# *Supporting Information*

# $PtI_2$-Catalyzed Cyclization of 3-Acyloxy-1,5-enynes with the Elimination of HOAc and a Benzyl Shift: Synthesis of Unsymmetrical *m*-Terphenyls

Kai M. Huang, Hong K. Wang, Jun Y. Wang, Chen C. Zhou, Xiao N. ke, Xiu F. Xu*[b], Ling Y. Liu*[a], Jing Li*[a]

[a] State key Laboratory of Elemento-Organic Chemistry, Nankai University, Weijin Road 94#, Nankai District, Tianjin 300071 (China); Synergetic Innovation Center of Chemical Science and Engineering (Tianjin 300071, China)
E-mail: lijing@nankai.edu.cn; liulingyan@nankai.edu.cn

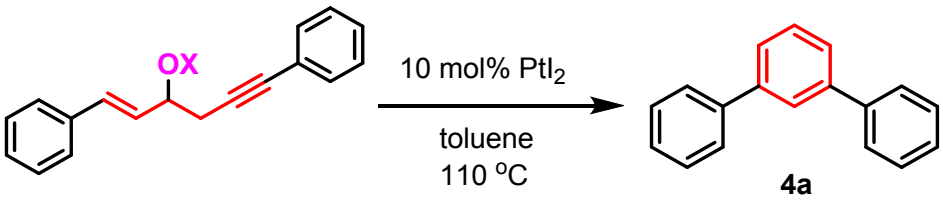
[b] Prof. Dr. X. F. Xu, the Department of Chemistry, Nankai University, Weijin Road 94#, Nankai District, Tianjin 300071 (China)
E-mail: xxfang@nankai.edu.cn

### *1. The true function of N-phenylmaleimide in this reaction system remains unclear currently*

The true function of N-phenylmaleimide in this reaction system remains unclear currently. To ascertain the exact function of N-phenylmaleimide, we had done some controlled experiments. One schlenk tube were added into the 0.1mmol **3a**, 10 mol% $PtI_2$ and 2 mL toluene as solvent, 50 mol% N-phenylmaleimide as additive; while the other tube was filled with the similar substrates and catalysis without the N-phenylmaleimide. These two reactions proceeded at 110 $^{o}$C and completed after about 90 mins (detected by TLC). It was observed that these two reaction systems had the differences as shown in the following figure: the left, the reaction system had less black precipitate than that of the right one. We presumed that the N-phenylmaleimide additive maybe act as a ligand to improve the solubility of platinum metal catalyst in toluene, and thus shortened the reaction time and reduced the possible oligomer formation or decomposition of this enyne substrate under the reaction condition. But unfortunately, no obvious change was observed in the $^{1}$H NMR and $^{13}$C NMR spectra of platinum and N-phenylmaleimide as possible ligand. Further study is ongoing.


**Figure S1** additive= N-phenylmaleimide

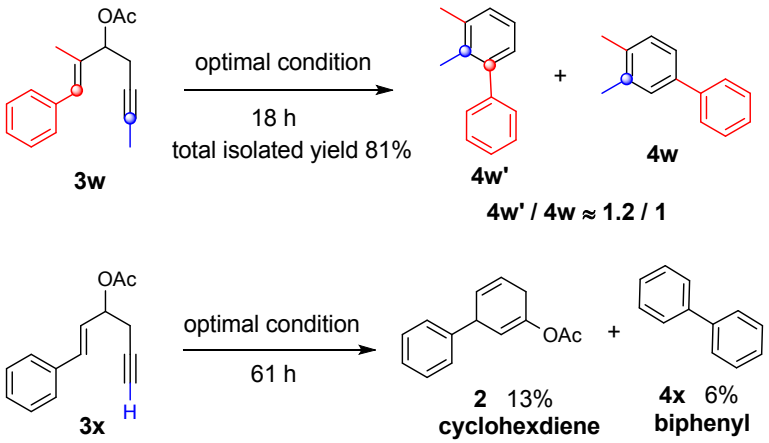
**Table S1.** The effect of the leaving group on the reaction




| Entry | Substrate | OX | t [c] | Yield (%) [a] |
|---|---|---|---|---|
| 1 | **3a** | OAc | 80 mins | 85 |
| 2 [b] | **3a'** | OTBS | 1.5 h | 73 |
| 3 | **3a'** | OTBS | 3.5 h | 57 |
| 4 | **2a** | OH | 12 h | 17 |
| 5 | **3a''** | $OCH_3$ | 43 h | 63 |

Standard procedure as Table 2 (main text)shows. [a] Isolated yield. [b] Using 20 mol% loading of $PtI_2$ catalyst. [c] The starting material disappeared traced by TLC.

To understand the effect of the leaving group at the C3-position of the 1,5-enyne substrate on the reaction, other hydroxy protecting groups were investigated (Table 3). It was found that the 3-acyloxy-1-en-5-yne **3a** gave better result than that of all other enyne substrates **3a'**, **2a**, **3a''** in the presence of $PtI_2$. Given upon a closer insight, the substrate with OAc leaving group could give the corresponding product in 85 % yield in 80 mins, For the OTBS protected 1,5-enyne substrate, it is necessary to prolong the reaction time to 90 mins and increase the amount of the $PtI_2$ to 20 mol%. Consequently, 73% isolated yield of *m*-terphenyls was obtained (entry 2). In the presence of 10 mol% $PtI_2$, the reaction time need to be extended to 3.5 h to consume the substrate completely which is detected once every 15 mins by TLC. Moreover, the isolated yield of **4a** is 57% which is lower than that of 3-OAC-1,5-enyne as substrate (85%) under the same reaction condition (entries 3 *vs* 1). Whereas for the 1,5-enyne with free hydroxy group, the starting material disappeared after 12 h traced by TLC, and resulted in only 17% target product with other side reactions (oligopolymerization or anything else) (entry 4). The direct elimination of water and methanol needs longer reaction time and afford a lower yield of 4a (entry 5). Summarily, the acetyl group is the best hydroxy protecting group in our methodology. We deduced the carbonyl group of the acetyl group formed available intra-molecule hydrogen bond with the hydrogen atom at C4 position, which makes the elimination of acetic acid more easily to occur.




**Scheme S1** The cyclization of enyne **3w** and **3x**

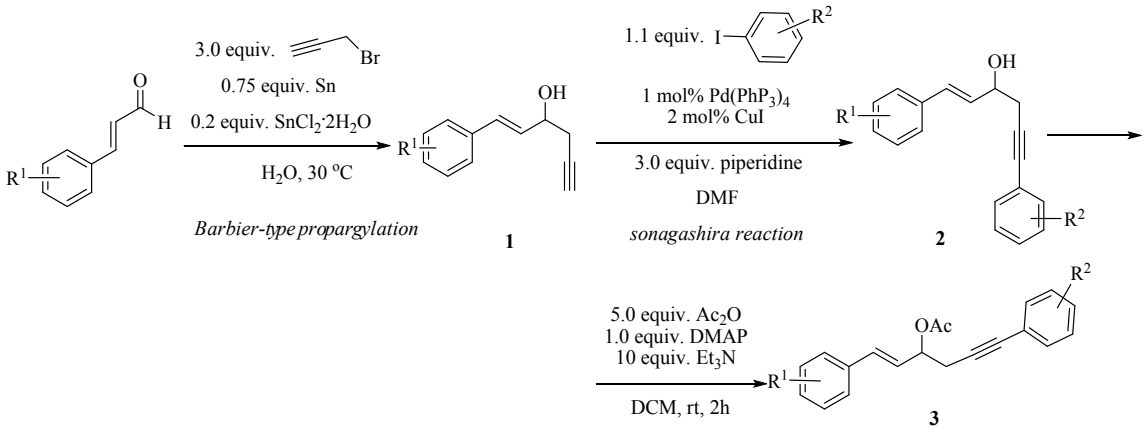
Optimal conditions: 5 mol% $PtI_2$, 50 mol% N-phenylmalimde, toluene, 110 °C. (b) The ratio of these cyclic products and its isomer were detected by proton NMR.

For the enyne **3w**, two regioselective products 2,3-dimethyl biphenyl **4w'** and 3,4-dimethyl biphenyl **4w** were generated (eq. 3, Scheme 3). In the case of terminal alkyne **3x** which was reported by Zhang's group (Scheme 1b in main text, reference 8), the biphenyl **4x** was obtained in a lower yield (6%) besides the cyclohexadiene **2** in 13% isolated yield. This result disclosed that the internal alkyne is important for this transformation into biphenyls or terphenyls derivatives. All these results demonstrated that substituents of the alkene moiety or alkyne terminal have a crucial effect on the regioselectivity or chemoselectivity of this cyclization reaction.

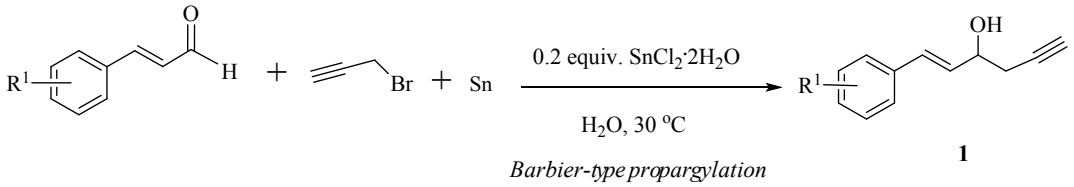
## I General Information

The $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded at Bruker AV 400MHz or 600 MHz. $^{1}H$ and $^{13}C$ NMR Chemical shifts were calibrated to tetramethylsilane as an internal reference. Chemical shifts are given in (ppm) and coupling constants (*J*) in Hz. The following abbreviations are used to indicate the multiplicity: s, singlet; d, doublet: t, triplet; q, quartet; m, multiplet; Infrared spectra were recorded on an Bruker Fourier transform spectrometer (FT-IR) and are reported in wave numbers ($cm^{-1}$). GC-MS spectra were recorded on Finnigan Polaris Q spectrometer. HRMS were obtained on an Agilent 6520 Q-TOF LC-MS with ESI resource. Mass spectra (MS) and high-resolution mass spectra (HRMS) were recorded on a GCT CA127 TOF-MS spectrometer (EI, 70 eV.). Compounds described in the literature were characterized by comparison of their $^{1}H$, and/or $^{13}C$ NMR spectra to the previously reported data.

**Enyne substrates were synthesized according to the following sequence:**



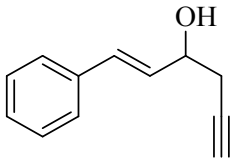

## II Synthesis and Characterization of Propargylic alcohols[1]




**Representative Procedure 1:**

To a vigorously stirred solution of cinnamaldehyde (2.64 g, 20 mmol) and 3 equiv. 3-bromopropyne (7.10 g, 60 mmol) in $H_2O$ (20 mL) 0.75 equiv. tin powder (1.78 , 15 mmol) and 20 mol% Lewis acid $SnCl_2 \cdot H_2O$ (0.83 g, 4 mmol) was added at 30 °C in a 50 mL flask. This solution was stirred at 30 °C until the complete consumption of the starting material as monitored by TLC. After adjusting the pH value to 8-9, the mixture was extracted three times with ethyl acetate (3×40 mL). The combined organic layer was dried over $MgSO_4$ and the solvent was removed in vacuum. The residue was purified by silica gel column chromatography (hexane /ethyl acetate : 10/1) to give the desired product.

**(*E*)-1-phenylhex-1-en-5-yn-3-ol**

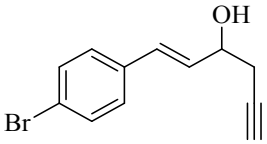


**1a**

Yellow oil, 2.03 g, Yield 59%; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.43-7.26 (ddd, *J* = 27.7, 19.6, 7.3 Hz, 6H), 6.69 (d, *J* = 15.9 Hz, 1H), 6.31 (dd, *J* = 15.9, 6.3 Hz, 1H), 4.50 (q, *J* = 6.0 Hz, 1H), 2.67-2.48 (m,

2H), 2.34(br, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.5, 131.5, 130.1, 128.8, 128.1, 126.8, 80.4, 71.3, 70.9, 27.9.

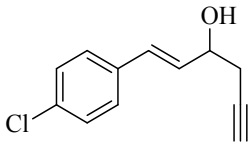
**(*E*)-1-(4-bromophenyl)hex-1-en-5-yn-3-ol**




**1b**

Yellow oil, 2.45 g, Yield 49%; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 6.60 (d, *J* = 15.9 Hz, 1H), 6.27 (dd, *J* = 15.9, 6.2 Hz, 1H), 4.46 (q, *J* = 5.6 Hz, 1H), 2.66-2.44 (m, 2H), 2.39-2.18 (m, 1H), 2.10 (t, *J* = 2.6 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 135.4, 131.9, 130.9, 130.3, 128.3, 121.8, 80.2, 71.5, 70.7, 27.8

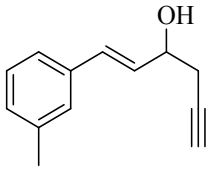
**(*E*)-1-(4-chlorophenyl)hex-1-en-5-yn-3-ol**




**1c**

Yellow oil, 2.18 g, Yield 53%; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.41-7.18 (m, 4H), 6.61 (d, *J* = 15.9 Hz, 1H), 6.25 (dd, *J* = 15.9, 6.2 Hz, 1H), 4.46 (p, *J* = 5.3 Hz, 1H), 2.66-2.45 (m, 2H), 2.33 (d, *J* = 4.7 Hz, 1H), 2.10 (t, *J* = 2.6 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 135.0, 133.7, 130.7, 130.2, 128.9, 128.0, 80.3, 71.5, 70.7, 27.9.

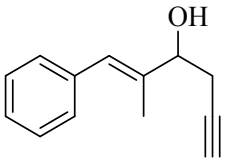
**(*E*)-1-m-tolylhex-1-en-5-yn-3-ol**




**1d**

Yellow oil, 2.08 g, Yield 56%; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.25-7.18 (m, 3H), 7.12-7.05 (m, 1H), 6.64 (d, *J* = 15.9 Hz, 1H), 6.27 (dd, *J* = 15.9, 6.4 Hz, 1H), 4.48 (dd, *J* = 11.2, 5.5 Hz, 1H), 2.65-2.48 (m, 2H), 2.35 (s, 3H), 2.25 (d, *J* = 4.5 Hz, 1H), 2.10 (t, *J* = 2.6 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 138.3, 136.4, 136.0, 131.6, 129.9, 128.9, 128.7, 127.5, 123.9, 80.5, 71.3, 70.9, 27.9, 21.6.

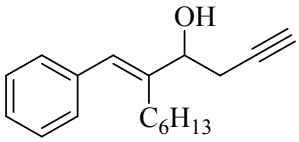
**(*E*)-2-methyl-1-phenylhex-1-en-5-yn-3-ol**




**1e**

Yellow oil, 2.26 g, Yield 61%; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.41-7.11 (m, 5H), 6.55 (s, 1H), 4.33 (t, *J* = 6.4 Hz, 1H), 2.73 (s, 1H), 2.53 (dd, *J* = 6.4, 2.7 Hz, 2H), 2.06 (t, *J* = 2.6 Hz, 1H), 1.85 (d, *J* = 1.3 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 138.2, 137.3, 129.1, 129.1, 129.1, 129.1, 129.0, 129.0, 129.0, 129.0, 128.3, 128.2, 128.1, 126.6, 126.6, 126.5, 126.5, 80.8, 75.6, 71.0, 26.0, 13.5.

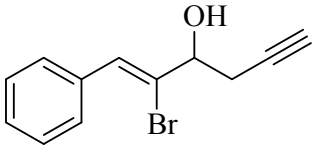
**(*E*)-5-benzylideneundec-1-yn-4-ol**




**1f**

Yellow oil, 2.30 g, Yield 45%; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.33-7.07 (m, 5H), 6.54 (s, 1H), 4.40-4.24 (m, 1H), 2.60-2.38 (m, 2H), 2.38-2.15 (m, 2H), 2.04 (ddd, *J* = 12.4, 9.5, 5.2 Hz, 2H), 1.52-1.31 (m, 2H), 1.30-1.07 (m, 7H), 0.78 (t, *J* = 6.8 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 143.3, 137.6, 128.8, 128.3, 126.7, 126.2, 81.0, 73.6, 71.1, 31.6, 29.7, 29.1, 28.7, 27.0, 22.7, 14.2.

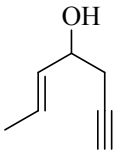
**(*Z*)-2-bromo-1-phenylhex-1-en-5-yn-3-ol**




**1g**

Yellow oil, 2.50 g, Yield 50%; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 6.0 Hz, 2H), 7.42 (d, *J* = 8.6 Hz, 3H), 7.23 (s, 1H), 4.57 (s, 1H), 3.53 (s, 1H), 2.92-2.68 (m, 2H), 2.21 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 134.7, 129.1, 128.2, 128.1, 127.1, 79.7, 75.5, 71.6, 26.2.

