500
	H	4.17795300	2.22335700	-0.86016900
	C	2.86476700	2.27590000	0.94898300
	H	3.63759400	2.83159600	1.49051100
	H	2.43546400	1.51482900	1.61061800
	O	3.10576300	0.52569300	-0.74229500
	C	-0.24761400	2.39022500	-1.03396400
	C	0.75782900	2.82670500	-0.28086100
	C	1.76902800	3.27399400	0.44888800
	C	1.95202900	4.72879600	0.85571600
	H	1.13378000	5.34993100	0.48149200
	H	1.98734000	4.82193800	1.95009700
	H	2.89590400	5.13094000	0.46117400
	H	-0.11753000	2.43545300	-2.11906700
	C	-1.54762200	1.85879100	-0.57286400
	C	-2.51079000	1.46555900	-1.52801900
	C	-3.76836400	0.96572700	-1.14336900
	C	-4.07887400	0.85262400	0.22897700
	C	-3.12377800	1.24154200	1.20100400
	C	-1.88055100	1.73778000	0.80317900
	H	-2.28562500	1.56484000	-2.58837600
	H	-4.49094800	0.69163500	-1.90503700
	H	-3.39971900	1.16956300	2.24896700

	H	-1.16624800	2.05949600	1.55787000
	Au	1.59770100	-0.88711600	-0.18173500
	P	-0.05992300	-2.49867600	0.29881900
	C	0.62287700	-4.24190100	0.38821300
	H	1.09418600	-4.50398900	-0.56316000
	H	1.37262400	-4.30588900	1.18180400
	H	-0.18746800	-4.94862400	0.59787700
	C	-0.93298700	-2.19344400	1.92785900
	H	-1.66767500	-2.98588500	2.10854800
	H	-0.20555800	-2.18279800	2.74426900
	H	-1.44562400	-1.22822600	1.88987000
	C	-1.40392600	-2.52673800	-1.00650000
	H	-2.16189200	-3.27241400	-0.74238200
	H	-1.87007900	-1.53961300	-1.07186500
	H	-0.96972700	-2.78033200	-1.97777500
	O	-5.27936900	0.37750800	0.73312100
	C	-6.37466200	0.07759800	-0.18900300
	H	-6.65144400	0.96644500	-0.77033000
	H	-6.10865600	-0.74600500	-0.86528800
	H	-7.20801500	-0.22254600	0.44743800
Product_PhCF3	**Total Energy** = -1138.16348258			
	C	0.21033000	1.03824800	-1.25036700
	H	-0.74383500	0.83810200	-1.75665100
	C	0.43120600	2.41291300	-0.69729800
	H	0.46032300	3.10578500	-1.55662700
	H	1.40651400	2.47422900	-0.19428600
	O	1.02981000	0.08294400	-1.19474700
	C	-2.26042600	1.06887800	1.45393900
	C	-1.48732400	1.95225500	0.83043300
	C	-0.70765700	2.84891100	0.24317900
	C	-0.84293500	4.34996500	0.46092100
	H	-1.61765900	4.57327600	1.19905100
	H	0.10454800	4.77774100	0.81781200
	H	-1.10328000	4.86144300	-0.47639100
	H	-1.92425300	0.69500300	2.42453100
	C	-3.55169200	0.52364600	0.97337300
	C	-4.18070100	-0.49760300	1.72266500
	C	-5.40134500	-1.04741600	1.30402400
	C	-6.00665100	-0.57689900	0.12495200
	C	-5.39857000	0.44665400	-0.62975200
	C	-4.17952700	0.99010500	-0.20742500
	H	-3.71456600	-0.86323600	2.63465600
	H	-5.87300400	-1.83663900	1.88117400
	H	-5.87480200	0.80604500	-1.53693500
	H	-3.72042300	1.79004300	-0.78271400
	Au	2.97954000	-0.26577300	-0.37934200
	P	5.12910200	-0.82022800	0.43360900
	C	6.03150400	-1.99517900	-0.71446300
	H	5.45585800	-2.91795000	-0.82835500
	H	6.15267400	-1.53255400	-1.69789400
	H	7.01833400	-2.23281200	-0.30256300
	C	6.24069000	0.67516500	0.63079700
	H	7.22634300	0.36109400	0.99086600
	H	6.35390100	1.18168200	-0.33172800
	H	5.80031000	1.37326900	1.34807700
	C	5.07149800	-1.66015200	2.10769500

	H	6.08803000	-1.89976400	2.43801200
	H	4.60015100	-0.99854100	2.83961200
	H	4.48777000	-2.58224900	2.03877100
	C	-7.33354300	-1.13101700	-0.30718200
	F	-7.51516300	-2.46257900	0.09032200
	F	-7.50153900	-1.09334100	-1.69960500
	F	-8.42227100	-0.41395300	0.23156000
Product_PhCN	**Total Energy** = -893.3338111			
	C	3.32559200	1.51130700	-0.29203500
	H	4.06566200	2.05029100	-0.89887000
	C	2.84778500	2.15239100	0.97224700
	H	3.69755500	2.60111400	1.49926700
	H	2.36975300	1.41546600	1.62869700
	O	2.89579100	0.42170000	-0.76053500
	C	-0.16705300	2.70083300	-1.05755900
	C	0.83699600	2.99882800	-0.24019600
	C	1.84574400	3.27885400	0.57122100
	C	2.10041200	4.65470600	1.16796800
	H	1.32123300	5.36484300	0.87816900
	H	2.13058200	4.59915200	2.26489800
	H	3.06824200	5.05163200	0.83161700
	H	-0.01604800	2.84606100	-2.13006900
	C	-1.49254900	2.17411900	-0.66033400
	C	-2.42230800	1.82507500	-1.66902900
	C	-3.67955600	1.29841600	-1.33936500
	C	-4.03385900	1.11283700	0.01771100
	C	-3.11627600	1.47800500	1.03576300
	C	-1.86281100	1.99989200	0.69718800
	H	-2.16169900	1.97071600	-2.71490400
	H	-3.40262100	1.36424300	2.07763600
	H	-1.17111500	2.29237500	1.48320700
	Au	1.38049700	-0.98670700	-0.19271100
	P	-0.28232500	-2.59437800	0.29458300
	C	0.37757700	-4.34790600	0.25527600
	H	0.79169000	-4.56549000	-0.73317700
	H	1.16794200	-4.46377000	1.00210800
	H	-0.43165000	-5.05381200	0.47176200
	C	-1.04967200	-2.35968200	1.98779500
	H	-1.80900600	-3.13005600	2.16120300
	H	-0.27828100	-2.43363100	2.75935100
	H	-1.51854700	-1.37346100	2.04466100
	C	-1.69912100	-2.53712800	-0.93063900
	H	-2.45000100	-3.28925100	-0.66489800
	H	-2.15968600	-1.54551400	-0.91755200
	H	-1.32445700	-2.74077300	-1.93772900
	H	-4.38903600	1.03988500	-2.11979100
	C	-5.31215400	0.55220700	0.36689700
	N	-6.35481400	0.07647800	0.65809400
Product_PhNO2	**Total Energy** = -1005.5845528			
	C	2.87882100	1.91603900	-0.88043000
	H	3.22338500	2.59117000	-1.67601600
	C	2.97719700	2.39702500	0.53641000
	H	3.98194400	2.81513100	0.69577200
	H	2.84011100	1.56287000	1.23787500
	O	2.40527400	0.80774600	-1.24502200
	C	-0.31020800	3.52854100	-0.61559700