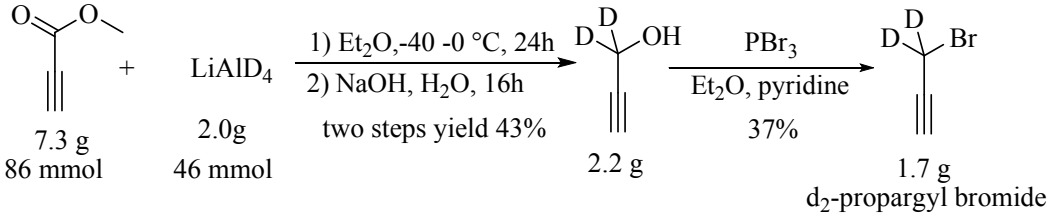
**(*E*)-hept-5-en-1-yn-4-ol**




**1h**

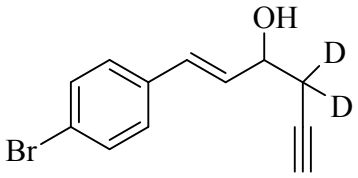
Yellow oil, 506 mg, Yield 23%; $^1$H NMR (400 MHz, $CDCl_3$) δ 5.81-5.67 (m, 1H), 5.54 (ddd, *J* = 15.3, 6.7, 1.4 Hz, 1H), 4.33-4.12 (m, 1H), 2.47-2.36 (m, 2H), 2.16 (d, *J* = 4.3 Hz, 1H), 2.04 (t, *J* = 2.6 Hz, 1H), 1.69 (d, *J* = 6.4 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 132.1, 128.2, 80.8, 70.9, 27.7, 17.8.

**Preparation of the deuterium-labeling homopropargylic alcohol**




The $d_2$-propargyl bromide is synthesized according to the reference[2] ; Spectral data obtained for the compound is in agreement with the data reported.

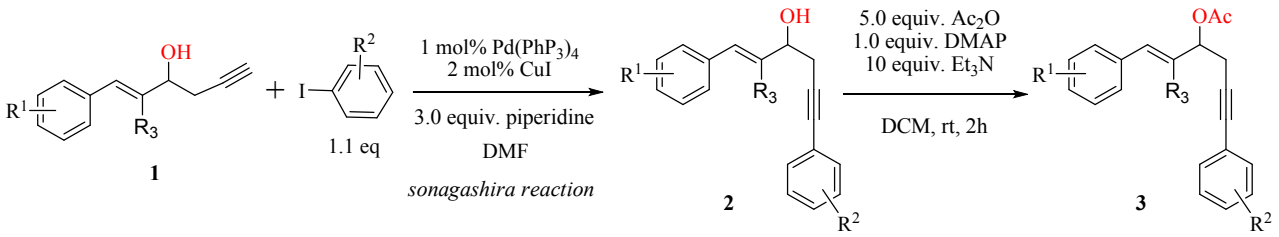
**(*E*)-1-(4-bromophenyl)-(4,4'-di-deuterium)-hex-1-en-5-yn-3-ol**



**1i**

According to the procedure **1a**; Yellow oil, 480 mg, Yield 52%; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 2H), 7.26 (d, *J* = 8.1 Hz, 2H), 6.61 (d, *J* = 15.9 Hz, 1H), 6.29 (dd, *J* = 16.0, 6.1 Hz, 1H), 4.47 (d, *J* = 6.1 Hz, 1H), 2.38 (s, 1H), 2.12 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 135.4, 131.8, 131.6, 130.9, 130.2, 128.3, 127.9, 121.8, 80.2, 77.5, 77.2, 76.9, 71.5, 70.5, 27.6, 27.4, 27.2, 27.0, 26.8, 1.2.

## III Synthesis and Characterization of 3-OH-1-en-5-ynes and 3-OAc-1-en-5-ynes

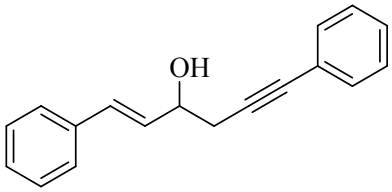



**Representative Procedure 1 to synthesis of 3-OH-1-en-5-ynes**[3]:

In a typical experiment, $Pd(PPh_3)_4$ (1 mol%, 11 mg) and CuI (3 mg, 2 mol%), piperidine (3 mmol, 360

uL) and the substituted Iodobenzene (1.1 mmol) were dissolved in DMF (10 mL) in a sealed Schlenk, after terminal alkynes **1** (1 mmol) was added, the solution is degassed by alternately freezing, evacuating and thawing. Under the nitrogen atmosphere, the reaction mixture was stirred at 80 °C for 16 h. After cooling to room temperature, the reaction mixture was quenched with saturated NaCl (aq), and the product was extracted three times with ethyl acetate (20 mL). The combined organic layer was washed with brine and was dried over magnesium sulfate and the solvent was removed in vacuo. The product was purified by silica gel column chromatography (petrol ether/EtOAc 10:1) to afford the compound **2**.

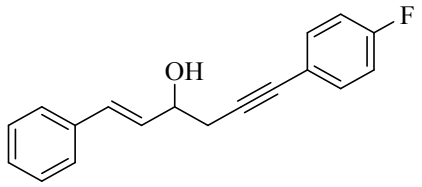
**(*E*)-1,6-diphenylhex-1-en-5-yn-3-ol**




**2a**

White solid, 196 mg, Yield 79%; m.p. 76-78 $^{o}$C. IR (FT-IR): 3389, 3027, 1598, 1444, 1245, 1041, 967, 915, 754, 692 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.53-7.21 (m, 10H), 6.73 (d, *J* = 15.9 Hz, 1H), 6.37 (dd, *J* = 15.9, 6.3 Hz, 1H), 4.64-4.51 (m, 1H), 2.91-2.69 (m, 2H), 2.22 (d, *J* = 4.5 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.6, 131.9, 131.4, 130.5, 128.8, 128.5, 128.2, 128.0, 126.8, 123.4, 85.6, 83.6, 77.5, 77.2, 76.9, 71.2, 29.0; HR-MS (ESI+) calculated for $C_{18}H_{16}O$ ($M+Na^{+}$) 271.1093, found 271.1093.

**(*E*)-6-(4-fluorophenyl)-1-phenylhex-1-en-5-yn-3-ol**

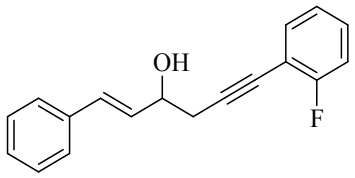



**2b**

White solid, 170 mg, Yield 64%; m.p. 67-69 $^{o}$C; IR (FT-IR): 3405, 2909, 1601, 1505, 1230, 1041, 968, 836, 750, 697, 529 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.54-7.21 (m, 7H), 7.01 (t, *J* = 8.3 Hz, 2H), 6.73 (d, *J* = 15.9 Hz, 1H), 6.37 (dd, *J* = 15.9, 6.1 Hz, 1H), 4.58 (d, *J* = 5.7 Hz, 1H), 2.93-2.72 (m, 2H), 2.38 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.7, 161.2, 136.6, 133.7, 133.7, 131.4, 130.4, 128.8,

128.0, 126.7, 119.5, 119.5, 115.8, 115.5, 85.5, 82.3, 77.5, 77.2, 76.9, 71.2, 28.8; HR-MS (ESI+) calculated for $C_{18}H_{15}FO$ ($M+Na^+$) 289.0999, found 289.1000.

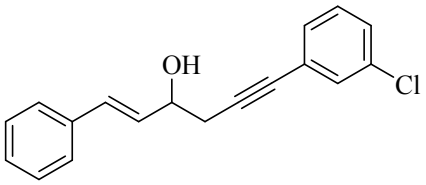
**(*E*)-6-(2-fluorophenyl)-1-phenylhex-1-en-5-yn-3-ol**




**2c**

Yellow oil, 215 mg, Yield 81%; IR (FT-IR): 3384, 3028, 2907, 1661, 1575, 1492, 1215, 1103, 967, 820, 754, 694 $cm^{-1}$;$^1$H NMR (400 MHz, $CDCl_3$) δ 7.35 (ddd, *J* = 29.1, 22.8, 7.3 Hz, 8H), 7.09 (d, *J* = 8.1 Hz, 2H), 6.73 (d, *J* = 15.9 Hz, 1H), 6.39 (dd, *J* = 15.9, 6.1 Hz, 1H), 4.60 (q, *J* = 5.8 Hz, 1H), 2.95-2.78 (m, 2H), 2.62 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.3, 161.8, 136.6, 133.7, 131.4, 130.3, 129.9, 129.8, 128.8, 128.0, 126.8, 124.1, 124.0, 115.7, 115.5, 112.0, 111.9, 91.3, 77.5, 77.2, 76.9, 76.8, 71.1, 29.1; HR-MS (ESI+) calculated for $C_{18}H_{15}FO$ ($M+Na^+$) 289.0999, found 289.0994

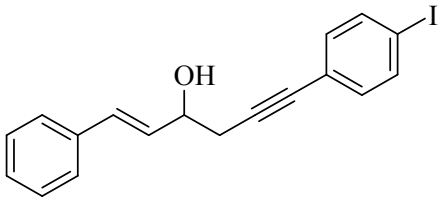
**(*E*)-6-(3-chlorophenyl)-1-phenylhex-1-en-5-yn-3-ol**




**2d**

Yellow solid, 208 mg, Yield 74%; m.p. 49-51 °C. IR (FT-IR): 3385, 3027, 1592, 966, 784, 748, 692 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.59-7.22 (m, 9H), 6.77 (d, *J* = 15.9 Hz, 1H), 6.40 (dd, *J* = 15.9, 6.2 Hz, 1H), 4.62 (d, *J* = 5.5 Hz, 1H), 2.98-2.73 (m, 2H), 2.25 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 134.2, 131.8, 131.6, 130.3, 130.0, 129.7, 128.8, 128.5, 128.1, 126.8, 125.2, 87.2, 82.1, 77.5, 77.2, 76.9, 71.2, 28.9; HR-MS (ESI+) calculated for $C_{18}H_{15}ClO$ ($M+Na^+$) 305.0709; found 305.0703.

**(*E*)-6-(4-iodophenyl)-1-phenylhex-1-en-5-yn-3-ol**

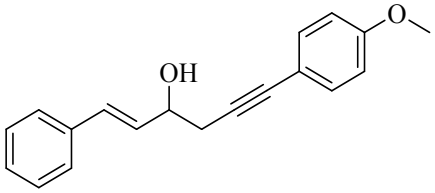



**2e**

White solid, 149 mg, Yield 40%; m.p. 112-114 °C. IR (FT-IR): 3302, 2921, 1657, 1578, 1446, 1389, 1096, 974, 826,750, 733, 694, 522 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.34

(ddd, *J* = 27.6, 19.9, 6.8 Hz, 6H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.34 (dd, *J* = 15.9, 6.3 Hz, 1H), 4.57 (d, *J* = 5.1H), 2.88-2.67 (m, 2H), 2.18 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 137.6, 136.5, 133.4, 131.5, 130.4, 128.8, 128.1, 126.8, 123.0, 93.9, 87.4, 82.6, 77.5, 77.2, 76.9, 71.2, 29.0; HR-MS (ESI+) calculated for $C_{18}H_{15}IO$ (M+$Na^+$) 397.0065, found 397.0057.

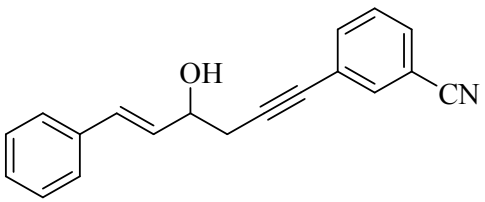
**(*E*)-6-(4-methoxyphenyl)-1-phenylhex-1-en-5-yn-3-ol**




**2f**

$Pd(PPh_3)_4$ (5 mol%, 11 mg) and CuI (1 mg, 3 mol%), piperidine (0.6 mmol, 100 uL) and the *p*-methoxyIodobenzene (1.1 mmol) were dissolved in DMF (3 mL) in a sealed Schlenk, after terminal alkynes **1a** (0.2 mmol) was added, the solution is degassed by alternately freezing, evacuating and thawing. Under the nitrogen atmosphere, the reaction mixture was stirred at the 60 °C for 16 h. After cooling to room temperature, the reaction mixture was quenched with saturated NaCl (aq), and the product was extracted three times with ethyl acetate (20 mL). The combined organic layer was washed with brine and was dried over magnesium sulfate and the solvent was removed in vacuo. The product was purified by silica gel column chromatography (petroleum ether/EtOAc 5:1) to afford the compound **2f**. White solid, 33 mg, Yield 59%; m.p. 87-89 °C; IR (FT-IR): 3460, 2930, 1605, 1510, 1035, 968, 833, 750, 696, 607 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.87-7.56 (m, 8H), 7.18 (d, J = 7.5 Hz, 2H), 7.06 (d, J = 15.9 Hz, 1H), 6.70 (dd, J = 15.9, 6.0 Hz, 1H), 4.90 (d, J = 5.4 Hz, 1H), 4.15 (s, 3H), 3.20-3.04 (m, 2H), 2.76 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.3, 136.5, 133.1, 131.1, 130.4, 128.6, 127.8, 126.6, 115.4, 113.9, 84.0, 83.2, 77.4, 77.1, 76.8, 71.1, 55.3, 28.9; HR-MS (ESI+) calculated for $C_{19}H_{18}O_2$ (M+ $H^+$) 279.1385, found 279.1380.

**(*E*)-3-(4-hydroxy-6-phenylhex-5-en-1-ynyl)benzonitrile**

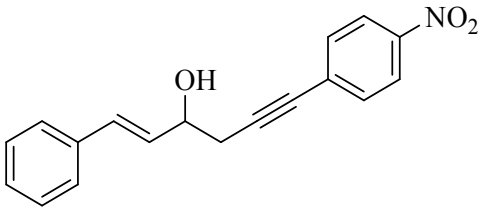



**2g**

Colorless oil, 229 mg, Yield 84%; IR (FT-IR): 3441, 3028, 2232, 1664, 1597, 1478, 967, 798, 750, 684 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.65 (s, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz,

1H), 7.47-7.21 (m, 6H), 6.70 (d, *J* = 15.9 Hz, 1H), 6.32 (dd, *J* = 15.9, 6.4 Hz, 1H), 4.68-4.44 (m, 1H), 2.81 (dd, *J* = 17.1, 5.8 Hz, 2H), 2.41 (s, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.4, 136.0, 135.2, 131.6, 131.3, 130.2, 129.3, 128.8, 128.1, 126.7, 125.1, 118.3, 112.7, 88.9, 81.0, 77.5, 77.2, 76.9, 71.1, 28.7; HR-MS (ESI+) calculated for $C_{19}H_{15}NO$ ($M+Na^+$) 296.1051; found 296.1046.

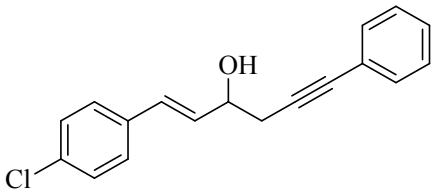
**(*E*)-6-(4-nitrophenyl)-1-phenylhex-1-en-5-yn-3-ol**




**2h**

According to the synthesis of **2f**; White solid, 28 mg, Yield 46%; m.p. 80-81 °C; IR (FT-IR): 3392, 3023, 2881, 1592, 1517, 1344, 1105, 970, 853, 750, 692 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.24-8.07 (m, 2H), 7.65-7.47 (m, 2H), 7.46-7.22 (m, 5H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.33 (dd, *J* = 15.9, 6.4 Hz, 1H), 4.68-4.50 (m, 1H), 2.94-2.72 (m, 2H), 2.30 (d, *J* = 4.3 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 147.0, 136.3, 132.6, 131.7, 130.5, 130.1, 128.8, 128.2, 126.7, 123.7, 92.1, 81.7, 77.5, 77.2, 76.9, 71.1, 28.9; HR-MS (ESI+) calculated for $C_{18}H_{15}NO_3$ ($M+Na^+$) 316.0950, found 316.1044.

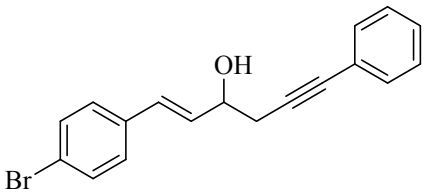
**(*E*)-1-(4-chlorophenyl)-6-phenylhex-1-en-5-yn-3-ol**




**2i**

White solid, 194 mg, Yield 69%; m.p. 95-96 °C; IR (FT-IR): 3403, 2925, 1596, 967, 806, 757, 693 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.48-7.19 (m, 10H), 6.66 (d, J = 15.9 Hz, 1H), 6.32 (dd, J = 15.9, 6.1 Hz, 1H), 4.55 (q, J = 5.9 Hz, 1H), 2.85-2.70 (m, 2H), 2.44 (br, 1H); $^{113}$C NMR (101 MHz, $CDCl_3$) δ 135.1, 133.6, 131.9, 131.1, 130.1, 128.9, 128.5, 128.2, 128.0, 123.3, 85.5, 83.6, 77.5, 77.2, 76.9, 71.0, 28.9; HR-MS (ESI+) calculated for $C_{18}H_{15}ClO$ ($M+Na^+$) 305.0709; found 305.0699.

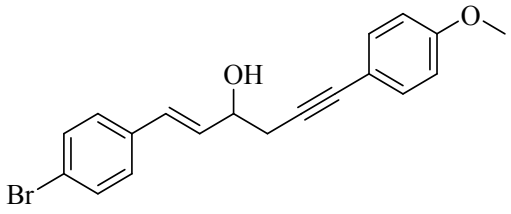
**(*E*)-1-(4-bromophenyl)-6-phenylhex-1-en-5-yn-3-ol**



**2j**

White solid, 215 mg Yield 66%; m.p. 95-97 °C; IR (FT-IR): 3418, 2925, 1597, 1487, 968, 803, 757, 693 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.65-7.07 (m, 11H), 6.59 (d, *J* = 15.9 Hz, 1H), 6.29 (dd, *J* = 15.9, 6.1 Hz, 1H), 4.50 (q, *J* = 5.8 Hz, 1H), 2.92-2.43 (m, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 135.5, 131.8, 131.2, 130.0, 128.4, 128.2, 128.2, 123.3, 121.7, 85.6, 83.5, 77.5, 77.2, 76.9, 71.0, 28.8; HR-MS (ESI+) calculated for $C_{18}H_{15}BrO$ ($M+Na^+$) 349.0204; found 349.0207.