	C	0.80869400	3.54829400	0.10225500
	C	1.92472000	3.49928300	0.81391500
	C	2.24287400	4.44104300	1.96531600
	H	1.40388500	5.11011800	2.17419800
	H	2.47302100	3.87545300	2.87906000
	H	3.12049300	5.05790400	1.72847000
	H	-0.38000900	4.15956800	-1.50361000
	C	-1.47937500	2.66640600	-0.33002800
	C	-2.56057300	2.63583200	-1.24293700
	C	-3.63135900	1.74780200	-1.06122200
	C	-3.60351800	0.88177200	0.04409500
	C	-2.57073400	0.92619800	1.00035700
	C	-1.51730800	1.82227500	0.80993500
	H	-2.55485800	3.29505000	-2.10741200
	H	-2.61875500	0.27571300	1.86706000
	H	-0.71541800	1.87661700	1.54136800
	Au	1.42571200	-0.90206100	-0.37360300
	P	0.32999300	-2.86288300	0.37337200
	C	1.03703300	-4.39359300	-0.44561400
	H	0.91314900	-4.32387800	-1.52998700
	H	2.10293300	-4.48003400	-0.21702600
	H	0.51400100	-5.28367900	-0.07904700
	C	0.50941200	-3.13247600	2.21916800
	H	0.00143700	-4.05863500	2.50954100
	H	1.56823500	-3.20395700	2.48259300
	H	0.06402400	-2.29458100	2.76258800
	C	-1.50753000	-2.87970600	0.01061600
	H	-1.94077500	-3.82077400	0.36692600
	H	-2.00986200	-2.05022600	0.51417700
	H	-1.67230400	-2.79439100	-1.06729000
	H	-4.45956300	1.70390700	-1.76017100
	N	-4.66040600	-0.13190400	0.19841000
	O	-5.70219300	-0.04452900	-0.53142600
	O	-4.45335800	-1.07725900	1.04503200
TS_Ph	**Total Energy** = -801.06749518 **, Frequency** = -143.6374			
	C	-1.73292100	-1.95003800	0.70421200
	H	-1.51037800	-1.72107700	1.75073400
	C	-2.70141400	-2.87396400	0.39265500
	H	-3.17893400	-3.44422200	1.18469500
	H	-2.87474000	-3.17212000	-0.63655600
	O	-1.12015100	-1.20855400	-0.24001700
	C	-2.61710700	0.47949400	-1.07998000
	C	-3.70811700	-0.23195100	-0.63021600
	C	-4.51214000	-1.07244600	-0.18337900
	C	-5.71914600	-1.81147700	0.21297400
	H	-2.21882300	0.19947700	-2.05510000
	C	-2.09102700	1.69326700	-0.48405500
	C	-1.06317200	2.39808600	-1.16904200
	C	-0.54344000	3.58663600	-0.63849700
	C	-1.03583700	4.08395800	0.58676200
	C	-2.05283300	3.38906900	1.27903200
	C	-2.58056500	2.20544500	0.74950400
	H	-0.69852500	2.01923800	-2.12201400
	H	0.22378800	4.13564100	-1.17738200
	H	-2.43349100	3.78320000	2.21709000
	H	-3.37571000	1.67813800	1.27024100

	H	-0.64194200	5.01176300	0.99359400
	H	-5.77698600	-1.93061900	1.30071600
	H	-6.60767600	-1.25100600	-0.11072100
	H	-5.75497700	-2.80292100	-0.25095600
	Au	0.89700400	-0.65574500	-0.04928900
	P	3.19975000	-0.12116700	0.08977100
	C	4.30984200	-1.61746100	-0.12405300
	H	5.36184000	-1.31899100	-0.05944700
	H	4.09299800	-2.35128100	0.65736700
	H	4.12342500	-2.07840500	-1.09820500
	C	3.68829300	0.63591200	1.73434300
	H	4.75912100	0.86687100	1.73967700
	H	3.11777400	1.55385100	1.90119700
	H	3.46636300	-0.06629900	2.54296600
	C	3.76221800	1.10691100	-1.21181400
	H	3.20619200	2.04209700	-1.10052600
	H	4.83341100	1.30779800	-1.10135400
	H	3.57307400	0.70004500	-2.20928500
TS_PhNH2	**Total Energy** = -856.43309785**, Frequency** = -169.6509			
	C	-0.88594200	-2.48055200	0.84880700
	H	-0.79186200	-2.13483100	1.88414700
	C	-1.55421100	-3.65522100	0.57910100
	H	-1.90046200	-4.27753900	1.39955300
	H	-1.54252500	-4.07573000	-0.42149900
	O	-0.43928900	-1.67279300	-0.12325600
	C	-2.66776200	-0.42351200	-1.18451900
	C	-3.30584500	-1.54079100	-0.69534700
	C	-3.69634200	-2.62935600	-0.22225100
	C	-4.58424200	-3.75294700	0.12776600
	H	-2.11202000	-0.54830200	-2.11471700
	C	-2.75097300	0.90059700	-0.64861900
	C	-2.10356900	1.97830600	-1.32891400
	C	-2.18902000	3.28409000	-0.86414800
	C	-2.93430400	3.57746600	0.31944300
	C	-3.57584900	2.50481900	1.01668500
	C	-3.48607300	1.20565800	0.54068800
	H	-1.54351700	1.76847400	-2.23813600
	H	-1.70418400	4.09363900	-1.40451800
	H	-4.14658500	2.72140400	1.91670300
	H	-3.99146300	0.40133700	1.06889600
	H	-4.68298100	-3.86163900	1.21370200
	H	-5.58560800	-3.56571900	-0.28483300
	H	-4.21712300	-4.69951900	-0.28299100
	Au	1.32674800	-0.58482100	0.00259900
	P	3.38392600	0.58737000	0.03582000
	C	4.86382000	-0.51700800	-0.29367700
	H	5.78803600	0.07056200	-0.26775600
	H	4.91219500	-1.30253100	0.46579600
	H	4.76058600	-0.98720600	-1.27578900
	C	3.74588000	1.42227900	1.67604500
	H	4.70711500	1.94584300	1.62983300
	H	2.95283700	2.13887900	1.90796000
	H	3.78162300	0.67116300	2.47030800
	C	3.49323100	1.95238500	-1.24705400
	H	2.69679100	2.68222100	-1.07587500
	H	4.46498400	2.45420000	-1.18351700