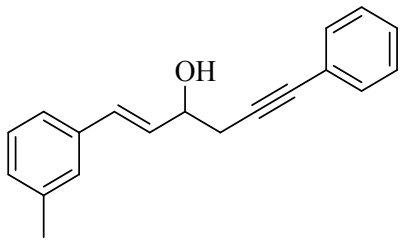
**(*E*)-1-(4-bromophenyl)-6-(4-methoxyphenyl)hex-1-en-5-yn-3-ol**




**2k**

Following the procedure of **2f**; White solid, 57 mg, Yield 80%; m.p. 141-142 °C; IR (FT-IR): 3352, 2931, 1604, 1031, 973, 835, 807, 540 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.10 (m, 6H), 6.73 (d, *J* = 8.8 Hz, 2H), 6.55 (d, *J* = 15.9 Hz, 1H), 6.23 (dd, *J* = 15.9, 6.0 Hz, 1H), 4.43 (d, *J* = 5.9 Hz, 1H), 3.71 (s, 3H), 2.77-2.57 (m, 2H), 2.26 (s, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ = 159.6, 135.6, 133.2, 131.9, 131.3, 130.0, 128.3, 121.7, 115.4, 114.1, 83.8, 83.5, 77.5, 77.2, 76.9, 71.0, 55.4, 29.0; HR-MS (ESI+) calculated for $C_{19}H_{18}BrO_2$ ($M+H^+$) 357.0490, found 357.0466.

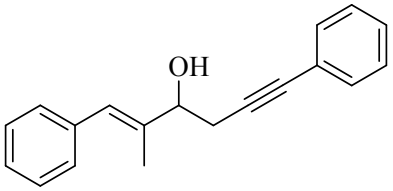
**(*E*)-6-phenyl-1-*m*-tolylhex-1-en-5-yn-3-ol**




**2l**

White solid, 201 mg, Yield 77%; m.p. 65-67°C; IR (FT-IR): 3432, 2924, 1601, 966, 778, 757, 692 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.31 (dt, *J* = 25.9, 4.3 Hz, 6H), 7.21-7.05 (m, 1H), 6.71 (dd, *J* = 15.9, 0.5 Hz, 1H), 6.37 (dd, *J* = 15.9, 6.3 Hz, 1H), 4.59 (q, *J* = 5.7 Hz, 1H), 2.95-2.72 (m, 2H), 2.55 (s, 1H), 2.40 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 138.2, 136.5, 131.8, 131.4, 130.3, 128.7, 128.6, 128.4, 128.1, 127.4, 123.9, 123.4, 85.8, 83.4, 77.5, 77.2, 76.9, 71.2, 28.9, 21.5; HR-MS (ESI+) calculated for $C_{19}H_{18}O$ ($M+Na^+$) 285.1255; found 285.1260.

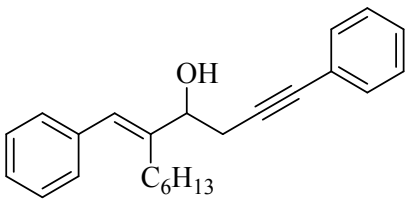
**(*E*)-2-methyl-1,6-diphenylhex-1-en-5-yn-3-ol**




**2m**

Colorless oil, 212 mg, Yield 81%; IR (FT-IR): 3441, 2914, 1715, 1599, 1491, 1444, 1070, 756, 695 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.34 (dt, *J* = 27.1, 22.7 Hz, 10H), 6.67 (s, 1H), 4.47 (s, 1H), 2.83 (d, *J* = 5.3 Hz, 2H), 2.33 (s, 1H), 1.96 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 138.5, 137.5, 131.8, 129.2, 128.4, 128.3, 128.1, 126.7, 126.6, 123.5, 86.1, 83.4, 77.5, 77.2, 76.9, 75.9, 27.3, 13.8; HR-MS (ESI+) calculated for $C_{19}H_{18}O$ ($M+H^+$) 263.1436, found 263.1441.

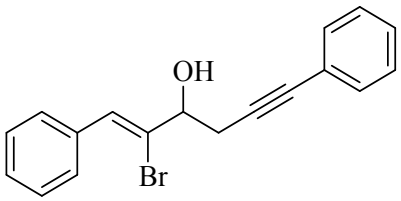
**(*E*)-5-benzylidene-1-phenylundec-1-yn-4-ol**




**2n**

Colorless oil, 199 mg, Yield 86%; IR (FT-IR): 3384, 3056, 2926, 1599, 1491, 1028, 916, 755, 694 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.47-7.16 (m, 11H), 6.67 (s, 1H), 4.47 (s, 1H), 2.80 (qd, *J* = 16.8, 6.1 Hz, 2H), 2.49-2.34 (m, 2H), 2.18 (dt, *J* = 13.8, 8.0 Hz, 1H), 1.51 (dd, *J* = 15.6, 7.9 Hz, 2H), 1.37-1.19 (m, 8H), 0.88 (dt, *J* = 13.6, 6.7 Hz, 4H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 143.6, 137.7, 131.8, 128.8, 128.4, 128.3, 128.0, 126.6, 126.2, 123.5, 86.3, 83.4, 77.5, 77.2, 76.9, 73.8, 31.6, 29.8, 29.8, 29.1, 28.8, 28.0, 22.7, 14.2; HR-MS (ESI+) calculated for $C_{24}H_{28}O$ ($M+Na^+$) 355.2038, found 355.2031.

**(*Z*)-2-bromo-1,6-diphenylhex-1-en-5-yn-3-ol**

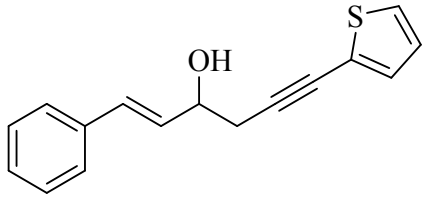



**2o**

Yellow oil, 218 mg, Yield 67%; IR (FT-IR): 3422, 2917, 2849, 1490, 1045, 755, 692 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 6.8 Hz, 2H), 7.58-7.28 (m, 9H), 4.61 (d, *J* = 5.0 Hz, 1H), 3.15-2.92 (m, 2H), 2.69 (s, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 135.1, 131.8, 129.3, 129.3, 128.4, 128.4, 128.2,

127.6, 123.3, 84.9, 83.9, 77.5, 77.2, 76.9, 75.9, 27.8; HR-MS (ESI+) calculated for $C_{18}H_{15}BrO$ ($M+Na^+$) 349.0204, found 349.0204.

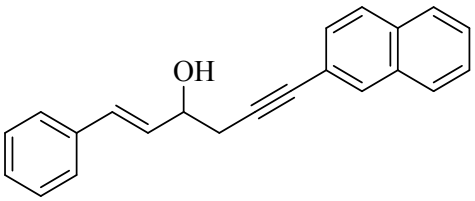
**(*E*)-1-phenyl-6-(thiophen-2-yl)hex-1-en-5-yn-3-ol**




**2p**

Yellow oil, 178 mg, Yield 70%; IR (FT-IR): 3394, 2905, 966, 848, 750, 695 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.28 (ddd, *J* = 44.1, 36.1, 8.6 Hz, 7H), 6.92 (d, *J* = 3.4 Hz, 1H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.31 (dd, *J* = 15.9, 5.4 Hz, 1H), 4.53 (s, 1H), 2.91-2.67 (m, 2H), 2.29 (s, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 136.5, 131.8, 131.5, 130.3, 128.8, 128.0, 127.0, 126.8, 126.7, 123.5, 89.9, 77.5, 77.2, 76.9, 76.5, 71.1, 29.2; HR-MS (ESI+) calculated for $C_{16}H_{14}OS$ ($M+Na^+$) 277.0663; found 277.0664.

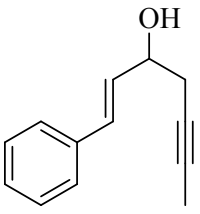
**(*E*)-6-(naphthalen-2-yl)-1-phenylhex-1-en-5-yn-3-ol**




**2q**

White solid, 211 mg, Yield 71%; m.p. 67-68 °C; IR (FT-IR): 3392, 3057, 2904, 1584, 1495, 1395, 1029, 966, 800, 774, 750,693 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.3 Hz, 1H), 7.83 (t, *J* = 9.8 Hz, 2H), 7.67 (d, *J* = 6.9 Hz, 1H), 7.60-7.24 (m, 8H), 6.79 (d, *J* = 15.9 Hz, 1H), 6.46 (dd, *J* = 15.9, 6.0 Hz, 1H), 4.67 (s, 1H), 2.99 (t, *J* = 8.0 Hz, 2H), 2.40 (s, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 136.5, 133.6, 133.3, 131.6, 130.6, 130.5, 128.8, 128.6, 128.4, 128.1, 126.8, 126.5, 126.4, 125.3, 121.1, 90.7, 81.5, 77.5, 77.2, 76.9, 71.4, 29.2; HR-MS (ESI+) calculated for $C_{22}H_{18}O$ ($M+Na^+$) 321.1255; found 321.1257.

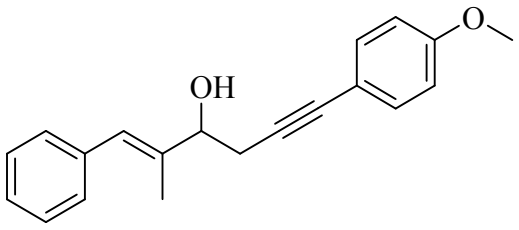
**(*E*)-1-phenylhept-1-en-5-yn-3-ol**[4]




**2r**

A round-bottomed flask was wrapped in aluminum foil and equipped with a dropping funnel and a thermometer. The flask was charged with (*E*)-1-phenylhex-1-en-5-yn- 3-ol (258 mg, 1.5 mmol, 1.0 equiv.) and tetrahydrofuran (4 mL). The resulting solution was cooled to –78 °C and a 2.5 M solution of *n*-butyllithium in hexane (1.2 mL, 3 mmol, 2.0 equiv.) was added dropwise. The mixture was stirred at -78 °C for a further 90 minutes and iodomethane (0.5 mL, 7.5 mmol, 5.0 equiv.) was added dropwise. The mixture was allowed to warm to room temperature for 1 hour and 1.0 M hydrochloric acid (10 mL) was added dropwise. The mixture was stirred for a further 30 minutes at room temperature, the organic layer separated and the aqueous layer extracted with diethyl ether (3 x 15 mL).The combined organic layers were dried over magnesium sulfate, filtered and concentrated *in vacuo*. The product was purified by silica gel column chromatography (hexane /ethyl acetate: 10/1) to give the desired product **2q**. Yellow oil, 176 mg, Yield 63%; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.42-7.14 (m, 6H), 6.62 (d, *J* = 15.9 Hz, 1H), 6.24 (dd, *J* = 15.9, 6.3 Hz, 1H), 4.38 (dd, *J* = 11.8, 5.9 Hz, 1H), 2.58-2.38 (m, 2H), 2.21 (s, 1H), 1.80 (t, *J* = 2.3 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 136.5, 131.0, 130.5, 128.6, 127.8, 126.6, 78.8, 77.4, 77.1, 76.7, 74.7, 71.0, 28.2, 3.6; GC-MS (EI, 70 eV): m/z (%) = 186 (2)[$M^+$], 168 (6), 153 (10), 133 (100), 115 (51).

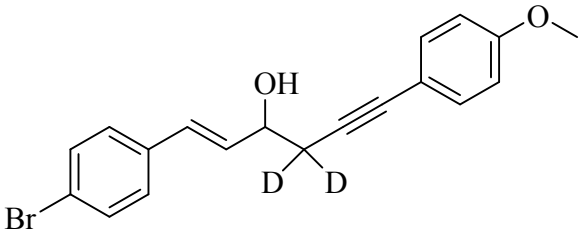
**(*E*)-6-(4-methoxyphenyl)-2-methyl-1-phenylhex-1-en-5-yn-3-ol**




**2s**

According to the synthesis of **2f**; Colorless oil, 42 mg, Yield 72%; IR (FT-IR): 3424, 2837, 1605, 1569, 1509, 1443, 1246, 1173, 1032, 832, 750,700,536 $cm^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.50-7.08 (m, 8H), 6.93-6.77 (m, 2H), 6.64 (s, 1H), 4.44 (t, *J* = 5.9 Hz, 1H), 3.80 (s, 3H), 2.86-2.72 (m, 2H), 2.37 (s, 1H), 1.93 (d, *J* = 1.2 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.5, 138.6, 137.6, 133.2, 129.2, 128.3, 126.7, 126.5, 115.6, 114.0, 114.0, 84.4, 83.2, 77.5, 77.2, 76.9, 75.9, 55.4, 27.4, 13.8; HR-MS (ESI+) calculated for $C_{20}H_{20}O_3$ ($M+H^+$) 293.1543, found 293.1535.

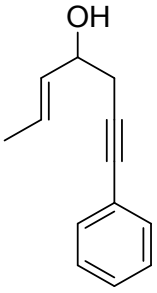
**(*E*)-1-(4-bromophenyl)-6-(4-methoxyphenyl)-(4,4'-di-deuterium)-hex-1-en-5-yn-3-ol**




**2t**

According to the procedure for the synthesis of **2f**; White solid, 56 mg, Yield 79%; m.p. 112-114 °C; IR (FT-IR): 3342, 3172, 1757, 1676, 1247, 1105, 1030, 974,800 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.57-7.20 (m, 7H), 6.82 (d, *J* = 8.6 Hz, 2H), 6.62 (d, *J* = 15.9 Hz, 1H), 6.32 (dd, *J* = 15.9, 6.0 Hz, 1H), 4.51 (d, *J* = 5.7 Hz, 1H), 3.79 (s, 3H), 2.41 (s, 1H);$^{13}C$ NMR (101 MHz, $CDCl_3$) δ 159.5, 135.6, 133.2, 133.1, 131.8, 131.3, 130.0, 128.3, 121.7, 115.4, 114.0, 83.8, 83.5, 77.5, 77.2, 76.9, 70.9, 55.4; HR-MS (ESI+) calculated for $C_{19}H_{15}D_2BrO_2$ ($M+H^+$) 359.0616, found 359.0594.

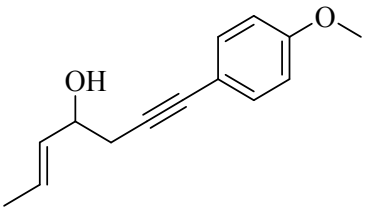
**(*E*)-1-phenylhept-5-en-1-yn-4-ol**




**2u**

Colorless oil, 152 mg, Yield 82%; IR (FT-IR): 3385, 2917, 1674, 1598, 1490, 1443, 1026, 966, 757, 692, 527 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.51-7.36 (m, 3H), 7.34-7.27 (m, 3H), 5.79 (dq, *J* = 12.8, 6.4 Hz, 1H), 5.62 (dd, *J* = 15.3, 6.6 Hz, 1H), 4.38-4.27 (m, 1H), 2.74-2.57 (m, 2H), 2.31 (d, *J* = 4.1 Hz, 1H), 1.74 (d, *J* = 6.4 Hz, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 159.4, 133.2, 132.3, 128.1, 115.6, 114.0, 84.4, 83.0, 77.5, 77.2, 76.9, 71.2, 55.4, 28.9, 17.9; HR-MS (ESI+) calculated for $C_{13}H_{14}O$ ($M+H^+$) 187.1123, found 187.1118.

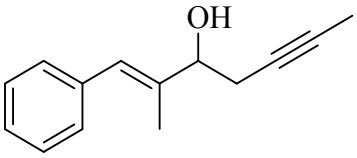
**(*E*)-1-(4-methoxyphenyl)hept-5-en-1-yn-4-ol**




**2v**

According to the synthesis of **2f**; Colorless oil, 34 mg, Yield 78%; IR (FT-IR): 3417, 2915, 1606, 1510, 1246, 1173, 1032, 966, 832, 536 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.7 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 5.77 (dt, *J* = 12.8, 6.4 Hz, 1H), 5.68-5.43 (m, 1H), 4.38-4.25 (m, 1H), 3.79 (s, 3H), 2.74-2.52 (m, 2H), 2.15 (d, *J* = 4.3 Hz, 1H), 1.73 (d, *J* = 6.3 Hz, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 159.4, 133.2, 132.3, 128.1, 115.6, 114.0, 84.4, 83.0, 77.5, 77.2, 76.9, 71.2, 55.4, 28.9, 17.9; HR-MS (ESI+) calculated for $C_{14}H_{16}O_2$ ($M+H^+$) 217.1229 , found 217.1221.

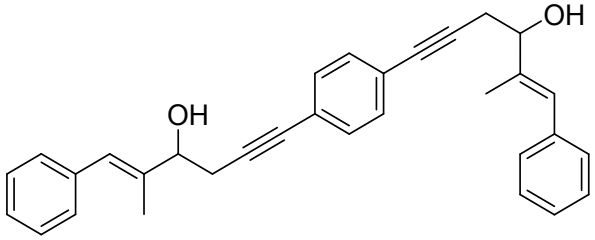
**(*E*)-2-methyl-1-phenylhept-1-en-5-yn-3-ol**




**2w**

According to the procedure of **2q**; Colorless oil, 111 mg, Yield 37%; $^1H$ NMR (400 MHz, CDCl3) δ 7.41-7.16 (m, 6H), 6.57 (s, 1H), 4.35-4.23 (m, 1H), 2.59-2.41 (m, 2H), 2.24 (s, 1H), 1.89 (d, J = 15.2 Hz, 3H), 1.82 (d, J = 1.9 Hz, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 138.5, 137.5, 129.0, 128.1, 126.5, 126.1, 78.7, 77.4, 77.1, 76.7, 75.7, 75.1, 26.6, 13.7, 3.6; GC-MS (EI, 70 eV): m/z (%) = 182 (2), 147 (97), 129 (100), 91 (22).

**(1E,1'E)-6,6'-(1,4-phenylene)bis(2-methyl-1-phenylhex-1-en-5-yn-3-ol)**



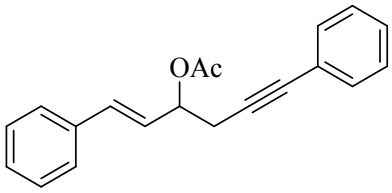

**2y**

Following the general procedure 2; White solid; Yield 56%; 124 mg; m.p. 113-114 °C. IR (FT-IR): 3326, 2911, 1739, 1444, 1244, 1046, 918, 747, 699, 548 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.38-7.18 (m, 15H), 6.62 (s, 2H), 4.43 (t, *J* = 6.1 Hz, 2H), 2.79 (d, *J* = 6.3 Hz, 4H), 2.28 (s, 2H), 1.91 (s, 6H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ = 138.3, 137.3, 131.5, 129.0, 128.2, 126.6, 126.5, 122.9, 87.7, 85.4, 82.8, 77.4, 77.1, 76.7, 75.8, 27.2, 13.6; HR-MS (ESI+) calculated for $C_{32}H_{30}O_2$ ($M+NH_4^+$) 464.2590, found 464.2583.

**Representative Procedure 3 to synthesis of 3-OAc-1-en-5-ynes[5]:**

To a solution of the 3-OH-1-en-5-ynes **2** (0.5 mmol), $Et_3N$ (0.7 mL, 5.0 mmol) and DMAP (0.06 g, 0.5 mmol) in anhydrous $CH_2Cl_2$ (5.0 mL) at 0°C, was slowly added acetic anhydride (0.25 mL, 2.5 mmol). The reaction was stirred at room temperature overnight, and then concentrated upon the disappearance of the enynyl alcohol (monitored by TLC). The residue obtained was purified through silica gel flash column chromatography (petrol ether/EtOAc: 20:1) to yield the desired acetate **3**.

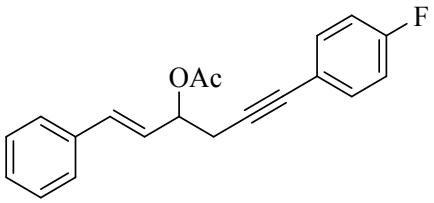
**(*E*)-1, 6-diphenylhex-1-en-5-yn-3-yl acetate**




**3a**

Colorless oil, 139 mg, Yield 96%; IR (FT-IR): 3028, 2913, 1738, 1598, 1491, 1444, 1371, 1232, 1021, 966, 754, 692 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.52-7.20 (m, 11H), 6.73 (d, *J* = 15.9 Hz, 1H), 6.30 (dd, *J* = 15.9, 7.1 Hz, 1H), 5.62 (q, *J* = 6.3 Hz, 1H), 2.95-2.72 (m, 2H), 2.13 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.3, 136.3, 133.6, 131.8, 128.8, 128.4, 128.3, 128.1, 126.9, 126.2, 123.5, 85.0, 83.0, 77.5, 77.2, 76.9, 72.8, 26.1, 21.4; HR-MS (ESI+) calculated for $C_{20}H_{18}O_2$ ($M+Na^+$) 313.1199, found 313.1202.

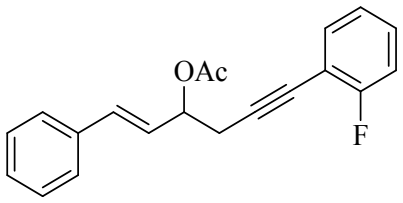
**(*E*)-6-(4-fluorophenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3b**

Colorless oil, 144 mg, Yield 94%; IR (FT-IR): 3028，2910，1738，1601，1506，1371，1232，1156，1021，966，836，750，693 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.50-7.25 (m, 7H), 6.98 (t, *J* = 8.1 Hz, 2H), 6.75 (d, *J* = 15.9 Hz, 1H), 6.30 (dd, *J* = 15.9, 7.1 Hz, 1H), 5.64 (q, *J* = 6.3 Hz, 1H), 2.97-2.77 (m, 2H), 2.14 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.2, 163.6, 161.2, 136.2, 133.6, 133.6, 128.8, 128.3, 126.8, 126.1, 119.6, 119.6, 115.7, 115.5, 84.7, 81.9, 77.5, 77.2, 76.9, 72.7, 26.0, 21.3; HR-MS (ESI+) calculated for $C_{20}H_{17}FO_2$ ($M+Na^+$) 331.1110, found 331.1111.

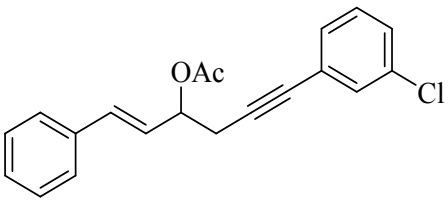
**(*E*)-6-(2-fluorophenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3c**

Colorless oil, 132 mg, Yield 86%; IR (FT-IR): 3028, 2930, 1737, 1658, 1575, 1492, 1448, 1371, 1231, 1021, 965, 818, 751, 692 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.56-7.22 (m, 7H), 7.09 (t, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 15.9 Hz, 1H), 6.79 (d, *J* = 15.9 Hz, 1H), 6.36 (dd, *J* = 15.9, 6.9 Hz, 1H), 6.36 (dd, *J* = 15.9, 6.9 Hz, 1H), 5.69 (d, *J* = 6.2 Hz, 1H), 5.69 (d, *J* = 6.2 Hz, 1H), 3.03-2.84 (m, 2H), 2.18 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.2, 164.3, 161.8, 136.2, 133.6, 133.5, 129.7, 129.6, 128.7, 128.2, 126.8, 126.0, 123.9, 123.9, 115.6, 115.4, 112.0, 111.9, 90.4, 77.5, 77.2, 76.8, 76.3, 72.5, 26.2, 21.3, 21.2; HR-MS (ESI+) calculated for $C_{20}H_{17}FO_2$ ($M+Na^+$) 331.1110, found 331.1109.

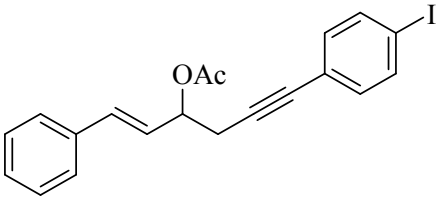
**(*E*)-6-(3-chlorophenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3d**

Yellow oil, 136 mg, Yield 84%; IR (FT-IR): 3027, 2924, 2853, 1738, 1592, 1560, 1474, 1370, 1231, 1020, 964, 784, 747, 682 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.42-7.00 (m, 9H), 6.62 (d, *J* = 15.9 Hz, 1H), 6.17 (dd, *J* = 15.9, 6.4 Hz, 1H), 5.52 (d, *J* = 6.0 Hz, 1H), 2.85-2.65 (m, 2H), 2.02 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.2, 136.1, 134.1, 133.7, 131.6, 129.9, 129.6, 128.8, 128.4, 128.3, 126.8, 126.0, 125.2, 86.5, 81.7, 77.5, 77.2, 76.9, 72.5, 26.0, 21.3; HR-MS (ESI+) calculated for $C_{20}H_{17}ClO_2$ ($M+Na^+$) 347.0815; found 347.0814.

**(*E*)-6-(4-iodophenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**

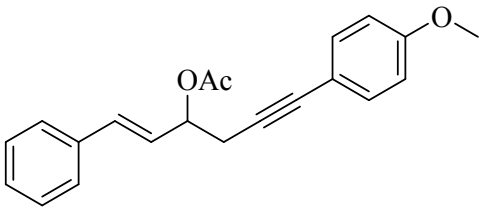



**3e**

White solid, 185 mg, Yield 89%; m.p. 72-73 °C; IR (FT-IR): 3058, 3027, 2930, 1739, 1483, 1371, 1233, 1021, 1007, 965, 820, 750, 693, 522 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.5-7.25 (m, 6H), 7.14 (d, *J* = 8.2 Hz, 2H), 6.76 (d, *J* = 15.9 Hz, 1H), 6.31 (dd, *J* = 15.9, 7.2 Hz,

1H), 5.66 (q, *J* = 6.4 Hz, 1H), 3.01-2.79 (m, 2H), 2.16 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.2, 137.5, 136.1, 133.6, 133.3, 128.8, 128.3, 126.8, 126.0, 123.0, 93.9, 86.6, 82.1, 77.5, 77.2, 76.9, 72.5, 26.1, 21.4; HR-MS (ESI+) calculated for $C_{20}H_{17}IO_2$ (M+Na$^+$) 439.0171, found 439.0163.

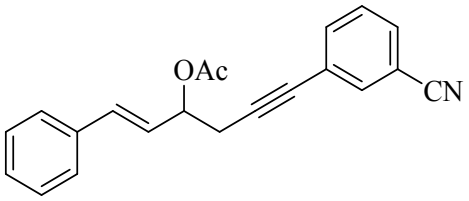
**(*E*)-6-(4-methoxyphenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3f**

White solid, 33 mg, Yield 86%; m.p. 62-63 °C; IR (FT-IR): 3027, 2932, 2837, 1739, 1606, 1510, 1447, 1371, 1290, 1244, 1030, 966, 832, 750, 694, 535 cm$^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.40-7.15 (m, 7H), 6.74 (d, *J* = 8.7 Hz, 2H), 6.65 (d, *J* = 15.9 Hz, 1H), 6.23 (dd, *J* = 15.9, 7.1 Hz, 1H), 5.54 (q, *J* = 6.5 Hz, 1H), 3.72 (s, 3H), 2.76 (dd, *J* = 6.2, 3.9 Hz, 2H), 2.06 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.3, 159.4, 136.3, 133.4, 133.1, 128.8, 128.7, 128.2, 126.8, 126.3, 115.7, 114.0, 83.4, 82.8, 77.5, 77.2, 76.8, 72.8, 55.4, 29.8, 26.1, 21.4; HR-MS (ESI+) calculated for $C_{21}H_{20}O_3$ (M+Na$^+$)343.1310, found 343.1311.

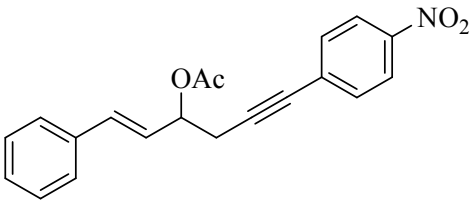
**(*E*)-6-(3-cyanophenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3g**

Colorless oil, 150 mg, Yield 95%; IR (FT-IR): 3029, 2917, 2232, 1738, 1372, 1233, 1021, 966, 799, 750, 684 cm$^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.68-7.43 (m, 3H), 7.41-7.15 (m, 6H), 6.66 (d, J = 15.9 Hz, 1H), 6.19 (dd, J = 15.9, 7.2 Hz, 1H), 5.55 (q, J = 6.3 Hz, 1H), 2.85-2.71 (m, 2H), 2.07 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.2, 136.0, 135.9, 135.1, 133.8, 131.3, 129.3, 128.8, 128.4, 126.8, 125.8, 125.0, 118.2, 112.8, 88.0, 80.8, 77.5, 77.2, 76.9, 72.4, 26.0, 21.3; HR-MS (ESI+) calculated for $C_{21}H_{17}NO_2$ (M+Na$^+$) 338.1157; found 338.1152.

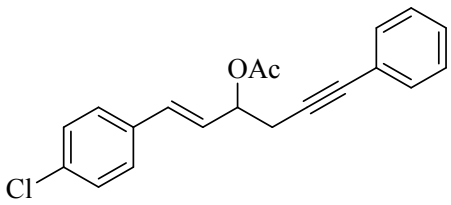
**(*E*)-6-(4-nitrophenyl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3h**

White solid, 28 mg, Yield 89%; m.p. 73-75 °C; IR (FT-IR): 3080, 2924, 2851, 1736, 1593, 1515, 1340, 1229, 1020, 853, 749, 690 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.8 Hz, 2H), 7.56-7.20 (m, 7H), 6.72 (d, *J* = 15.9 Hz, 1H), 6.25 (dd, *J* = 15.9, 7.2 Hz, 1H), 5.63 (q, *J* = 6.4 Hz, 1H), 2.89 (dd, *J* = 6.2, 1.7 Hz, 2H), 2.12 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.2, 147.0, 136.0, 133.9, 132.5, 130.4, 128.8, 128.4, 126.8, 125.7, 123.6, 123.6, 91.1, 81.5, 77.5, 77.2, 76.9, 72.4, 29.8, 26.2, 21.3; HR-MS (ESI+) calculated for $C_{20}H_{17}NO_4$ ($M+Na^+$) 358.1055; found 358.0724.

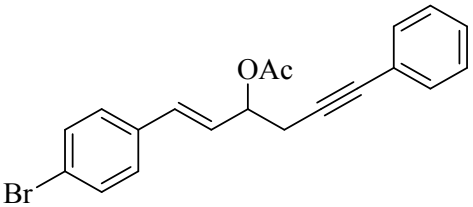
**(*E*)-1-(4-chlorophenyl)-6-phenylhex-1-en-5-yn-3-yl acetate**




**3i**

Colorless oil, 143 mg, Yield 88%; IR (FT-IR): 3034, 2909, 1739, 1491, 1371, 1231, 1093, 1014, 967, 806, 756, 692 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.43-7.14 (m, 9H), 6.61 (d, *J* = 15.9 Hz, 1H), 6.21 (dd, *J* = 15.9, 7.0 Hz, 1H), 5.65-5.49 (m, 1H), 2.89-2.70 (m, 2H), 2.06 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.1, 134.6, 133.8, 132.1, 131.7, 128.8, 128.3, 128.1, 128.0, 128.0, 126.8, 123.4, 84.8, 83.1, 77.5, 77.2, 76.9, 72.4, 25.9, 21.2; HR-MS (ESI+) calculated for $C_{20}H_{17}ClO_2$ ($M+Na^+$) 347.0815; found 347.0812.

**(*E*)-1-(4-bromophenyl)-6-phenylhex-1-en-5-yn-3-yl acetate**

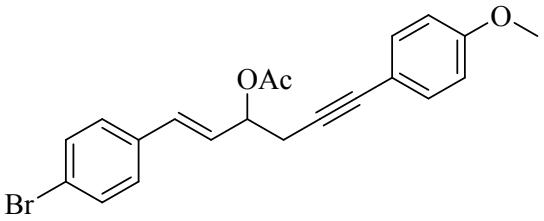



**3j**

Colorless oil, 167 mg, Yield 91%; IR (FT-IR): 3033, 2928, 1739, 1488, 1371, 1232, 1071, 967, 803, 756, 692 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.43-7.28 (m, 4H), 7.19 (dt, *J* = 14.5, 10.0 Hz, 5H), 6.58 (d, *J* = 15.9 Hz, 1H), 6.21 (dd, *J* = 15.9, 7.0 Hz, 1H), 5.55 (q, *J* = 6.3 Hz, 1H), 2.91-2.67 (m, 2H), 2.05

(s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.0, 135.0, 132.1, 131.7, 131.6, 131.6, 131.5, 128.3, 128.2, 128.0, 126.9, 123.3, 122.0, 84.8, 83.0, 77.5, 77.2, 76.9, 73.2, 72.4, 27.4, 25.8, 21.2; HR-MS (ESI+) calculated for $C_{20}H_{17}BrO_2$ ($M+Na^+$) 391.0310; found 391.0310.

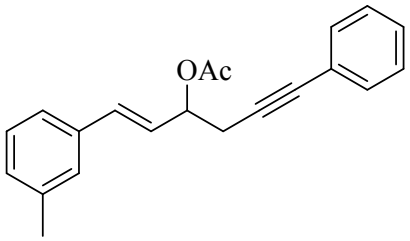
**(*E*)-1-(4-bromophenyl)-6-(4-methoxyphenyl)hex-1-en-5-yn-3-yl acetate**




**3k**

Colorless oil, 58 mg, Yield 92%; IR (FT-IR): 3002, 1734, 1606, 1510, 1371, 1245, 1173, 1071, 1030, 967, 832, 536 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.1 Hz, 2H), 7.27 (dd, *J* = 17.4, 7.9 Hz, 5H), 6.79 (d, *J* = 8.3 Hz, 2H), 6.64 (d, *J* = 16.0 Hz, 1H), 6.26 (dd, *J* = 15.9, 7.0 Hz, 1H), 5.57 (q, *J* = 6.4 Hz, 1H), 3.78 (s, 3H), 2.81 (dd, *J* = 13.7, 8.3 Hz, 2H), 2.11 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.3, 159.6, 135.3, 133.2, 132.3, 131.9, 128.4, 127.3, 122.1, 115.7, 114.1, 83.2, 83.0, 77.5, 77.2, 76.9, 72.7, 55.5, 26.0, 21.4; HR-MS (ESI+) calculated for $C_{21}H_{19}BrO_3$ ($M+Na^+$) 421.0415, found 421.0410.