	H	3.37205500	1.52701300	-2.24747100
	N	-3.04060300	4.86709500	0.77942900
	H	-3.58321500	5.08513200	1.60410700
	H	-2.62088500	5.63890000	0.27946600
TS_PhOMe	**Total Energy** = -915.58064762 **, Frequency** = -131.6745			
	C	-0.75588100	-2.75441500	0.83955200
	H	-0.66454200	-2.40027500	1.87150500
	C	-1.34833300	-3.96814400	0.58191400
	H	-1.64761000	-4.60943700	1.40624300
	H	-1.35774000	-4.37668000	-0.42368300
	O	-0.37892400	-1.91740300	-0.14397800
	C	-2.48460800	-0.81783000	-1.16140500
	C	-3.18687200	-1.89879000	-0.67442200
	C	-3.62115300	-2.96580000	-0.19895300
	C	-4.48305200	-4.09085600	0.19397600
	H	-1.94270600	-0.96831600	-2.09533300
	C	-2.52510800	0.52062000	-0.63820700
	C	-1.86322400	1.56320100	-1.34637700
	C	-1.90390800	2.88601800	-0.89955200
	C	-2.61252000	3.19309100	0.29055200
	C	-3.26873900	2.16373500	1.02036900
	C	-3.22930100	0.85464900	0.56110600
	H	-1.33017800	1.32550300	-2.26488700
	H	-1.41079400	3.66547700	-1.47044700
	H	-3.80412700	2.43874100	1.92333000
	H	-3.74700100	0.07221200	1.10918700
	H	-4.55573900	-4.17740400	1.28388600
	H	-5.49652900	-3.92472700	-0.19805100
	H	-4.11347200	-5.04032600	-0.20769600
	Au	1.32181900	-0.71722300	-0.01461500
	P	3.31467200	0.56020900	0.04944400
	C	4.79437100	-0.35259000	-0.65447500
	H	5.68808000	0.27871300	-0.60177700
	H	4.96476300	-1.26989600	-0.08376700
	H	4.60094400	-0.62105900	-1.69694900
	C	3.81871400	1.05811800	1.78611500
	H	4.75032200	1.63383200	1.75909400
	H	3.02993000	1.66456000	2.24026000
	H	3.96591900	0.16241600	2.39631300
	C	3.21587100	2.16377500	-0.91871000
	H	2.40566500	2.78176300	-0.52151700
	H	4.16150700	2.71148500	-0.84211500
	H	3.01048900	1.94524000	-1.97064000
	O	-2.73119100	4.45246600	0.82314800
	C	-2.15939800	5.60873200	0.12546600
	H	-2.60213300	5.71784700	-0.87209700
	H	-2.42099800	6.46699200	0.74457000
	H	-1.06809800	5.51918600	0.05245300
TS_PhCF3	**Total Energy** = -1138.11193740, **Frequency** = -136.3178			
	C	-3.11349900	-0.86277900	0.73694200
	H	-2.71081500	-0.84398200	1.75324600
	C	-4.46706700	-0.95273200	0.53408900
	H	-5.13246700	-1.10266400	1.37982400
	H	-4.88117300	-1.02219100	-0.46703800
	O	-2.24085600	-0.67316800	-0.27967700
	C	-2.40548700	1.45072200	-1.14428000

	C	-3.58718400	1.74001000	-0.49238100
	C	-4.67422700	1.71588100	0.11150100
	C	-5.97639200	1.99159500	0.72915700
	H	-2.49396200	0.99536500	-2.13059600
	C	-1.08107000	1.93316300	-0.77469600
	C	-0.01304900	1.72607500	-1.68657800
	C	1.28867600	2.11568000	-1.35507500
	C	1.53546700	2.70241200	-0.09745300
	C	0.48284700	2.94306600	0.80884900
	C	-0.82183400	2.56909200	0.46662900
	H	-0.21048500	1.26880700	-2.65291700
	H	2.10123500	1.97321000	-2.06113700
	H	0.68633100	3.41984400	1.76238500
	H	-1.63960300	2.75646400	1.15653500
	H	-5.93198900	1.89284500	1.81963900
	H	-6.27426100	3.02449100	0.49900500
	H	-6.75302000	1.32119600	0.34566200
	Au	-0.27466400	-1.44869100	-0.09284400
	P	1.88784200	-2.39456200	0.13230900
	C	1.96281600	-4.17443300	-0.45324100
	H	2.97476900	-4.57109900	-0.31712900
	H	1.25608800	-4.78205900	0.11893600
	H	1.69331500	-4.22655900	-1.51197800
	C	2.47954300	-2.41672600	1.91125100
	H	3.47357900	-2.87330800	1.96973100
	H	2.53131300	-1.39307100	2.29245700
	H	1.78152200	-2.99020500	2.52755400
	C	3.22335500	-1.48868900	-0.82218900
	H	3.31669900	-0.46636200	-0.44601600
	H	4.18143700	-2.00503200	-0.69682900
	H	2.96695400	-1.46182500	-1.88507700
	C	2.95602700	3.00052600	0.29058800
	F	3.63773300	1.80318300	0.65520100
	F	3.06424900	3.85499500	1.38337100
	F	3.70231500	3.55063200	-0.75495200
TS_PhCN	**Total Energy** = -893.27936929**, Frequency** = -129.6852			
	C	1.94421700	-2.05735500	-0.78424800
	H	1.66735600	-1.79869200	-1.81015300
	C	2.99253900	-2.91133200	-0.54870000
	H	3.48859600	-3.40105900	-1.38217000
	H	3.24046200	-3.22911000	0.45923600
	O	1.29870300	-1.41554500	0.21524100
	C	2.63138500	0.27009100	1.13445100
	C	3.78752900	-0.23190100	0.57325600
	C	4.67968500	-0.90875000	0.03087900
	C	5.93287400	-1.46628500	-0.49214900
	H	2.33948500	-0.13966900	2.10100500
	C	1.92005800	1.45859300	0.69116200
	C	0.86607500	1.95987400	1.50123400
	C	0.15195200	3.09904300	1.11809700
	C	0.47305600	3.75494000	-0.09628300
	C	1.52726900	3.26509600	-0.91032800
	C	2.24457600	2.13275900	-0.51707000
	H	0.62616900	1.46198300	2.43794500
	H	-0.63890400	3.49424700	1.74818700