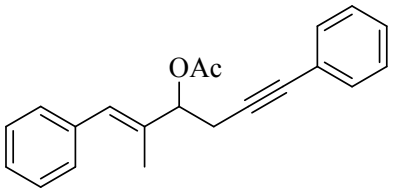
**(*E*)-6-phenyl-1-m-tolylhex-1-en-5-yn-3-yl acetate**




**3l**

Colorless oil, 130 mg, Yield 86%; IR (FT-IR): 3031, 2921, 1738, 1489, 1370, 1231, 1020, 964, 778, 756, 692 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.42 (ddd, *J* = 13.5, 8.1, 5.9 Hz, 6H), 7.26 (dd, *J* = 5.7, 2.6 Hz, 1H), 6.90 (d, *J* = 15.9 Hz, 1H), 6.48 (dd, *J* = 15.9, 7.2 Hz, 1H), 5.84 (q, *J* = 6.5 Hz, 1H), 3.18-2.96 (m, 2H), 2.52 (s, 3H), 2.29 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.0, 138.1, 136.0, 133.5, 131.6, 128.9, 128.5, 128.5, 128.2, 127.9, 127.4, 125.9, 123.9, 123.4, 85.0, 82.9, 77.5, 77.2, 76.9, 72.6, 29.7, 25.9, 21.3, 21.1; HR-MS (ESI+) calculated for $C_{21}H_{20}O_2$ ($M+Na^+$) 327.1361; found 327.1361.

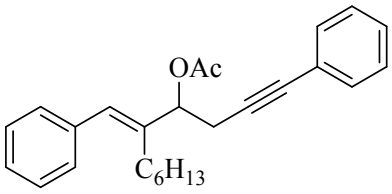
**(*E*)-2-methyl-1, 6-diphenylhex-1-en-5-yn-3-yl acetate**




**3m**

Colorless oil, 141 mg, Yield 93%; IR (FT-IR): 3057, 2963, 2857, 1739, 1370, 1234, 1020, 800, 756, 694 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.52-7.22 (m, 10H), 6.72 (s, 1H), 5.60 (t, *J* = 6.8 Hz, 1H), 2.92 (qd, *J* = 16.8, 6.8 Hz, 2H), 2.17 (s, 3H), 2.01 (dd, *J* = 6.7, 1.4 Hz, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.1, 137.0, 134.7, 131.6, 129.1, 128.7, 128.3, 128.2, 128.0, 126.9, 123.5, 85.3, 82.9, 77.5, 77.2, 77.1, 76.9, 24.6, 21.3, 13.9; HR-MS (ESI+) calculated for $C_{21}H_{20}O_2$ ($M+Na^+$) 327.1361; found 327.1355.

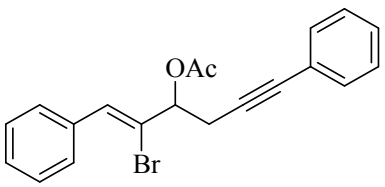
**(*E*)-5-benzylidene-1-phenylundec-1-yn-4-yl acetate**




**3n**

Colorless oil, 177 mg, Yield 95%; IR (FT-IR): 3057, 3024, 2928, 2857, 1742, 1598, 1491, 1443, 1233, 1027, 756, 694 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.41-7.07 (m, 11H), 6.57 (s, 1H), 5.49 (t, *J* = 6.5 Hz, 1H), 2.79 (d, *J* = 6.5 Hz, 2H), 2.36-2.11 (m, 2H), 2.06 (s, 3H), 1.49 (dd, *J* = 9.3, 4.7 Hz, 3H), 1.22 (dd, *J* = 16.1, 10.0 Hz, 7H), 0.79 (t, *J* = 6.6 Hz, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.3, 140.0, 137.3, 131.8, 128.9, 128.4, 128.2, 128.0, 126.9, 123.6, 85.6, 82.9, 77.5, 77.2, 76.9, 75.4, 31.7, 29.8, 29.0, 29.0, 25.4, 22.8, 21.5, 14.3; HR-MS (ESI+) calculated for $C_{26}H_{30}NaO_2$ ($M+Na^+$) 397.2143, found 397.2142.

**(*Z*)-2-bromo-1,6-diphenylhex-1-en-5-yn-3-yl acetate**

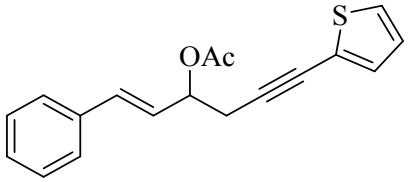



**3o**

Colorless oil, 149 mg, Yield 81%; IR (FT-IR): 3056, 2926, 1740, 1488, 1442, 1368, 1219, 1018, 916, 753, 689 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.0 Hz, 2H), 7.38-7.18 (m, 9H), 7.16 (s, 1H), 5.59 (t, *J* = 6.8 Hz, 1H), 3.01-2.86 (m, 2H), 2.10 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 169.8, 134.8,

132.1, 131.8, 131.8, 129.4, 128.7, 128.4, 128.4, 128.2, 123.4, 122.9, 84.2, 83.5, 77.5, 77.2, 76.9, 76.6, 25.1, 21.3; HR-MS (ESI+) calculated for $C_{20}H_{17}BrO_2$ ($M+NH_4^+$) 386.0756; found 386.0753.

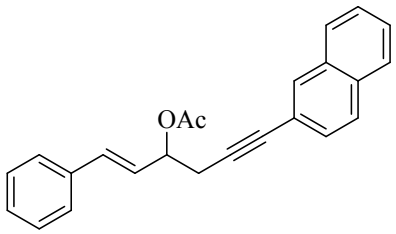
**(*E*)-1-phenyl-6-(thiophen-2-yl)hex-1-en-5-yn-3-yl acetate**




**3p**

Yellow oil, 136 mg, Yield 92%; IR (FT-IR): 3105, 3027, 2925, 1733, 1652, 1598, 1518, 1494, 1370, 1228, 1016, 964, 847, 748, 692, 601 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.52-7.24 (m, 5H), 7.25-7.11 (m, 2H), 6.96 (dd, *J* = 5.1, 3.7 Hz, 1H), 6.76 (d, *J* = 15.9 Hz, 1H), 6.32 (dd, *J* = 15.9, 7.2 Hz, 1H), 5.66 (q, *J* = 6.3 Hz, 1H), 3.00-2.81 (m, 2H), 2.15 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.1, 136.1, 133.5, 131.6, 128.7, 128.2, 126.9, 126.9, 126.8, 126.8, 126.7, 126.6, 126.6, 126.0, 123.5, 89.1, 77.5, 77.2, 76.9, 76.2, 72.4, 26.2, 21.2; HR-MS (ESI+) calculated for $C_{18}H_{16}O_2S$ ($M+Na^+$) 319.0769; found 319.0768.

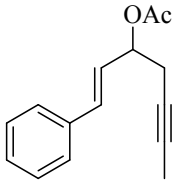
**(*E*)-6-(naphthalen-2-yl)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3q**

White solid, 153 mg, Yield 90%; m.p. 62-63 °C. IR (FT-IR): 3058, 2934, 1738, 1371, 1234, 1020, 966, 800, 775, 750, 693 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.2 Hz, 1H), 7.87 (dd, *J* = 14.2, 8.2 Hz, 2H), 7.75 (d, *J* = 7.1 Hz, 1H), 7.66-7.30 (m, 9H), 6.92 (d, *J* = 15.9 Hz, 1H), 6.50 (dd, *J* = 15.9, 7.2 Hz, 1H), 5.85 (q, *J* = 6.5 Hz, 1H), 3.13 (d, *J* = 6.2 Hz, 2H), 2.24 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.1, 136.1, 133.7, 133.5, 133.2, 130.2, 128.7, 128.6, 128.5, 128.4, 128.2, 126.8, 126.8, 126.7, 126.3, 126.3, 126.2, 125.2, 121.1, 90.0, 81.1, 77.5, 77.2, 76.9, 72.8, 26.2, 21.3; HR-MS (ESI+) calculated for $C_{24}H_{20}O_2$ ($M+Na^+$) 363.1361; found 363.1360.

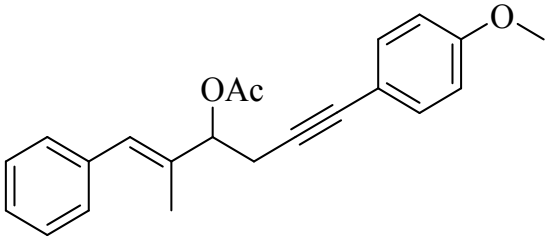
**(*E*)-1-phenylhept-1-en-5-yn-3-yl acetate**




**3r**

Yellow oil, 93 mg, Yield 82%; IR (FT-IR): 3028, 2920, 1739, 1494, 1371, 1234, 1021, 966, 750, 694 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.43-7.06 (m, 6H), 6.59 (d, *J* = 15.9 Hz, 1H), 6.16 (dd, *J* = 16.0, 7.0 Hz, 1H), 5.41 (d, *J* = 5.8 Hz, 1H), 2.49 (s, 2H), 2.04 (s, 4H), 1.71 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.4, 136.4, 133.4, 129.2, 128.8, 128.2, 126.9, 126.5, 78.3, 77.6, 77.5, 77.2, 76.9, 74.2, 73.0, 25.4, 21.5, 3.8; HR-MS (ESI+) calculated for $C_{15}H_{16}O_2$ ($M+Na^+$) 251.1048, found 251.1036.

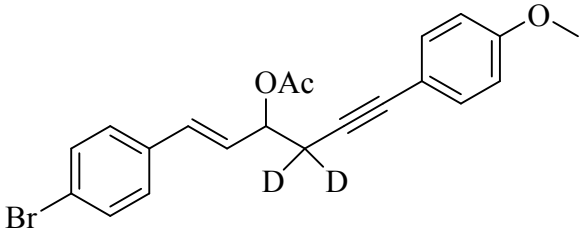
**(E)-6-(4-methoxyphenyl)-2-methyl-1-phenylhex-1-en-5-yn-3-yl acetate**




**3s**

Colorless oil, 42 mg, Yield 88%; IR (FT-IR): 3054, 2999, 2955, 2934, 1738, 1606, 1569, 1509, 1443, 1369, 1242, 1173, 1028, 832, 749, 700, 536 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.44-7.11 (m, 8H), 6.79 (d, *J* = 8.8 Hz, 2H), 6.63 (s, 1H), 5.51 (t, *J* = 6.8 Hz, 1H), 3.77 (s, 3H), 2.83 (qd, *J* = 16.8, 6.8 Hz, 2H), 2.12 (s, 3H), 1.93 (d, *J* = 1.1 Hz, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.3, 159.4, 137.2, 134.9, 133.1, 129.2, 128.7, 128.3, 126.9, 115.7, 114.0, 83.7, 82.7, 77.5, 77.4, 77.2, 76.9, 55.4, 24.7, 21.4, 14.0; HR-MS (ESI+) calculated for $C_{22}H_{22}O_3$ ($M+H^+$) 335.1647, found 335.1641.

**(*E*)-1-(4-bromophenyl)-6-(4-methoxyphenyl)-4,4-di-deuterium-hex-1-en-5-yn-3-yl acetate**

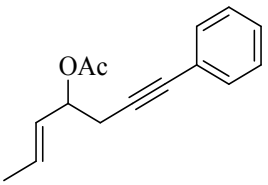



**3t**

Colorless oil, 54 mg, Yield 94%; IR (FT-IR): 3038, 2832, 2837, 1738, 1606, 1509, 1370, 1244, 1173, 1071, 1029, 967，832，804，535 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.1 Hz, 2H), 7.34 (dd, *J* = 17.4, 7.9 Hz, 4H), 6.86 (d, *J* = 8.3 Hz, 2H), 6.70 (d, *J* = 16.0 Hz, 1H), 6.33 (dd, *J* = 15.9, 7.0

Hz, 1H), 5.64 (q, *J* = 6.4 Hz, 1H), 3.85 (s, 3H), 2.87 (t, *J* = 5.6 Hz, 2H), 2.18 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.3, 159.5, 135.3, 133.2, 132.2, 131.9, 128.4, 127.2, 122.1, 115.6, 114.0, 83.2, 83.0, 77.5, 77.2, 76.9, 72.6, 55.4, 21.4; HR-MS (ESI+) calculated for $C_{21}H_{17}D_2BrO$ ($M+Na^+$) 423.0541, found 423.0533.

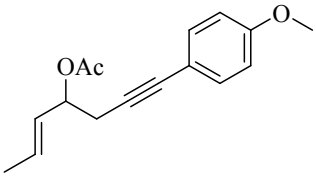
**(*E*)-1-phenylhept-5-en-1-yn-4-yl acetate**




**3u**

Colorless oil, 93 mg, Yield 82%; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 6.4, 3.0 Hz, 2H), 7.28 (dd, *J* = 8.2, 5.2 Hz, 4H), 5.86 (dq, *J* = 13.1, 6.4 Hz, 1H), 5.59 (ddd, *J* = 15.3, 7.3, 1.4 Hz, 1H), 5.40 (q, *J* = 6.5 Hz, 1H), 2.73 (dd, *J* = 6.2, 2.1 Hz, 2H), 2.09 (s, 3H), 1.81-1.70 (m, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.4, 131.8, 130.5, 128.4, 128.3, 128.0, 123.7, 85.4, 82.7, 77.5, 77.2, 76.9, 72.9, 26.0, 21.4, 18.0; HR-MS (ESI+) calculated for $C_{15}H_{16}O_2$ ($M+Na^+$) 251.1048, found 251.1036.

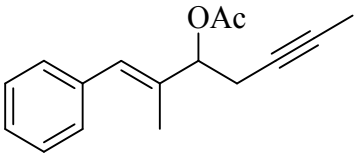
**(*E*)-1-(4-methoxyphenyl)hept-5-en-1-yn-4-yl acetate**




**3v**

Colorless oil, 111 mg, Yield 87%; IR (FT-IR): 3300, 2957, 2933, 2838, 1740, 1607, 1510, 1442, 1371, 1289, 1244, 1173, 1031, 965, 833, 536 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.7 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 5.84 (dd, *J* = 15.2, 6.6 Hz, 1H), 5.58 (ddd, *J* = 15.3, 7.3, 1.5 Hz, 1H), 5.38 (q, *J* = 6.5 Hz, 1H), 3.79 (s, 3H), 2.81-2.64 (m, 2H), 2.08 (s, 3H), 1.80-1.69 (m, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 170.4, 159.4, 133.1, 130.4, 128.3, 115.8, 114.0, 83.8, 82.4, 77.5, 77.2, 76.9, 73.0, 55.4, 26.0, 21.4, 18.0; HR-MS (ESI+) calculated for $C_{16}H_{18}O_3$ ($M+H^+$) 259.1334, found 259.1331.

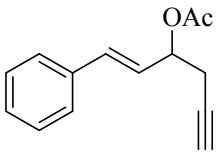
**(*E*)-2-methyl-1-phenylhept-1-en-5-yn-3-yl acetate**




**3w**

Colorless oil, 107 mg, Yield 89%; IR (FT-IR): 3056, 3024, 2920, 1739, 1492, 1443, 1369, 1235, 1019, 748, 699 $cm^{-1}$; $^1H$ NMR (400 MHz, CDCl3) δ 7.29 (ddd, J = 21.2, 14.0, 7.2 Hz, 5H), 6.58 (s, 1H), 5.38 (t, J = 6.6 Hz, 1H), 2.70-2.48 (m, 2H), 2.11 (s, 3H), 1.88 (s, 3H), 1.77 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.3, 137.3, 135.0, 129.2, 128.5, 128.3, 126.9, 78.1, 77.6, 77.5, 77.2, 76.9, 74.5, 24.0, 21.4, 13.9, 3.7; HR-MS (ESI+) calculated for $C_{16}H_{18}O_2$ ($M+Na^+$) 265.1204, found 265.1201.

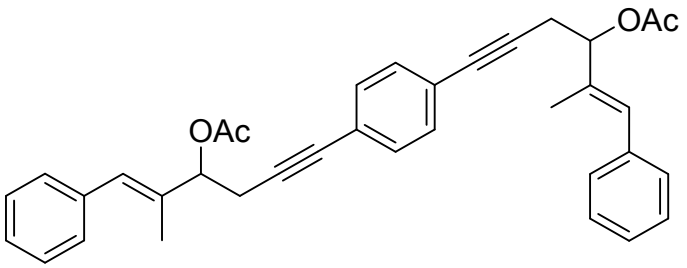
**(*E*)-1-phenylhex-1-en-5-yn-3-yl acetate**




**3x**

Colorless oil, 101 mg, Yield 94%; IR (FT-IR): 3295, 3028, 1738, 1494, 1450, 1372, 1234, 1023, 967, 751, 694, 645 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.56-7.17 (m, 6H), 6.71 (d, *J* = 15.9 Hz, 1H), 6.26 (dd, *J* = 15.9, 7.2 Hz, 1H), 5.56 (q, *J* = 6.3 Hz, 1H), 2.65 (dd, *J* = 6.1, 2.6 Hz, 2H), 2.13 (s, 3H), 2.06 (t, *J* = 2.6 Hz, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 170.3, 136.2, 133.7, 128.8, 128.4, 126.9, 125.8, 79.5, 77.5, 77.2, 76.9, 72.4, 71.0, 25.1, 21.4. Spectral data obtained for the compound are in agreement with the data reported. [5]

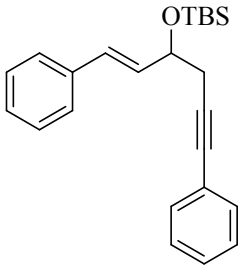
**(1E,1'E)-6,6'-(1,4-phenylene)bis(2-methyl-1-phenylhex-1-en-5-yne-6,3-diyl) diacetate**




**3y**

Following the general procedure 3. Colorless oil, Yield 81%, 107 mg. IR (FT-IR): 3025, 2920, 1739, 1505, 1494, 1369, 1233, 1018, 838, 747, 699 $cm^{-1}$; $^1H$ NMR (400 MHz, CDCl3) δ 7.40 – 7.21 (m, 17H), 6.66 (s, 2H), 5.54 (t, J = 6.7 Hz, 2H), 2.89 (qd, J = 16.9, 6.8 Hz, 4H), 2.15 (s, 6H), 1.96 (d, J = 1.1 Hz, 6H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ = 170.1, 136.9, 134.5, 131.4, 129.0, 128.7, 128.2, 126.8, 122.9, 86.8, 82.5, 77.4, 77.1, 77.0, 76.7, 24.6, 21.2, 13.8; HR-MS (ESI+) calculated for $C_{36}H_{34}O_4$ ($M+NH_4^+$) 548.2801, found 548.2801.