	H 1.77386300 3.78172700 -1.83279200 H 3.06028300 1.76576900 -1.13368600 H 5.92451600 -1.51239400 -1.58701200 H 6.76950700 -0.81982100 -0.19107800 H 6.12139900 -2.47092200 -0.09881300 Au -0.76416400 -1.01895000 0.04636200 P -3.10522700 -0.68346200 -0.09620500 C -3.96110100 -0.74591400 1.57160600 H -5.03982800 -0.60303800 1.44590400 H -3.77827600 -1.71576800 2.04285300 H -3.56658500 0.04027200 2.22145200 C -3.95518600 -1.98438300 -1.14557300 H -5.03331200 -1.79356800 -1.17957700 H -3.55200700 -1.96045100 -2.16189800 H -3.77680300 -2.97604800 -0.72022600 C -3.58230100 0.96438900 -0.85308300 H -3.18454800 1.03138500 -1.86962300 H -4.67279600 1.06260000 -0.88509400 H -3.16349900 1.78119100 -0.25882500 C -0.27487000 4.91365700 -0.50450200 N -0.90198200 5.85708400 -0.84279600
TS_PhNO2	**Total Energy** = -1005.52848708**, Frequency =** -131.7636 C -2.60047600 -1.54663300 0.79032700 H -2.23398200 -1.36222300 1.80366100 C -3.85696100 -2.06061300 0.59286900 H -4.45510100 -2.37114700 1.44507300 H -4.21627000 -2.29666800 -0.40398300 O -1.81849300 -1.13908200 -0.23612700 C -2.61777100 0.78657300 -1.18142000 C -3.85182100 0.72474000 -0.56496200 C -4.89476000 0.39763900 0.02772800 C -6.23163300 0.27936400 0.61996100 H -2.52786900 0.28728700 -2.14574600 C -1.51843400 1.66365600 -0.80133700 C -0.37510200 1.70559100 -1.64263900 C 0.75053600 2.45016300 -1.27744900 C 0.71865100 3.15513900 -0.06195400 C -0.41900800 3.18496300 0.76673200 C -1.53697900 2.43231200 0.39287600 H -0.37576500 1.15233000 -2.57837700 H 1.63583600 2.49132800 -1.90160700 H -0.40465300 3.77478300 1.67682000 H -2.42204400 2.42688400 1.02239600 H -6.18399500 0.24628700 1.71427600 H -6.83063100 1.15707600 0.33798300 H -6.75230400 -0.61519900 0.26169000 Au 0.29347700 -1.28785600 -0.05781500 P 2.64615200 -1.52386800 0.13913400 C 3.26317300 -3.18235400 -0.48263200 H 4.34971400 -3.24615900 -0.35823400 H 2.78703600 -3.98975800 0.08083600 H 3.01312200 -3.29756300 -1.54107300 C 3.23765300 -1.40070400 1.91434600 H 4.32352000 -1.53922600 1.95537500 H 2.98500000 -0.41787900 2.32203200

	H	2.75184200	-2.17033600	2.52068500
	C	3.62711400	-0.23569700	-0.80765600
	H	3.37286800	0.77020900	-0.46149900
	H	4.69878000	-0.40390500	-0.65428200
	H	3.40308100	-0.31351700	-1.87553200
	N	1.93956700	3.86776700	0.37245500
	O	1.83912600	4.71096900	1.32257300
	O	3.03721700	3.56771500	-0.21845000

	Uncatalyzed Rearrangement	
	B3LYP/LANL2DZ	B3LYP/6-31g**
Reactant_Ph	**Total Energy** = -539.5454573	**Total Energy** = -539.6423393
	C 1.00694600 2.01321600 0.64009900	C 1.00077500 2.00021400 0.58825100
	H 0.80801000 1.24385400 1.38512500	H 0.99755000 1.19601100 1.32017900
	C 1.36624700 3.26745400 0.96586800	C 1.16740500 3.27764900 0.92409900
	H 1.46311400 3.54949000 2.00898500	H 1.30635700 3.54722200 1.96353200
	H 1.56243600 4.01817100 0.20611100	H 1.17238400 4.06520300 0.17880500
	O 0.85349700 1.62456600 -0.69625900	O 0.83854900 1.61450900 -0.71627300
	C 0.56345300 0.18703100 -0.95416000	C 0.57738700 0.21316700 -0.94399800
	C 1.66975700 -0.67439900 -0.50272800	C 1.68529900 -0.63178900 -0.47908600
	C 2.62024300 -1.36451500 -0.16427300	C 2.62394800 -1.30505700 -0.11992000
	C 3.77445400 -2.18048400 0.24218100	C 3.76300200 -2.11033700 0.30886300
	H 4.59503700 -1.54096100 0.59131800	H 4.65204000 -1.48538400 0.44634000
	H 3.51125500 -2.86673400 1.05694300	H 3.56011300 -2.61731900 1.25838500
	H 0.53465100 0.17460500 -2.05077700	H 0.54652200 0.15855200 -2.03944700
	C -0.82164800 -0.19903400 -0.41854000	C -0.79882000 -0.19992300 -0.41259500
	C -1.91436100 0.64187200 -0.72606900	C -1.87790100 0.67520700 -0.59570900
	C -3.20849500 0.31381800 -0.28969100	C -3.15536300 0.31809400 -0.16934100
	C -3.42687300 -0.86130500 0.45843500	C -3.37171100 -0.91982500 0.44106100
	C -2.34154100 -1.70138700 0.76647300	C -2.30178900 -1.79486600 0.62351700
	C -1.04313700 -1.37125600 0.32955300	C -1.02009300 -1.43600900 0.20005800
	H -1.74147300 1.55524100 -1.28983300	H -1.70547600 1.64037200 -1.06097300
	H -4.04233300 0.96979700 -0.52811200	H -3.98294200 1.00696100 -0.31213300
	H -4.42885500 -1.11582500 0.79603900	H -4.36773700 -1.19778000 0.77326600
	H -2.50225500 -2.60879200 1.34403300	H -2.46024800 -2.75788100 1.10045300
	H -0.20631700 -2.02273000 0.56556400	H -0.18638100 -2.11491500 0.34602500
	H 4.14849100 -2.77870600 -0.59821400	H 4.00658200 -2.87626800 -0.43546400
Reactant_PhNH2	**Total Energy** = -594.89799568	**Total Energy** = -595.00126664
	C 1.55719600 1.91821600 0.73073600	C 1.57288600 1.87979600 0.69185700
	H 1.15903200 1.17182300 1.41714700	H 1.21128600 1.11651600 1.37677100
	C 2.07286800 3.08822000 1.15005700	C 2.06481400 3.04444200 1.11063700
	H 2.09951200 3.32001000 2.20970800	H 2.10972800 3.26044200 2.17078100
	H 2.46482200 3.82008400 0.44995400	H 2.42068000 3.79436000 0.41295800
	O 1.48110600 1.59965300 -0.62772300	O 1.47596800 1.57599900 -0.63859000
	C 1.03800800 0.21255300 -0.97827400	C 1.04034000 0.23212000 -0.96159100
	C 2.01435000 -0.78645300 -0.50986200	C 2.00324400 -0.77302000 -0.49316400
	C 2.86169400 -1.58887100 -0.14574500	C 2.82940000 -1.57564900 -0.12358800
	C 3.89285300 -2.54321300 0.28959400	C 3.83385600 -2.53877900 0.31630600
	H 4.75230100 -2.01354200 0.72004200	H 4.82778600 -2.07947900 0.34970500
	H 3.50469200 -3.23137400 1.05123200	H 3.60924000 -2.92287500 1.31730500
	H 1.08322000 0.26257700 -2.07302700	H 1.07004400 0.24515400 -2.05811000
	C -0.40281400 -0.03677100 -0.53769300	C -0.39898500 -0.01802600 -0.51887100
	C -1.40897400 0.84925500 -0.98428400	C -1.38012800 0.92554500 -0.85570900