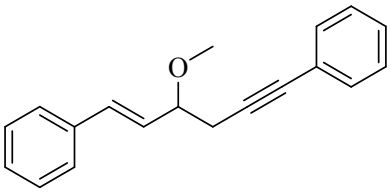
**(*E*)-*tert*-butyl(1,6-diphenylhex-1-en-5-yn-3-yloxy)dimethylsilane**[6]




**3a'**

The (*E*)-1,6-diphenylhex-1-en-5-yn-3-ol **3a**, upon treatment with dimethyl-tert- butylsilyl chloride (1.2 equiv.) and imidazole (2.5 equiv) in dry DMF (2 mL/g of 3a) at 35 °C for 10 hours, produced the (*E*)-tert-butyl(1,6-diphenylhex- 1-en-5-yn-3-yloxy)dimethylsilane **3a'**. Yellow oil, 322 mg, Yield 89%; IR (FT-IR): 2954, 2858, 1491, 1253, 1071, 835, 777, 754, 691 $cm^{-1}$; $^{1}H$ NMR (400 MHz, $CDCl_3$) δ 7.48-7.08 (m, 13H), 6.59 (d, *J* = 15.8 Hz, 1H), 6.29 (dd, *J* = 15.9, 6.0 Hz, 1H), 4.60-4.44 (m, 1H), 2.64 (qd, *J* = 16.5, 6.5 Hz, 2H), 0.91 (s, 9H), 0.09 (d, *J* = 13.1 Hz, 6H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 137.0, 132.0, 131.8, 130.0, 128.8, 128.4, 127.9, 127.7, 126.7, 124.0, 87.3, 82.4, 77.5, 77.2, 76.9, 72.6, 29.9, 26.1, 18.5, -4.2, -4.5; GC-MS (EI, 70 eV): m/z (%) = 305 (10), 248 (20), 247 (100), 231 (21), 73 (91).

**(*E*)-(3-methoxyhex-1-en-5-yne-1,6-diyl)dibenzene**[7]

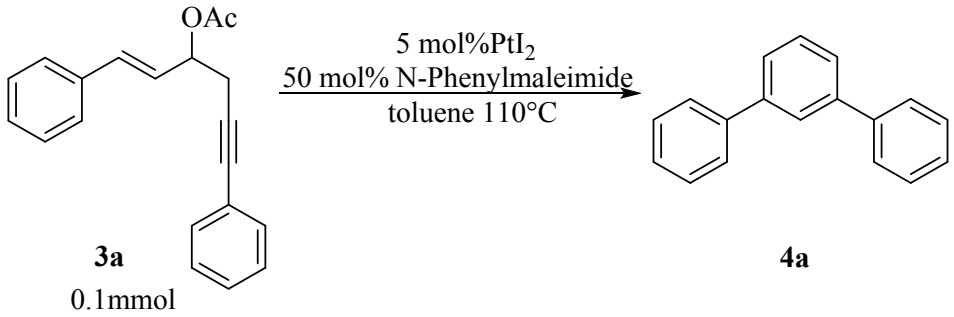



**3a''**

A 50 mL two necked round-bottomed flask was charged with a 60% dispersion of NaH (38 mg, 1.6 mmol) in paraffin oil, which was washed with hexane (5 mL x 2). To this was added THF (5mL) and the suspension was cooled to 0 °C. (*E*)-1, 6-diphenylhex-1-en-5-yn-3-ol (92 mg, 0.4 mmol) was added dropwise and the resulting solution was warmed up to room temperature. After being stirred for 1 h, 1-iodobutane (170 mg, 1.2 mmol) was added dropwise over a period of 5 min, and the mixture was stirred for 20 h. The solution was diluted with $Et_2O$ (20 mL) and washed with saturated $NH_4Cl$ aqueous solution (5 mL x 2). The aqueous solution was extracted with $Et_2O$ (10 mL x 2) and the combined organic layer was washed with saturated $NaHCO_3$ aqueous solution (5 mL) and brine (5 mL), and then dried over anhydrous sodium sulfate. The product was purified by silica gel column chromatography (hexane /ethyl acetate : 20/1) to give the desired product **3a''**. Yellow oil, 79 mg,

Yield 76%; IR (FT-IR): 3027, 2929, 2822, 1598, 1491, 1446, 1361, 1093, 968, 753, 692, 533 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.40-7.06 (m, 10H), 6.58 (d, *J* = 15.9 Hz, 1H), 6.12 (dd, *J* = 15.9, 7.7 Hz, 1H), 3.89 (dd, *J* = 13.6, 6.4 Hz, 1H), 3.31 (s, 3H), 2.69 (ddd, *J* = 23.4, 16.7, 6.2 Hz, 2H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 136.6, 133.3, 131.8, 128.8, 128.8, 128.3, 128.0, 127.9, 126.8, 123.9, 86.4, 82.5, 81.0, 77.5, 77.2, 76.9, 56.8, 26.9, 1.2; GC-MS (EI, 70 eV): m/z (%) = 229 (8), 148 (11), 147 (100), 116 (17), 115 (48), 91 (13).

## IV $PtI_2$ catalyzed 3-OAc-1-en-5-yne to synthesis of *m*-terphenyls and biphenyl derivatives

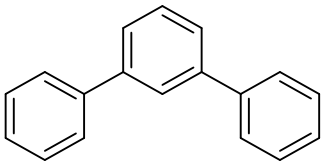



**3a**
0.1mmol

**4a**

Under the nitrogen atmosphere, $PtI_2$ (5 mol%, 2.2 mg) and N-Phenylmaleimide (50 mol%, 8.6 mg) were added to a solution of 3-OAc-1-en-5-yne **3a** (0.1 mmol, 29 mg) in anhydrous toluene (2 mL). The reaction mixture was stirred at 110 ºC until complete disappearance of **3a** observed by TLC. Solvent was removed under reduced pressure and the crude mixture was purified by flash chromatography on silica gel.

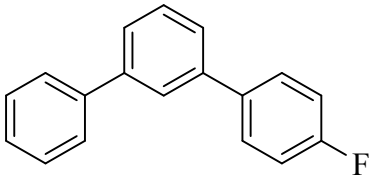
***m*-Terphenyl**



**4a**

White solid, 21 mg, Yield 92%; m.p. 83-84 $^oC$; IR (FT-IR): 3058, 2958, 1597, 1568, 1262, 1098, 801, 750, 699 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.67 (d, *J* = 7.6 Hz, 4H), 7.60 (dd, *J* = 6.9, 1.5 Hz, 2H), 7.53 (dd, *J* = 8.7, 6.5 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 4H), 7.39 (t, *J* = 7.3 Hz, 2H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 142.0, 141.4, 129.4, 129.0, 127.6, 127.5, 126.4, 126.3. GC-MS (EI, 70 eV): m/z (%) 231 (20), 230 (100) [$M^+$], 202 (6), 152 (3), 115 (1). Spectral data obtained for the compound are in agreement with the data reported.[8]

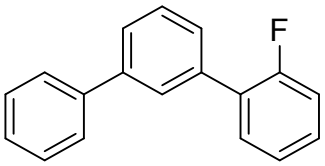
**4-fluoro-[1,1';3',1"] terphenyl**




**4b**

White solid, 22 mg, Yield 87%,. m.p. 85-86 $^{o}$C; IR (FT-IR): 3061, 1595, 1513, 886, 842, 797, 758, 700 cm$^{-1}$; $^{1}$H NMR (40 0 MHz, $CDCl_3$) δ 7.77 (d, *J* = 1.3 Hz, 1H), 7.70 -7.56 (m, 5H), 7.52 (ddd, *J* = 21.5, 10.9, 4.8 Hz, 4H), 7.43-7.36 (m, 1H), 7.21-7.12 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.0, 161.5, 142.1, 141.3, 141.0, 137.5, 129.5, 129.0, 129.0, 127.7, 127.5, 126.3, 126.2, 126.2, 116.0, 115.8, 1.2. GC-MS (EI, 70 eV): m/z (%) 249 (20), 248 (100) [$M^+$], 247 (9), 220 (3), 170 (1). Spectral data obtained for the compound are in agreement with the data reported.[9]

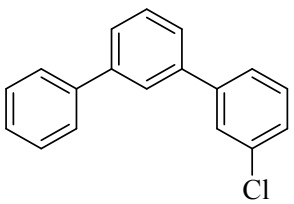
**2-fluoro-[1,1';3',1"] terphenyl**




**4c**

Colorless oil, 22 mg, Yield 87%; IR (FT-IR): 3060, 3032, 1599, 1496, 1473, 1406, 1210, 834, 802, 753, 730, 699 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 1.0 Hz, 1H), 7.74-7.64 ( m, 3H), 7.62-7.48 (m, 5H), 7.46-7.36 (m, 2H), 7.33-7.19 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.2, 158.8, 141.7, 141.2, 136.5, 131.0, 131.0, 129.3, 129.3, 129.1, 129.0, 128.2, 127.6, 127.5, 126.7, 124.6, 124.6, 116.5, 116.2; MS (EI, 70 eV): m/z (%) 250 (1), 249 (11), 248 (100), 247 (6), 226 (6), 149 (5); HR-MS (EI+) calculated for $C_{18}H_{13}F$ ($M^+$) 248.1001, found 248.1005.

**3-chloro-[1,1';3',1"] terphenyl**

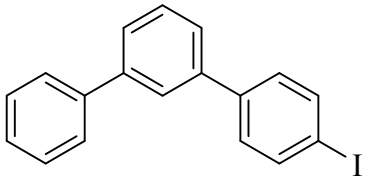



**4d**

Colorless oil, 40 mg, Yield 90%; IR (FT-IR): 3059, 3032, 1593, 1565, 1468, 1394, 1079, 880, 782, 756, 739, 696, 613 cm$^{-1}$; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 1.7 Hz, 1H), 7.69-7.64 (m, 3H), 7.62 (dt, *J* = 6.7, 1.9 Hz, 1H), 7.58-7.52 (m, 3H), 7.49 (dd, *J* = 10.3, 4.7 Hz, 2H), 7.43-7.33 (m, 3H);

$^{13}$C NMR (101 MHz, $CDCl_3$) δ 143.2, 142.2, 141.1, 140.6, 134.9, 130.2, 129.5, 129.0, 127.7, 127.6, 127.6, 127.5, 126.9, 126.3, 126.2, 125.6; MS (EI, 70 eV): m/z (%) 267 (4), 266 (21), 265 (12), 264 (100), 228 (17), 227 (7), 226 (10), 132 (4); HR-MS (EI+) calculated for $C_{18}H_{13}Cl$ ($M^+$) 264.0706, found 264.0709.

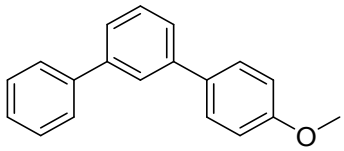
**4-iodo-[1,1';3',1"] terphenyl**




**4e**

White solid, 30 mg, Yield 80%; m.p. 96-100 $^o$C; IR (FT-IR): 3077, 2920, 1582, 1492, 827, 794, 757, 697, 515 cm$^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.85-7.76 (m, 3H), 7.69-7.63 (m, 2H), 7.63-7.58 (m, 1H), 7.57-7.45 (m, 4H), 7.40 (dt, *J* = 7.1, 1.8 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.2, 141.1, 140.8, 140.8, 138.1, 129.5, 129.3, 129.0, 127.7, 127.4, 126.7, 126.0, 126.0, 93.4; MS (EI, 70 eV): m/z (%) 358 (1), 357 (14), 356 (100), 230 (3), 229 (7), 228 (19), 227 (8), 226 (9), 202 (5), 178 (3); HR-MS (EI+) calculated for $C_{18}H_{13}I$ ($M^+$) 356.0062, found 356.0068.

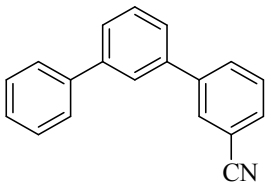
**4-methoxy-[1,1';3',1"] terphenyl**




**4f**

White solid, 24 mg, Yield 89%; m.p. 128-130 $^o$C; IR (FT-IR): 2955, 1605, 1495, 1246, 836, 796, 760, 697 cm$^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.66 (d, *J* = 7.5 Hz, 2H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.51 (ddd, *J* = 18.7, 11.2, 4.8 Hz, 5H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 8.7 Hz, 2H), 3.87 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.4, 141.9, 141.5, 141.5, 133.9, 129.3, 129.0, 128.5, 127.6, 127.5, 125.9, 125.9, 125.8, 114.4, 55.6; GC-MS (EI, 70 eV): m/z (%) 261 (22), 260 (100) [$M^+$], 245 (40), 217 (28), 215 (13), 189 (4), 151 (1). Spectral data obtained for the compound are in agreement with the data reported.[10]

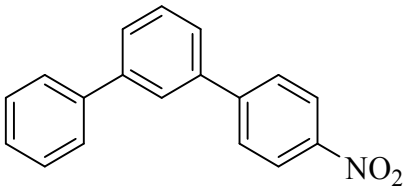
**[1,1';3',1"] terphenyl-3-carbonitrile**




**4g**

Colorless oil, 18 mg, Yield 69%; IR (FT-IR): 3059, 2229, 1597, 1472, 889, 793, 756, 699 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.68 (s, 1H), 7.61-7.53 (m, 4H), 7.53-7.44 (m, 3H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 142.5, 140.9, 139.6, 131.8, 131.0, 131.0, 129.8, 129.8, 129.1, 127.9, 127.4, 126.2, 126.2, 119.0, 113.2; MS (EI, 70 eV): m/z (%) 257 (2), 256 (16), 255 (100), 254 (12), 253 (7), 227 (4), 226 (5), 152 (2); HR-MS (EI+) calculated for $C_{19}H_{13}N(M^+)$ 255.1048, found 255.1052.

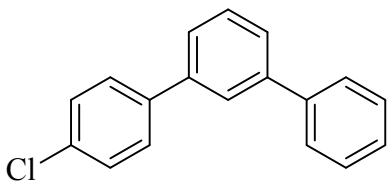
**4-nitro-[1,1';3',1"] terphenyl**




**4h**

White solid, 21 mg, Yield 75%; m.p. 78-79 °C; IR (FT-IR): 2917, 1594, 1513, 1344, 853, 798, 746, 697 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.37-8.29 (m, 2H), 7.80 (ddd, *J* = 9.4, 4.7, 2.0 Hz, 3H), 7.67 (ddd, *J* = 11.9, 6.0, 4.5 Hz, 3H), 7.63-7.54 (m, 2H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 147.8, 147.3, 142.5, 140.8, 139.5, 129.8, 129.1, 128.1, 128.0, 127.9, 127.4, 126.5, 126.4, 124.3; GC-MS (EI, 70 eV): m/z (%) 276 (20), 275 (100) [$M^+$], 245 (23), 228 (26), 202 (13), 152 (3), 113 (2). Spectral data obtained for the compound are in agreement with the data reported.[11]

**4-chloro-[1,1';3',1"] terphenyl**

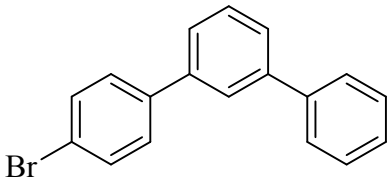



**4i**

White solid, 22 mg, Yield 82%; m.p. 70-71 °C; IR (FT-IR): 3060, 2924, 1595, 1494, 837, 795, 757, 698, 521 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 1.5 Hz, 1H), 7.66-7.61 (m, 2H), 7.61-7.55

(m, 3H), 7.53 (dt, *J* = 8.5, 4.3 Hz, 2H), 7.44 (tt, *J* = 9.1, 2.1 Hz, 4H), 7.37 (dd, *J* = 8.3, 6.4 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ = 142.2, 141.2, 140.7, 139.8, 133.7, 129.5, 129.2, 129.0, 128.7, 127.7, 127.5, 126.7, 126.2, 126.1, 77.5, 77.2, 76.9; MS (EI, 70 eV): m/z (%) 267 (4), 266 (23), 265 (14), 264 (100), 229 (8), 228 (20), 227 (8), 226 (11), 202 (5), 152 (4), 132 (4), 113 (4); HR-MS (EI+) calculated for $C_{18}H_{13}Cl$ ($M^+$)264.0706, found 264.0709.

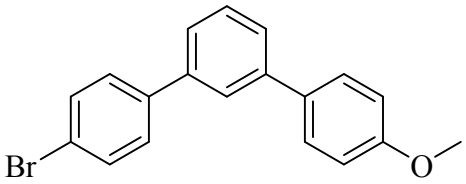
**4-bromo-[1,1';3',1"] terphenyl**




**4j**

White solid, 32 mg, Yield 93%; m.p. 85-86 °C; IR (FT-IR): 3055, 1657, 1561, 1491, 831, 795, 698 $cm^{-1}$; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 1.3 Hz, 1H), 7.67-7.62 (m, 2H), 7.60 (dq, *J* = 8.7, 2.1 Hz, 3H), 7.56-7.50 (m, 4H), 7.48 (dd, *J* = 10.3, 4.8 Hz, 2H), 7.39 (ddd, *J* = 7.3, 3.8, 1.1 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 142.2, 141.2, 140.7, 140.3, 132.1, 129.5, 129.0, 127.7, 127.5, 126.7, 126.1, 126.1, 121.9; MS (EI, 70 eV): m/z (%) 312 (1), 311 (14), 310 (92), 309 (15), 308 (100), 228 (32), 227 (15), 226 (20), 202 (9), 152 (6), 113(7); HR-MS (EI+) calculated for $C_{18}H_{13}{}^{79}Br$ ($M^+$) 308.0201, found 308.0205.

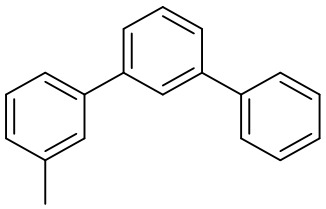
**4"-bromo-4-methoxyl-[1,1';3',1"] terphenyl**




**4k**

10 mol% $PtI_2$ without additive; White solid, 47 mg, Yield 76%; m.p. 138-140 °C; IR (FT-IR): 2924, 1606, 1515, 1033, 833, 789, 694 $cm^{-1}$; $^1$H NMR (600 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.60-7.56 (m, 4H), 7.56-7.53 (m, 1H), 7.51 (dd, *J* = 8.6, 1.9 Hz, 2H), 7.49 (d, *J* = 5.0 Hz, 2H), 7.02-6.98 (m, 2H), 3.87 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 159.5, 141.8, 140.7, 140.4, 133.7, 132.1, 129.5, 129.0, 128.5, 126.3, 125.7, 125.5, 121.8, 114.5, 55.6; MS (EI, 70 eV): m/z (%) 342 (2), 341 (14), 340 (93), 338 (100), 325 (22), 323(22), 297 (15), 295 (15), 216 (10), 216 (37), 213 (8), 189 (8), 170 (5); HR-MS (EI+) calculated for $C_{19}H_{15}{}^{79}BrO$ ($M^+$) 338.0306, found 338.0310

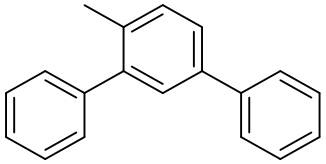
**3-methyl-[1,1';3',1"] terphenyl**



**4l**

Colorless oil, 21 mg, Yield 84%; IR (FT-IR): 3031, 2920, 1599, 1474, 1093, 1022, 893, 784, 755, 699, 629 $cm^{-1}$; $^{1}H$ NMR (400 MHz, $CDCl_3$) δ 7.84 (t, *J* = 1.6 Hz, 1H), 7.69 (dd, *J* = 5.1, 3.4 Hz, 2H), 7.60 (dd, *J* = 6.8, 1.5 Hz, 2H), 7.57-7.45 (m, 5H), 7.44-7.35 (m, 2H), 7.22 (d, *J* = 7.5 Hz, 1H), 2.47 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 142.1, 141.9, 141.4, 141.4, 138.6, 129.3, 129.0, 128.9, 128.3, 128.3, 127.6, 127.5, 126.4, 126.3, 126.2, 124.6, 21.8; MS (EI, 70 eV): m/z (%) 246 (1), 245 (15), 244 (100), 243 (8), 229 (5), 228 (11), 202 (3), 165(6), 152 (2); HR-MS (EI+) calculated for $C_{19}H_{16}$ ($M^+$) 244.1252, found 244.1256.

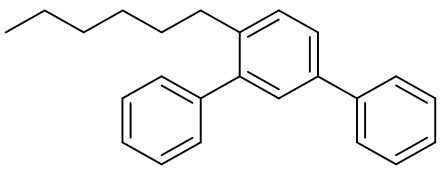
**4'-methyl-[1,1';3',1"] terphenyl**



**4m**

Colorless oil, 25 mg, Yield 97%; IR (FT-IR): 3057, 3026, 1600, 1479, 1442, 825, 759, 698, 585 $cm^{-1}$; $^{1}H$ NMR (400 MHz, $CDCl_3$) δ 7.68-7.62 (m, 2H), 7.57-7.51 (m, 2H), 7.50-7.32 (m, 9H), 2.35 (s, 3H); $^{3}C$ NMR (101 MHz, $CDCl_3$) δ 142.5, 134.7, 131.0, 129.4, 128.9, 128.8, 128.3, 128.3, 127.3, 127.2, 127.1, 126.0, 20.3; MS (EI, 70 eV): m/z (%) 246 (1), 245 (15), 244 (100), 243 (22), 239 (5), 239 (5), 229 (13), 228 (13), 165 (16), 152 (3), 115 (3); HR-MS (EI+) calculated for $C_{19}H_{16}$ ($M^+$) 244.1252, found 244.1256.

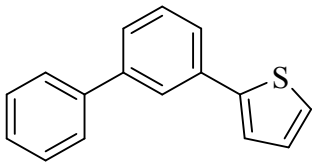
**4'-hexyl-[1,1';3',1"] terphenyl**



**4n**

Colorless oil, 32 mg, Yield 92%; IR (FT-IR): 3058, 3027, 2926, 2856, 1600, 1479, 1378, 1073, 895, 829, 760, 700 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.69-7.61 (m, 2H), 7.57 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.51-7.42 (m, 5H), 7.42-7.31 (m, 5H), 2.72 -2.53 (m, 2H), 1.58-1.44 (m, 2H), 1.29-1.12 (m, 6H), 0.86 (t, *J* = 6.9 Hz, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 142.4, 142.1, 141.0, 139.8, 138.6, 129.9, 129.5, 128.9, 128.9, 128.2, 127.3, 127.2, 127.0, 126.1, 32.9, 31.7, 31.5, 29.3, 22.7, 14.3; MS (EI, 70 eV): m/z (%) 315 (6), 314 (28), 244 (15), 243 (100), 242 (5), 241 (10), 228 (10), 215 (4), 202 (3), 165 (12); HR-MS (EI+) calculated for $C_{24}H_{26}$ ($M^+$) 314.2035, found 314.2039.

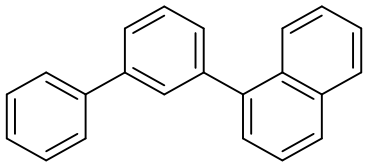
**2-(biphenyl-3-yl)thiophene**




**4p**

White solid, 15 mg, Yield 56%; m.p. 67-68 °C; IR (FT-IR): 3059, 1595, 1571, 797, 770, 696 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 1.5 Hz, 1H), 7.63 (ddd, *J* = 10.3, 7.9, 1.3 Hz, 3H), 7.55-7.44 (m, 4H), 7.43-7.36 (m, 2H), 7.32 (dd, *J* = 5.1, 0.9 Hz, 1H), 7.12 (dd, *J* = 5.0, 3.6 Hz, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 144.5, 142.2, 141.1, 135.1, 129.5, 129.0, 128.2, 127.7, 127.4, 126.6, 125.2, 125.1, 125.1, 123.5; MS (EI, 70 eV): m/z (%) 238 (3), 237 (10), 236 (100), 235 (5), 234 (6), 203 (3), 202 (7), 191 (3), 189 (5), 165 (2), 149 (2); HR-MS (EI+) calculated for $C_{16}H_{12}S$ ($M^+$) 236.0660, found 236.0664.

**1-(biphenyl-3-yl)naphthalene**

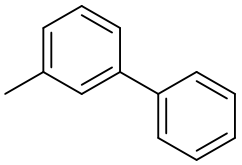


**4q**

White solid, 26 mg, Yield 87%; IR (FT-IR): 3057, 2923, 1595, 1479, 1392, 1019, 799, 779, 755, 704, 613 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.3 Hz, 1H), 7.93 (dd, *J* = 15.7, 8.1 Hz, 2H), 7.78 (s, 1H), 7.75-7.66 (m, 3H), 7.64-7.44 (m, 8H), 7.39 (t, *J* = 6.9 Hz, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 141.4, 141.4, 141.2, 140.3, 134.0, 131.8, 129.2, 129.1, 129.0, 128.9, 128.5, 128.0, 127.6, 127.4, 127.2, 126.3, 126.2, 126.0, 125.6; MS (EI, 70 eV): m/z (%) 281 (14), 280 (100), 279 (35), 276

(10), 252 (5), 228 (10), 203 (10), 202 (11), 191(4), 138(3); HR-MS (EI+) calculated for $C_{22}H_{16}$ ($M^+$) 280.1252, found 280.1255.

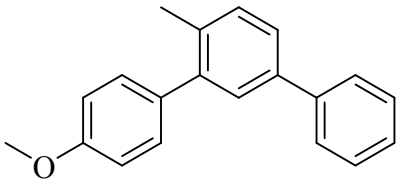
**3-methylbiphenyl**



**4r**

Colorless oil, 17 mg, Yield 79 %; IR (FT-IR): 3031, 2921, 1603, 1482, 1075, 791, 753, 698 $cm^{-1}$; $^1H$ NMR (400 MHz, CDCl3) δ 7.6-7.58 (m, 2H), 7.50-7.40 (m, 4H), 7.40-7.33 (m, 2H), 7.19 (d, J = 7.3 Hz, 1H), 2.45 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ = 141.4, 141.3, 138.4, 128.7, 128.0, 127.2, 124.3, 21.6. GC-MS (EI, 70 eV): m/z (%) = 169 (14), 168 (100) [$M^+$], 167 (67), 165 (20), 153 (22). Spectral data obtained for the compound are in agreement with the data reported.[12]

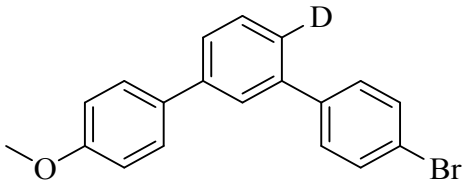
**6'-methyl-4-methoxyl-[1,1';3',1''] terphenyl**




**4s**

Colorless oil, 24 mg, Yield 91%; IR (FT-IR): 3030, 2925, 1609, 1514, 1481, 1245, 1176, 1030, 832, 761, 698, 576 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.3 Hz, 2H), 7.52 (d, *J* = 6.3 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 4H), 7.01 (d, *J* = 7.5 Hz, 2H), 3.89 (s, 3H), 2.35 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 158.8, 142.1, 141.1, 138.9, 134.8, 134.4, 131.0, 130.5, 128.9, 128.9, 127.3, 127.2, 125.8, 113.7, 55.5, 20.4; GC-MS (EI, 70 eV): m/z (%) 276 (1), 275 (13), 274 (100), 273 (4), 259 (10), 241 (5), 228 (4), 216 (6), 215 (12), 202 (5), 165 (5); HR-MS (EI+) calculated for $C_{20}H_{18}O$ ($M^+$) 274.1358, found 274.1362.

**4''-bromo-4'-deuterium-4-methoxyl-[1,1';3',1''] terphenyl**

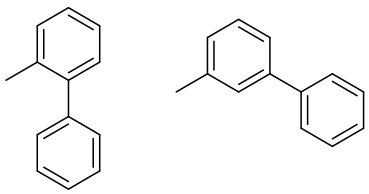



**4t**

10 mol% $PtI_2$ without additive; White solid, 48 mg, Yield 78%; m.p. 141-142 °C; IR (FT-IR): 2927,

1606, 1513, 1033, 913, 830, 744 $cm^{-1}$; $^1H$ NMR (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 1.7 Hz, 1H), 7.60-7.53 (m, 5H), 7.50 (dd, *J* = 11.9, 8.0 Hz, 3H), 7.00 (d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 159.5, 141.7, 140.6, 140.3, 133.6, 132.1, 129.4, 129.0, 128.5, 126.3, 125.6, 121.8, 114.5, 55.6; MS (EI, 70 eV): m/z (%) 343 (2), 342 (14), 341 (96), 339 (100), 326 (23), 324 (22), 298 (14), 296 (15), 217 (9), 216 (32), 202 (9), 190 (7); HR-MS (EI+) calculated for $C_{19}H_{14}{}^2HO^{79}Br$ ($M^+$) 339.0369, found 339.0365.

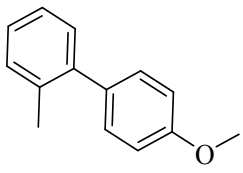
**A mixture of 2-methylbiphenyl and 3-methylbiphenyl**



**4u (left) / 4r (right) = 10/1**

Colorless oil, 10 mg, Total yield 57%; IR (FT-IR): 3060, 3022, 2924, 2853, 1600, 1479, 1380, 1010, 774, 748, 725, 701 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.3 Hz, 0H), 7.46 (dd, *J* = 8.5, 6.5 Hz, 3H), 7.39 (td, *J* = 6.4, 1.7 Hz, 3H), 7.35-7.27 (m, 4H), 2.47 (s, 0H), 2.33 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 142.1, 142.1, 130.5, 130.0, 129.4, 128.2, 127.4, 126.9, 126.0, 20.7; GC-MS (EI, 70 eV): $t_{R\ major}$ = 6.1 min, m/z (%) 169 (14), 168 (100) [$M^+$], 167 (84), 165 (25), 153 (36), $t_{R\ minor}$ = 6.8 min, m/z (%) 169 (14), 168 (100) [$M^+$], 167 (67), 165 (24), 153 (23); Spectral data obtained for the compound are in agreement with the data reported.[12]

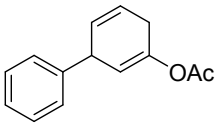
**4'-methoxy-2-methylbiphenyl**




**4v**

Colorless oil, 20 mg, Yield 90%; IR (FT-IR): 2926, 2835, 1612, 1515, 1484, 1243, 1177, 1039, 834, 761, 731 $cm^{-1}$; $^1H$ NMR (400 MHz, Chloroform-*d*) δ 7.16 (dd, *J* = 10.5, 4.9 Hz, 6H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.77 (s, 3H), 2.20 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 158.5, 141.6, 135.5, 134.4, 130.3, 130.3, 129.9, 127.0, 125.8, 113.5, 77.4, 77.1, 76.7, 55.3, 20.6; GC-MS (EI, 70 eV): m/z (%) 199 (16), 198 (100) [$M^+$], 183 (15), 167 (18), 155 (14), 115 (2). Spectral data obtained for the compound are in agreement with the data reported.[13]

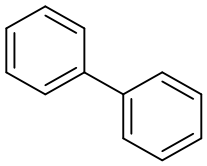
**3-phenylcyclohexa-1,4-dienyl acetate**




**2**

Colorless oil, 6 mg, Yield 13%; IR (FT-IR): 2829, 1757, 1698, 1457, 1362, 1218, 1122 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.36-7.18 (m, 6H), 5.78-5.67 (m, 2H), 5.46 (dd, *J* = 3.6, 1.5 Hz, 1H), 4.24-4.16 (m, 1H), 3.00-2.84 (m, 2H), 2.15 (s, 3H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 168.3, 144.9, 142.8, 127.6, 127.2, 126.9, 125.6, 120.8, 114.80, 42.4, 26.7, 20.0. Spectral data obtained for the compound are in agreement with the data reported.[5]

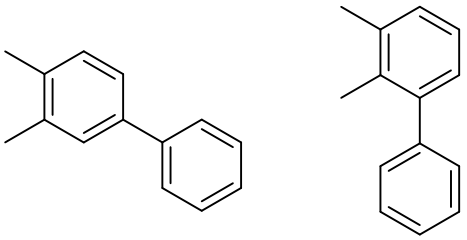
**Biphenyl**



**4x**

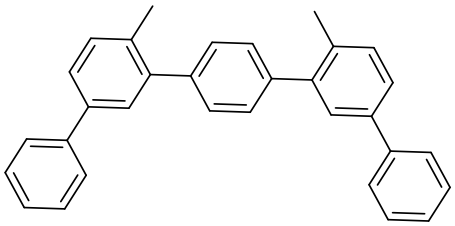
White solid, 2 mg, Yield 6%, m.p 68-69; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.64-7.56 (m, 4H), 7.50-7.41 (m, 4H), 7.40-7.31 (m, 2H). GC-MS (EI, 70 eV): m/z (%) 155 (13), 154 (100), 153 (39), 152 (32), 128 (2), 76 (2). Spectral data obtained for the compound are in agreement with the data reported.[12]

**A mixture of 3,4-dimethylbiphenyl and 2,3-dimethylbiphenyl**



**4w (left) / 4w' (right) ≈ 1/1.2**

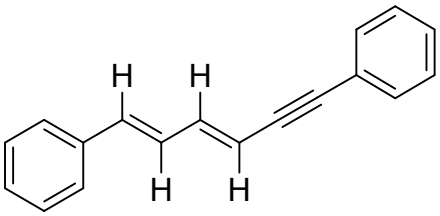
Colorless oil, 30mg, Total yield 81%; IR (FT-IR): 3025, 2923, 2856, 1602, 1486, 1466, 759, 700 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.52, 7.52, 7.50, 7.50, 7.36, 7.36, 7.35, 7.35, 7.33, 7.31, 7.28, 7.27, 7.26, 7.24, 7.24, 7.22, 7.16, 7.14, 7.12, 7.09, 7.07, 7.05, 7.03, 7.01, 7.01, 2.27, 2.26, 2.24, 2.09; $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 142.6, 142.3, 141.3, 138.9, 137.2, 136.9, 135.7, 134.0, 130.1, 129.4, 128.9, 128.7, 128.5, 128.0, 127.7, 127.0, 126.9, 126.6, 125.3, 124.5, 20.8, 20.0, 19.5, 17.0; GC-MS (EI, 70 eV): m/z (%) 183 (13) 182 (100) [$M^+$], 167 (77), 152 (11), 115 (2). Spectral data obtained for the compound are in agreement with the data reported.[14]

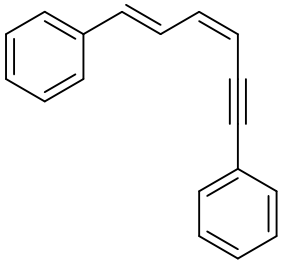


**4y**

White solid, 26 mg, Yield 66%; m.p. 203-205 °C; IR (FT-IR): 3026，2963，2921，1595，802，757，696 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.53 (m, 4H), 7.48 (d, *J* = 1.8 Hz, 2H), 7.44 (dd, *J* = 7.8, 1.9 Hz, 2H), 7.40 – 7.31 (m, 8H), 7.27 (dd, *J* = 12.5, 7.6 Hz, 5H), 2.30 (s, 6H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ = 142.0, 140.9, 140.5, 138.8, 134.6, 130.9, 129.0, 128.8, 128.7, 127.2, 127.1, 125.9, 20.3, 1.1; MS (EI, 70 eV): m/z (%) = 412 (5), 411 (29), 410 (100), 334 (13), 319 (5), 241 (9), 205 (6), 165 (9), 91 (8); HR-MS (EI+) calculated for $C_{32}H_{26}$ ($M^+$) 410.2035, found 410.2030.