	C -2.74872000 0.66748900 -0.62490700 C -3.12959300 -0.42313200 0.20211400 C -2.12279000 -1.31426200 0.64992500 C -0.78229900 -1.11731300 0.28226900 H -1.13195100 1.69795200 -1.60585500 H -3.50621900 1.36563300 -0.97671400 H -2.39374600 -2.15742100 1.28309600 H -0.02496000 -1.81499700 0.62997300 H 4.25595500 -3.14248100 -0.55497200 N -4.46360300 -0.61058500 0.56154400 H -5.17888000 0.02725400 0.24792100 H -4.73809100 -1.38295900 1.14889700	C -2.70998500 0.73773400 -0.50392600 C -3.10887800 -0.41403000 0.19988100 C -2.12830300 -1.36055600 0.53536500 C -0.79592400 -1.15954800 0.18169800 H -1.09000800 1.82584200 -1.38945200 H -3.45175800 1.48754800 -0.76792500 H -2.41253000 -2.25495200 1.08442700 H -0.05367300 -1.90485200 0.44914700 H 3.88569300 -3.39400900 -0.36649100 N -4.43350300 -0.57881700 0.60310300 H -5.11793800 -0.07731100 0.05418700 H -4.71580200 -1.53283400 0.78032900
Reactant_PhNO2	**Total Energy** = -744.01757330 C 2.39319700 1.85231500 0.75291400 H 2.24114800 1.02176600 1.44081900 C 2.74058000 3.08597100 1.15605800 H 2.87663600 3.29193200 2.21234700 H 2.89685900 3.89385800 0.44739700 O 2.22803500 1.55596500 -0.60996200 C 1.73729900 0.20266700 -0.95533500 C 2.61462800 -0.86013700 -0.43585300 C 3.37838400 -1.73196100 -0.04759700 C 4.30976000 -2.76878600 0.42166400 H 5.28014300 -2.32643800 0.67943900 H 3.92283700 -3.27903900 1.31236400 H 1.81647500 0.21620000 -2.05032200 C 0.25405200 0.05010100 -0.58201100 C -0.60725100 1.15343400 -0.77639000 C -1.97650000 1.04699100 -0.50069800 C -2.47507200 -0.18088200 -0.02922200 C -1.64256200 -1.29339800 0.17315800 C -0.27261400 -1.16788600 -0.10642900 H -0.19426400 2.09347200 -1.12859900 H -2.65235300 1.88313900 -0.63986300 H -2.06629600 -2.22149400 0.54005500 H 0.38895800 -2.01459700 0.04687000 H 4.48021100 -3.52360100 -0.35609000 N -3.91719100 -0.30439900 0.26289100 O -4.66199100 0.71836600 0.07181500 O -4.35272100 -1.42870200 0.69237200	**Total Energy** = -744.14224900 C 2.37132800 1.83122900 0.70233400 H 2.30985000 0.98259700 1.37945200 C 2.60838500 3.07302000 1.11683600 H 2.75121600 3.27002400 2.17187600 H 2.67553700 3.90199500 0.42109800 O 2.22570600 1.53520500 -0.63087000 C 1.74105100 0.21937600 -0.94951400 C 2.60775100 -0.84222400 -0.42223600 C 3.34737200 -1.70667100 -0.01105100 C 4.24990200 -2.74210500 0.48151600 H 5.23943300 -2.32439900 0.69559300 H 3.87096900 -3.19776400 1.40244600 H 1.80759300 0.19972900 -2.04509500 C 0.26164800 0.05963300 -0.57810300 C -0.58856500 1.16737900 -0.70562000 C -1.94691700 1.05295400 -0.43098400 C -2.44673000 -0.18510400 -0.03084500 C -1.62676200 -1.30201700 0.10204300 C -0.26778400 -1.17052500 -0.17314000 H -0.17541600 2.12245200 -1.00944600 H -2.61951500 1.89665200 -0.51879900 H -2.05587000 -2.24398800 0.41916300 H 0.38954800 -2.02649800 -0.06762000 H 4.37739100 -3.53754400 -0.26054300 N -3.88303500 -0.31500100 0.26234100 O -4.58504400 0.68821000 0.13741700 O -4.29735900 -1.41940400 0.61446100
Product_Ph	**Total Energy** = -539.5822027 C -3.23834000 1.22306300 -0.50276900 H -2.33726300 1.86180600 -0.39546000 C -2.94467300 -0.22686100 -0.87156700 H -2.44686900 -0.23202800 -1.85055700 H -3.89500700 -0.76889800 -0.95227900 O -4.37580600 1.68915400 -0.31896100 C 0.51406700 -1.40411300 -0.36269000 C -0.75549800 -1.12597500 -0.08418600 C -2.03049600 -0.88078800 0.17545500 C -2.67710900 -1.21041800 1.51661800 H -1.95540000 -1.64773600 2.21273300 H -3.10466100 -0.30928700 1.97878300 H -3.50216800 -1.92319300 1.37694100	**Total Energy** = -539.6848573 C -3.11246600 1.22821000 -0.61550500 H -2.20588300 1.85156400 -0.78654800 C -2.92345000 -0.24792100 -0.92322400 H -2.44607300 -0.34821200 -1.90316500 H -3.90747800 -0.72798500 -0.94133500 O -4.13142700 1.71163300 -0.17568900 C 0.48369600 -1.42859700 -0.32166300 C -0.77609600 -1.13943000 -0.07584700 C -2.03963100 -0.87476300 0.15548400 C -2.70252900 -1.13369500 1.49333200 H -1.98365800 -1.48990600 2.23324700 H -3.17845800 -0.22246300 1.87362900 H -3.49424400 -1.88550200 1.38673500

	H 0.73874600 -2.38280900 -0.79520900 C 1.68520400 -0.51975300 -0.15045900 C 1.57214300 0.76635300 0.43307000 C 2.70761300 1.57132900 0.61416300 C 3.97992600 1.10952700 0.21666200 C 4.10401300 -0.16744900 -0.36256900 C 2.96651200 -0.97406200 -0.54332200 H 0.59437400 1.12550800 0.74637700 H 2.60619600 2.55626400 1.06452000 H 5.08097600 -0.53213200 -0.67098700 H 3.06943200 -1.96094300 -0.99159500 H 4.85791600 1.73510900 0.35798500	H 0.71264200 -2.42350800 -0.70789500 C 1.64504800 -0.53876200 -0.12908000 C 1.51870100 0.75913700 0.39569700 C 2.63746700 1.56921000 0.56119700 C 3.90722000 1.10198000 0.20774800 C 4.04608700 -0.18478200 -0.31255300 C 2.92507600 -0.99712500 -0.47846000 H 0.53428600 1.12408900 0.67416800 H 2.52122100 2.56941100 0.96885700 H 5.02769500 -0.55824600 -0.58966300 H 3.03785100 -1.99939600 -0.88401700 H 4.77878300 1.73632000 0.33873800
TS_Ph	**Total Energy (Boat)** = -539.5100001, **Frequency** = -369.7238 cm^{-1} C -1.65205400 -1.44583700 1.07836900 H -1.23351500 -1.23401600 2.07289500 C -2.97601400 -1.09680700 0.82337500 H -3.62061900 -0.77076400 1.63832200 H -3.45149300 -1.40976800 -0.10201600 O -0.82844200 -1.84674200 0.12851200 C -0.22864500 -0.30668800 -1.04687400 C -1.33280600 0.52650900 -0.90182000 C -2.44140700 0.87463100 -0.43082800 C -3.63465000 1.72682800 -0.23632800 H -0.22958100 -0.98818100 -1.89607500 C 1.10586900 0.01238400 -0.49555300 C 2.20361600 -0.80869800 -0.84662300 C 3.48235500 -0.55295300 -0.32711100 C 3.68371200 0.53039400 0.55182500 C 2.59618200 1.35505800 0.90534100 C 1.31707500 1.10031700 0.38503000 H 2.04442900 -1.65533300 -1.51088200 H 4.31757800 -1.19286300 -0.60102400 H 2.74971700 2.19448600 1.57956600 H 0.48077300 1.74327300 0.64804600 H 4.67420400 0.73070600 0.95363700 H -3.71281500 2.06794800 0.80300300 H -3.57527700 2.61283200 -0.88261400 H -4.55526400 1.18480200 -0.48378200	**Total Energy (Boat)** = -539.6051151, **Frequency** = -388.1644 cm^{-1} C -1.59768000 -1.40862700 1.06968900 H -1.15809100 -1.16440900 2.05074200 C -2.92378500 -1.10516800 0.85511800 H -3.55392700 -0.78056000 1.67827100 H -3.41233900 -1.43939400 -0.05287900 O -0.81492700 -1.81443100 0.13186700 C -0.24364700 -0.34611900 -1.03727000 C -1.32531700 0.51192200 -0.93563600 C -2.40926500 0.86922700 -0.45141700 C -3.58828200 1.71434700 -0.23636400 H -0.23098500 -1.01529900 -1.89373200 C 1.08480800 -0.00824800 -0.49277100 C 2.18890400 -0.80517400 -0.83563000 C 3.45184800 -0.52820100 -0.31942200 C 3.63157000 0.55080200 0.54911200 C 2.53969700 1.35033800 0.89645900 C 1.27648300 1.07545700 0.37945000 H 2.04648400 -1.65126900 -1.50202100 H 4.29645500 -1.15340200 -0.59369400 H 2.67509500 2.19304100 1.56826300 H 0.42877400 1.70180000 0.63891700 H 4.61686500 0.76951700 0.95016100 H -3.66336600 2.03533800 0.80747300 H -3.52491600 2.61088100 -0.86360900 H -4.51263500 1.18586900 -0.49073000
	Total Energy (Chair) = -539.5096829, **Frequency** = -362.4901 cm^{-1} C 2.07469800 1.76050300 0.56209400 H 2.72507900 2.49361100 0.06260100 C 2.67230400 0.74852600 1.30726200 H 3.74072400 0.78322300 1.51387600 H 2.06377600 0.07616700 1.90491300 O 0.78381600 1.78388900 0.27990700 C 0.22351100 0.32424100 -0.99639100 C 1.31809200 -0.52851300 -0.89082100 C 2.43731300 -0.88737600 -0.45628400 C 3.67453900 -1.69048100 -0.35670500 H 0.23755400 1.04076600 -1.81704000 C -1.11886500 0.00053900 -0.47147300 C -2.19834600 0.85874400 -0.78510200	**Total Energy** = -539.6048925, **Frequency** = -388.1415 cm^{-1} C 2.03116800 1.74076800 0.53803700 H 2.67135200 2.47501100 0.02086300 C 2.64278200 0.77346500 1.30207400 H 3.70770500 0.82917800 1.50744800 H 2.04561000 0.10080500 1.90610500 O 0.76935600 1.74249100 0.27420600 C 0.24003800 0.34316100 -0.97456000 C 1.30522900 -0.53903900 -0.89560500 C 2.41072500 -0.88752700 -0.45652500 C 3.63979100 -1.67775000 -0.33719000 H 0.24921800 1.02901900 -1.81828200 C -1.10324300 0.01354900 -0.46295700 C -2.17750800 0.86579400 -0.75978600

	C -3.48568100 0.59837900 -0.28808900 C -3.71183300 -0.52777300 0.52791100 C -2.64137000 -1.38982600 0.84353400 C -1.35424700 -1.12823500 0.34822400 H -2.01976500 1.73661200 -1.40226600 H -4.30743600 1.26750300 -0.53105900 H -2.81450400 -2.26062300 1.47158700 H -0.52897700 -1.79498700 0.58568200 H -4.70845400 -0.73208900 0.91227800 H 3.80749400 -2.09660800 0.65309500 H 3.63627000 -2.53197600 -1.06159500 H 4.55703100 -1.08507600 -0.59629300	C -3.45363500 0.59427300 -0.27227000 C -3.67381300 -0.53565000 0.51791000 C -2.61007900 -1.39055400 0.81907800 C -1.33422900 -1.11855900 0.33360900 H -2.00241900 1.75010100 -1.36603100 H -4.27619300 1.26286800 -0.50844700 H -2.77769700 -2.27172600 1.43157600 H -0.50628000 -1.78346900 0.55948400 H -4.66908300 -0.75074300 0.89574100 H 3.75786000 -2.09122800 0.66938900 H 3.61814000 -2.51200500 -1.04775400 H 4.52359000 -1.06933400 -0.55462100
TS_PhNH2	**Total Energy (Chair)** = -594.86394796, **Frequency** = -316.7991 cm^{-1} C 2.57434600 1.66628800 0.73377100 H 3.29972900 2.38127800 0.31423900 C 3.07134800 0.58972200 1.46222500 H 4.12770700 0.54748300 1.72286300 H 2.39411200 -0.08472900 1.97843500 O 1.30812700 1.79251100 0.38597300 C 0.69953800 0.40439100 -1.03439600 C 1.75329800 -0.49705800 -0.90806700 C 2.82496500 -0.95741000 -0.45733700 C 4.01471700 -1.82539900 -0.34105900 H 0.80926100 1.18453300 -1.78629500 C -0.67225700 0.12895700 -0.60705000 C -1.70190100 1.04288300 -0.94085600 C -3.02124400 0.83612700 -0.53007900 C -3.36018400 -0.30855800 0.23971800 C -2.33259000 -1.23191400 0.57697300 C -1.01794900 -1.01063600 0.16164600 H -1.45418300 1.93332700 -1.51507500 H -3.79519900 1.55448600 -0.79353100 H -2.57914900 -2.11483200 1.16426400 H -0.24173000 -1.72455300 0.42648600 H 4.06743500 -2.30068400 0.64574400 H 3.98276200 -2.61816300 -1.10118100 H 4.93674400 -1.24984400 -0.48719800 N -4.67055300 -0.52538600 0.65271400 H -5.40016100 0.13424900 0.42897000 H -4.91099100 -1.32929700 1.21256500	**Total Energy (Chair)** = -594.96515139, **Frequency** = -350.9187 cm^{-1} C -2.53222500 -1.64303100 0.70260800 H -3.24567000 -2.36128700 0.26156400 C -3.04641500 -0.60840700 1.44907900 H -4.10136100 -0.58723400 1.70610800 H -2.38188700 0.06630700 1.97588300 O -1.29010900 -1.74489300 0.37908600 C -0.71592000 -0.43443200 -0.99963800 C -1.73395800 0.50342200 -0.91543400 C -2.79031000 0.96240300 -0.46486000 C -3.96514800 1.82737900 -0.33281100 H -0.81701600 -1.18114300 -1.78314100 C 0.65836100 -0.15477200 -0.58267400 C 1.68405000 -1.05997700 -0.90193900 C 2.99394000 -0.83825400 -0.50297300 C 3.32845800 0.30963000 0.23933500 C 2.30408400 1.22064000 0.56450400 C 0.99850100 0.98735600 0.16255400 H 1.44365300 -1.95642800 -1.46691100 H 3.76979800 -1.55522100 -0.75912400 H 2.54509300 2.11187000 1.13861600 H 0.22081900 1.70125300 0.41654600 H -4.00242800 2.30981400 0.64905800 H -3.94205100 2.61320300 -1.09702100 H -4.89138100 1.25768300 -0.45978000 N 4.62773300 0.51531800 0.68431100 H 5.35453700 0.03414500 0.17438300 H 4.87414500 1.46721100 0.91444500
TS_PhNO2	**Total Energy (Chair)** = -743.98245718, **Frequency** = -372.8858 cm^{-1} C -3.18413700 -1.52628800 0.95708600 H -3.93327400 -2.27081900 0.65425200 C -3.61882800 -0.35417800 1.56785300 H -4.65754600 -0.25570200 1.87803300 H -2.90039300 0.34885600 1.97896300 O -1.93422200 -1.70836600 0.56310200 C -1.44962000 -0.56128000 -1.00204200 C -2.44268900 0.41046500 -0.93794600 C -3.46940900 0.94944100 -0.46306800 C -4.61412600 1.88018200 -0.37478200 H -1.61677900 -1.39391200 -1.68422500	**Total Energy (Chair)** = -744.10495879, **Frequency** = -401.7594 cm^{-1} C -3.14706500 -1.51176600 0.91458400 H -3.89609500 -2.25173900 0.59049900 C -3.58546200 -0.37717200 1.55792700 H -4.62143500 -0.29119100 1.87150100 H -2.87028500 0.31856900 1.98015700 O -1.92476300 -1.67722600 0.53460100 C -1.45232500 -0.56892900 -0.97641600 C -2.41365600 0.42732500 -0.94433200 C -3.42602300 0.95392500 -0.45909600 C -4.55762300 1.87946800 -0.34908300 H -1.61407700 -1.37145700 -1.69185700

	C	-0.03303800	-0.29332800	-0.67252900	C	-0.03504400	-0.30370200	-0.65620700
	C	0.91714100	-1.32403000	-0.86639300	C	0.91023300	-1.32642300	-0.83826800
	C	2.26521900	-1.12654600	-0.54638000	C	2.24834400	-1.12342000	-0.52428200
	C	2.65692400	0.12225200	-0.03064000	C	2.63504200	0.11969600	-0.02608900
	C	1.73680600	1.16760500	0.17284700	C	1.72144400	1.15553100	0.16720000
	C	0.39275200	0.95166000	-0.15083000	C	0.38709500	0.93622700	-0.14963600
	H	0.58928100	-2.28602400	-1.25047500	H	0.58602900	-2.29097600	-1.21576900
	H	3.00583600	-1.90617300	-0.68327400	H	2.99144100	-1.89936900	-0.65635800
	H	2.08419400	2.11424200	0.57109300	H	2.06845700	2.10481800	0.55481900
	H	-0.33405100	1.74618300	-0.00947600	H	-0.34081800	1.72930800	-0.01508600
	H	-4.59291600	2.45395200	0.55915800	H	-4.52092000	2.45324700	0.58215700
	H	-4.58729300	2.58946000	-1.21272800	H	-4.54217600	2.58626700	-1.18637400
	H	-5.56613900	1.33789300	-0.41835600	H	-5.51094200	1.34215100	-0.37553400
	N	4.07483600	0.34524100	0.30412700	N	4.04982900	0.34777300	0.30189300
	O	4.90134800	-0.61315900	0.10911600	O	4.83753800	-0.58004300	0.11602000
	O	4.41328100	1.48772800	0.77391700	O	4.36375600	1.45369400	0.74322600

HOMA (harmonic oscillator model of aromaticity): The HOMA, a geometry-based criterion for aromaticity, was calculated using following equation.

$$rHOMA = 1 - \Sigma\alpha / n (R_0 - R_i)^2,$$

$$\alpha = 2\{(R_0 - R_S)^2 - (R_0 - R_D)^2\}^{-1}$$

R_0 = Values corresponding to the bond distances in the Claisen rearrangement of the allyl vinyl ether

α = normalizing factor

n = number of bonds involved

R_D = Double bond

R_S = Single bond

Ri = Bond length under investigation

$R_{S(C-O)}$: 1.425 Å

$R_{D(C=O)}$: 1.202 Å

$R_{S(C-C)}$: 1.530 Å

$R_{S(C=C)}$: 1.329 Å

For standard HOMA calculations, Ro is the C=C bond distance in fully aromatic benzene ring. However in order to calculate the aromaticity of the transition states, we took the Ro bond

distances from the optimized geometry of the cyclic aromatic transition state of the allyl vinyl ether Claisen rearrangements. Thus, the HOMA in the present study is relative to the HOMA values of the TS of the allyl vinyl ether.

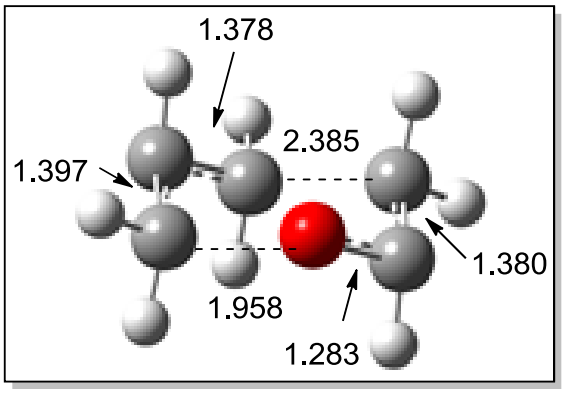

Figure 2 Optimized geometry for the transition states of the Claisen rearrangement of the allyl vinyl ether calculated at B3LYP/6-311+G** level by the Schleyer group.

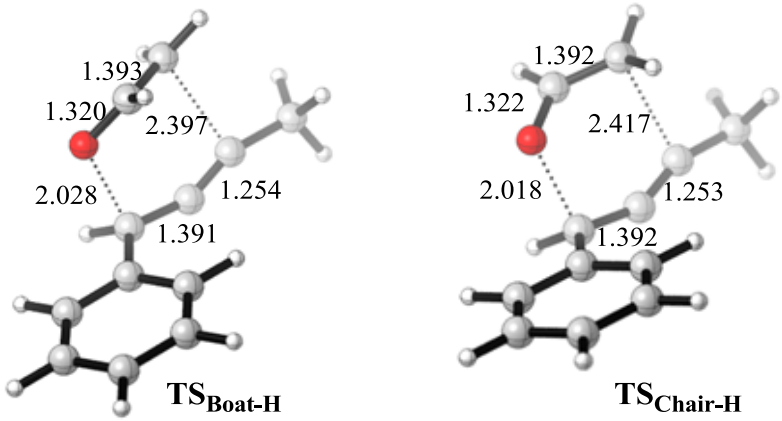

Figure 3 B3LYP/6-31G(d,p) transition state structures for the uncatalyzed Claisen rearrangement of the phenyl-substituted propargyl vinyl ether with selected bond distances.

Isotropic Shifts of Bq calculated at the geometric center of the transition state ring.

Uncatalyzed Rearrangement	
TS_{PhNH2}	Bq Isotropic = 17.5677 Anisotropy = 24.7684 XX= 16.2067 YX= 8.6287 ZX= 11.7000 XY= 9.6791 YY= 15.4964 ZY= 7.7754 XZ= 8.5132 YZ= 2.1051 ZZ= 20.9998 Eigenvalues: 5.4628 13.1602 34.0800

TS_{Ph}	Bq Isotropic = 18.8452 Anisotropy = 28.4570 XX= 14.4757 YX= 10.6374 ZX= 9.9223 XY= 9.0070 YY= 19.7603 ZY= 6.9618 XZ= 11.5161 YZ= 8.3066 ZZ= 22.2996 Eigenvalues: 5.4028 13.3163 37.8165
TS_{PhNO2}	Bq Isotropic = 19.2135 Anisotropy = 27.7936 XX= 19.7488 YX= 10.4626 ZX= 12.5174 XY= 11.8479 YY= 17.3882 ZY= 8.5214 XZ= 8.4856 YZ= 2.8960 ZZ= 20.5036 Eigenvalues: 6.4196 13.4784 37.7426
<u>Gold(I)-catalyzed cyclization-mediated rearrangement</u>	
TS_{PhNH2}	Bq Isotropic = 12.7905 Anisotropy = 10.7503 XX= 15.1347 YX= 2.3371 ZX= 0.8421 XY= 0.0225 YY= 8.8693 ZY= -4.6831 XZ= 4.2362 YZ= -10.1135 ZZ= 14.3676 Eigenvalues: 3.2296 15.1846 19.9574
TS_{Ph}	Bq Isotropic = 12.8404 Anisotropy = 10.8675 XX= 14.3811 YX= 3.5968 ZX= -1.6612 XY= 1.8336 YY= 8.6861 ZY= 3.8462 XZ= -6.0384 YZ= 8.8852 ZZ= 15.4538 Eigenvalues: 3.1698 15.2659 20.0853
TS_{PhNO2}	Bq Isotropic = 13.2140 Anisotropy = 10.3801 XX= 15.4222 YX= 0.3007 ZX= -1.3065 XY= -1.3315 YY= 9.5023 ZY= -4.5139 XZ= 0.5400 YZ= -10.6634 ZZ= 14.7174 Eigenvalues: 4.0495 15.4584 20.1340
<u>Gold(I)-catalyzed cation-accelerated oxonia Claisen rearrangement</u>	
TS_{PhNH2}	Bq Isotropic = 12.5498 Anisotropy = 11.7573 XX= 10.6661 YX= -3.4061 ZX= -0.2171 XY= -7.2406 YY= 11.1814 ZY= 5.1046 XZ= 1.2299 YZ= 6.1623 ZZ= 15.8018 Eigenvalues: 3.9136 13.3477 20.3880
TS_{PhOMe}	Bq Isotropic = 14.0190 Anisotropy = 16.0978 XX= 11.0207 YX= -3.9256 ZX= -1.0600 XY= -7.8432 YY= 12.0895 ZY= 7.1136 XZ= 0.4725 YZ= 7.9691 ZZ= 18.9468 Eigenvalues: 3.7845 13.5216 24.7508
TS_{Ph}	Bq Isotropic = 15.6001 Anisotropy = 19.9677 XX= 7.6113 YX= -2.2600 ZX= 1.6460 XY= -5.9551 YY= 16.1904 ZY= 8.6394 XZ= 2.6228 YZ= 8.6752 ZZ= 22.9985 Eigenvalues: 4.1560 13.7323 28.9118
TS_{PhCN}	Bq Isotropic = 15.6693 Anisotropy = 19.7918 XX= 7.0803 YX= 0.7302 ZX= 3.4430 XY= 4.2906 YY= 18.1113 ZY= -8.7324 XZ= 4.3380 YZ= -8.4702 ZZ= 21.8162

	Eigenvalues: 4.2132 13.9307 28.8638
TS_{PhCF3}	Bq Isotropic = 15.6086 Anisotropy = 20.1185 XX= 9.5591 YX= 6.0679 ZX= 8.9198 XY= 3.0664 YY= 16.1126 ZY= 4.6490 XZ= 9.4836 YZ= 3.9349 ZZ= 21.1542 Eigenvalues: 4.1239 13.6810 29.0210
TS_{PhNO2}	Bq Isotropic = 15.7083 Anisotropy = 19.3978 XX= 7.1963 YX= 3.2945 ZX= 6.4989 XY= 0.3981 YY= 18.8494 ZY= 6.9785 XZ= 6.9445 YZ= 6.3599 ZZ= 21.0792 Eigenvalues: 4.4230 14.0617 28.6402
Claisen rearrangement *via*. gold(I)-coordinated to the vinyl ether	
TS_{PhNH2}	Bq Isotropic = 8.1015 Anisotropy = 6.7593 XX= 11.8809 YX= -1.8059 ZX= -2.2257 XY= -0.9433 YY= 9.5520 ZY= -0.9927 XZ= -0.4956 YZ= -0.5322 ZZ= 2.8717 Eigenvalues: 2.5375 9.1594 12.6077
TS_{PhOMe}	Bq Isotropic = 8.7569 Anisotropy = 5.8700 XX= 12.0097 YX= -1.9754 ZX= -1.4243 XY= -0.7504 YY= 9.7318 ZY= -0.5363 XZ= 0.1555 YZ= -0.1303 ZZ= 4.5293 Eigenvalues: 4.4365 9.1640 12.6702
TS_{Ph}	Bq Isotropic = 9.9398 Anisotropy = 4.6780 XX= 12.7880 YX= -1.6920 ZX= -0.1145 XY= -0.1436 YY= 9.3781 ZY= 0.5065 XZ= 1.4148 YZ= 0.9511 ZZ= 7.6534 Eigenvalues: 7.2277 9.5333 13.0585
TS_{PhCl}	Bq Isotropic = 10.2233 Anisotropy = 4.5354 XX= 12.8379 YX= -1.8512 ZX= 0.3673 XY= -0.0790 YY= 9.9281 ZY= 0.3570 XZ= 1.5761 YZ= 0.6731 ZZ= 7.9039 Eigenvalues: 7.5133 9.9097 13.2470
TS_{PhCN}	Bq Isotropic = 10.9980 Anisotropy = 4.5166 XX= 13.2248 YX= -1.7761 ZX= 1.2307 XY= 0.2388 YY= 10.0816 ZY= 0.9332 XZ= 2.3749 YZ= 1.0998 ZZ= 9.6877 Eigenvalues: 8.1389 10.8460 14.0091
TS_{PhNO2}	Bq Isotropic = 11.7102 Anisotropy = 5.5768 XX= 13.6864 YX= -1.7417 ZX= 2.1478 XY= 0.3422 YY= 10.2650 ZY= 1.2829 XZ= 3.2852 YZ= 1.3796 ZZ= 11.1792 Eigenvalues: 8.2980 11.4045 15.4281