**A mixture of (*1E,3E*)/ (*1E,3Z*)-hexa-1,3-dien-5-yne-1,6-diyldibenzene 5 and 6**



***trans*-5** ***cis*-6**

Under the protection of nitrogen, $FeCl_3 \cdot 6H_2O$ (50 mol %, 21.5 mg) was added to a solution of 3-OAc-1-en-5-yne **3a** (0.16 mmol, 47 mg) in anhydrous toluene (3 mL). The reaction mixture was stirred at 30 ºC until complete disappearance of **3a** was observed by TLC. Solvent was removed under reduced pressure and the crude mixture was purified by flash chromatography on silica gel. Yellow oil, Mixture, 37 mg, total yield 48%; $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.51-7.11 (m, 19H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.93 (dq, *J* = 5.9, 3.0 Hz, 2H), 6.80-6.70 (m, 1H), 6.63 (d, *J* = 15.7 Hz, 1H), 6.59 – 6.55 (m, 1H), 6.54-6.45 (m, 1H), 5.88-5.79 (m, 1H), 5.62 (d, *J* = 10.6 Hz, 1H); $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 109.3, 111.4, 126.2, 126.7, 126.9, 127.6, 128.0, 128.1, 128.1, 128.2, 128.3, 128.3, 128.4, 128.4, 128.6, 128.8, 131.5, 134.8, 135.0, 135.5, 140.0, 141.9; MS (EI, 70 eV): m/z (%) 231 (12), 230 (74) [$M^+$], 229 (100), 215 (50), 202 (17).[15]

## V The X-ray structure of compound 4a

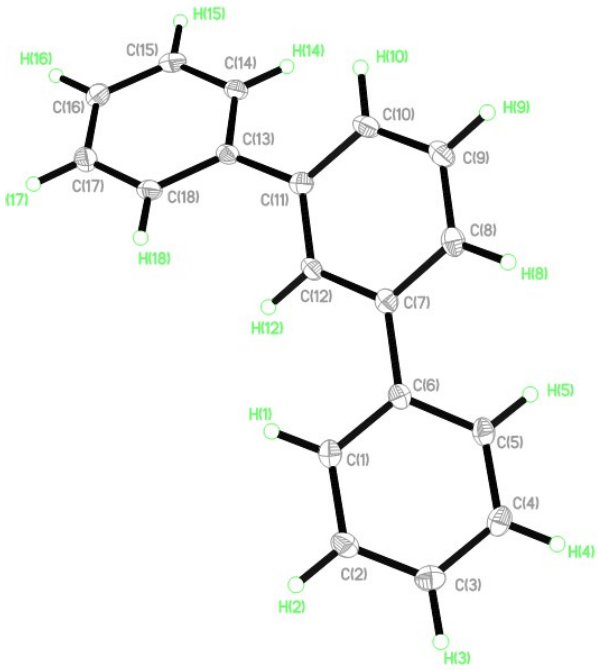



**Table S2.** Crystal data and structure refinement for **4a**.

| | | |
|---|---|---|
| Identification code | **4a** | |
| Empirical formula | C18 H14 | |
| Formula weight | 230.29 | |
| Temperature | 113(2) K | |
| Wavelength | 0.71073 A | |
| Crystal system, space group | Triclinic, P-1 | |
| Unit cell dimensions | a = 6.84(2) A | alpha = 89.97(10) deg. |
| | b = 7.37(2) A | beta = 89.69(8) deg. |
| | c = 24.89(7) A | gamma = 89.72(7) deg. |
| Volume | 1255(6) A^3 | |
| Z, Calculated density | 4, 1.219 Mg/m^3 | |
| Absorption coefficient | 0.069 mm^-1 | |
| F(000) | 488 | |
| Crystal size | 0.20 x 0.18 x 0.12 mm | |

| | |
|---|---|
| Theta range for data collection | 1.64 to 25.02 deg. |
| Limiting indices | -8<=h<=8, -8<=k<=8, -29<=l<=29 |
| Reflections collected / unique | 10505 / 4369 [R(int) = 0.0808] |
| Completeness to theta = 25.02 | 99.0 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.9918 and 0.9864 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4369 / 0 / 325 |
| Goodness-of-fit on F^2 | 0.818 |
| Final R indices [I>2sigma(I)] | R1 = 0.0411, wR2 = 0.0752 |
| R indices (all data) | R1 = 0.0781, wR2 = 0.0827 |
| Largest diff. peak and hole | 0.183 and -0.212 e.A^-3 |

---

## *VI References*


(1) Zhang, Y.; Zhang, H.; Liu, L. Y.; Wang, X.; Chang, W. X.; Li, J. *Chem. J. Chin. U.* **2012**, *33*, 2447.

(2) Nag, S.; Lehmann, L.; Kettschau, G.; Toth, M.; Heinrich, T.; Thiele, A.; Varrone, A.; Halldin, C. *Bioorg. Med. Chem.* **2013**, *21*, 6634.

(3) Wang, X.; Liu, L.; Chang, W.; Li, J. *Eur. J. Org. Chem.* **2010**, *2010*, 5391.

(4) Dobbs, A. P.; Guesne, S. J. J.; Parker, R. J.; Skidmore, J.; Stephenson, R. A.; Hursthouse, M. B. *Org. & Biomol. Chem.* **2010**, *8*, 1064.

(5) Wang, S. Z.; Zhang, L. M. *J. Am. Chem. Soc.* **2006**, *128*, 14274.

(6) Corey, E. J.; Venkateswarlu, A. *J. Am. Chem. Soc.* **1972**, *94*, 6190.

(7) Tsuchimoto, T.; Matsubayashi, H.; Kaneko, M.; Shirakawa, E.; Kawakami, Y. *Angew. Chem. Int. Edit.* **2005**, *44*, 1336.

(8) Yoshikai, N.; Matsuda, H.; Nakamura, E. *J. Am. Chem. Soc.* **2009**, *131*, 9590.

(9) Miguez, J. M. A.; Adrio, L. A.; Sousa-Pedrares, A.; Vila, J. M.; Hii, K. K. *J. Org. Chem.* **2007**, *72*, 7771.

(10) Garcia-Garcia, P.; Fernandez-Rodriguez, M. A.; Aguilar, E. *Angew. Chem. Int. Edit.* **2009**, *48*, 5534.

(11) Beaumard, F.; Dauban, P.; Dodd, R. H. *Org. Lett.* **2009**, *11*, 1801.

(12) Sun, C. L.; Li, H.; Yu, D. G.; Yu, M. A.; Zhou, X. A.; Lu, X. Y.; Huang, K.; Zheng, S. F.; Li, B. J.; Shi, Z. J. *Nat. Chem.* **2010**, *2*, 1044.

(13) Denmark, S. E.; Smith, R. C.; Chang, W. T. T.; Muhuhi, J. M. *J. Am. Chem. Soc.* **2009**, *131*,

3104.
(14) Kawai, H.; Kobayashi, Y.; Oi, S.; Inoue, Y. *Chem. Commun*. **2008**, 1464.
(15) Zhu, Y.; Li, T. Y.; Qu, X. M.; Sun, P.; Yang, H. L.; Mao, J. C. *Org. & Biomol. Chem.* **2011**, *9*, 7309.

## VII Computational results for PtI2-Catalyzed Cyclization of 3-Acyloxy-1,5-Enynes

## Contents

# The Cartesian Coordinates of the stationary points discussed in the text and in the supporting information

**General remarks:**

All geometry optimizations, frequency and solvation energy calculations were performed with the B3LYP[1] functional in Gaussian 09.[2] All the transition states have been verified by IRC (intrinsic reaction coordinate)[3] calculations. The Stuttgart/Dresden effective core potential[4] was used on rhodium and iodine, and the 6-31G(d) basis set was employed for other atoms. Solvation free energy corrections in toluene solvent were computed on gas-phase optimized geometries by single point SMD calculations[5] at the B3LYP/6-311+G(d,p) level (SDD for Rh and I). Since dispersion interactions were expected to be essential in the regiochemical control in some reaction systems, Grimme's DFT-D3(BJ)[6] dispersion corrections were calculated using the DFTD3 program.[7] Single point dispersion energy corrections were calculated and added to the B3LYP Gibbs free energies in solution. Entropic contributions to the reported free energies were calculated from partition functions evaluated using Truhlar's quasiharmonic approximation.[8] Figures of three-dimensional molecular structures were prepared using CYLView.[9]

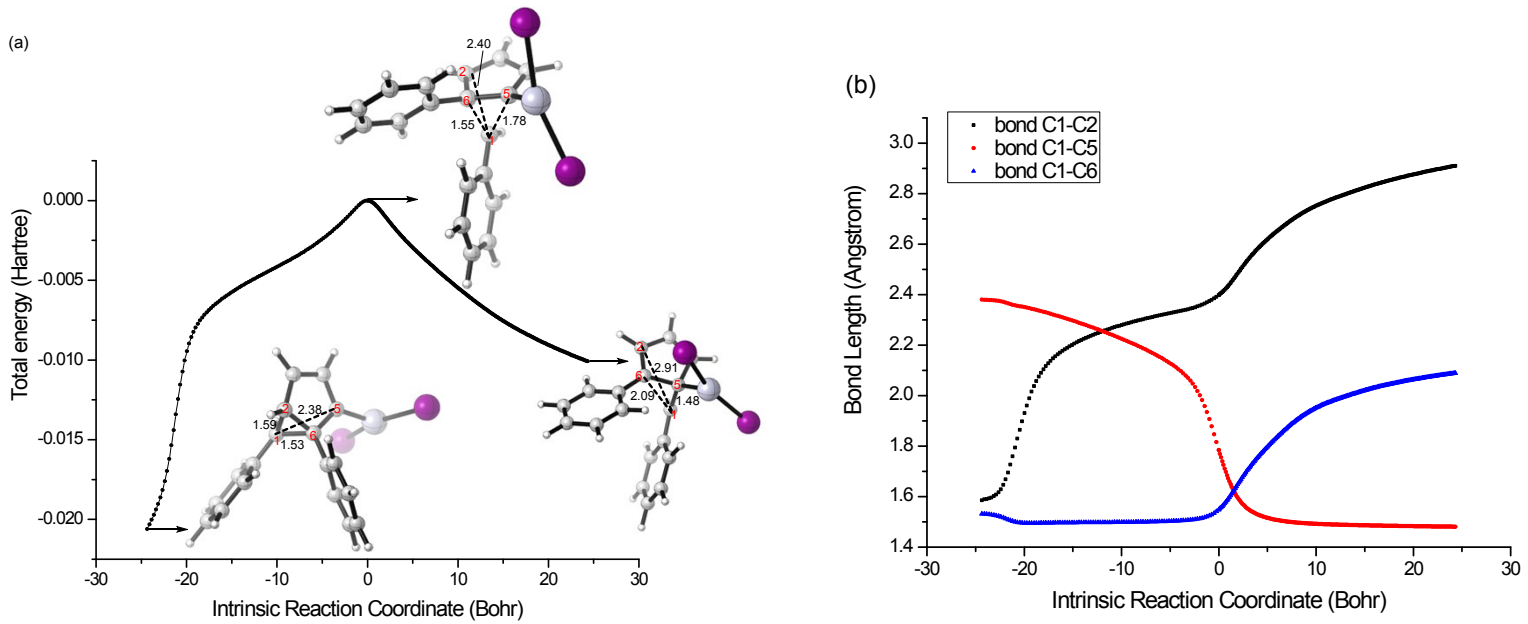
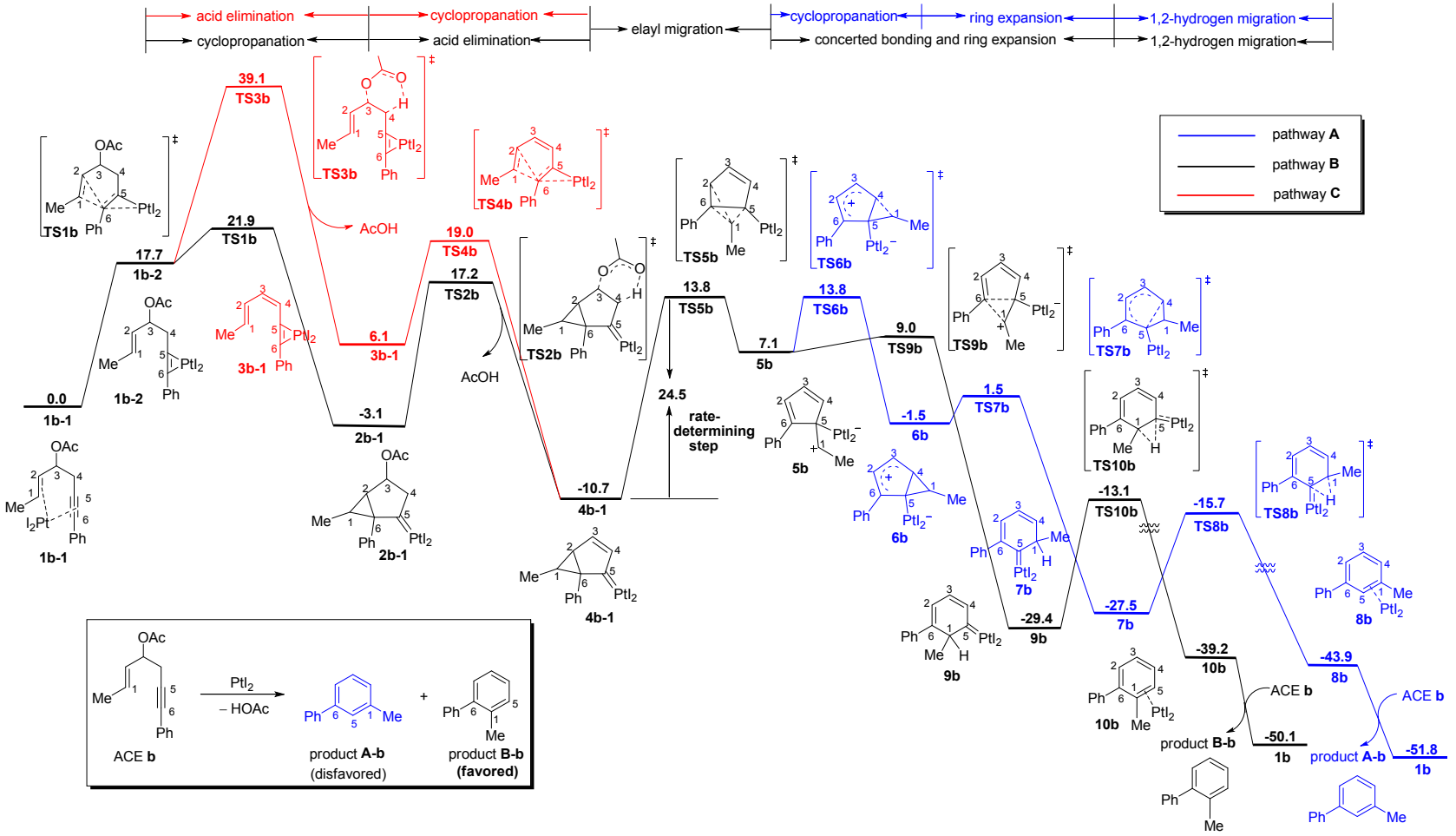



***Figure S2.*** Calculation result of IRC (intrinsic reaction coordinate) for **TS5a**. (a) Dependence of total energy on the intrinsic reaction coordinate. (b) Dependence of bond length of C1-C2, C1-C5 and C1-C6 on the intrinsic reaction coordinate.

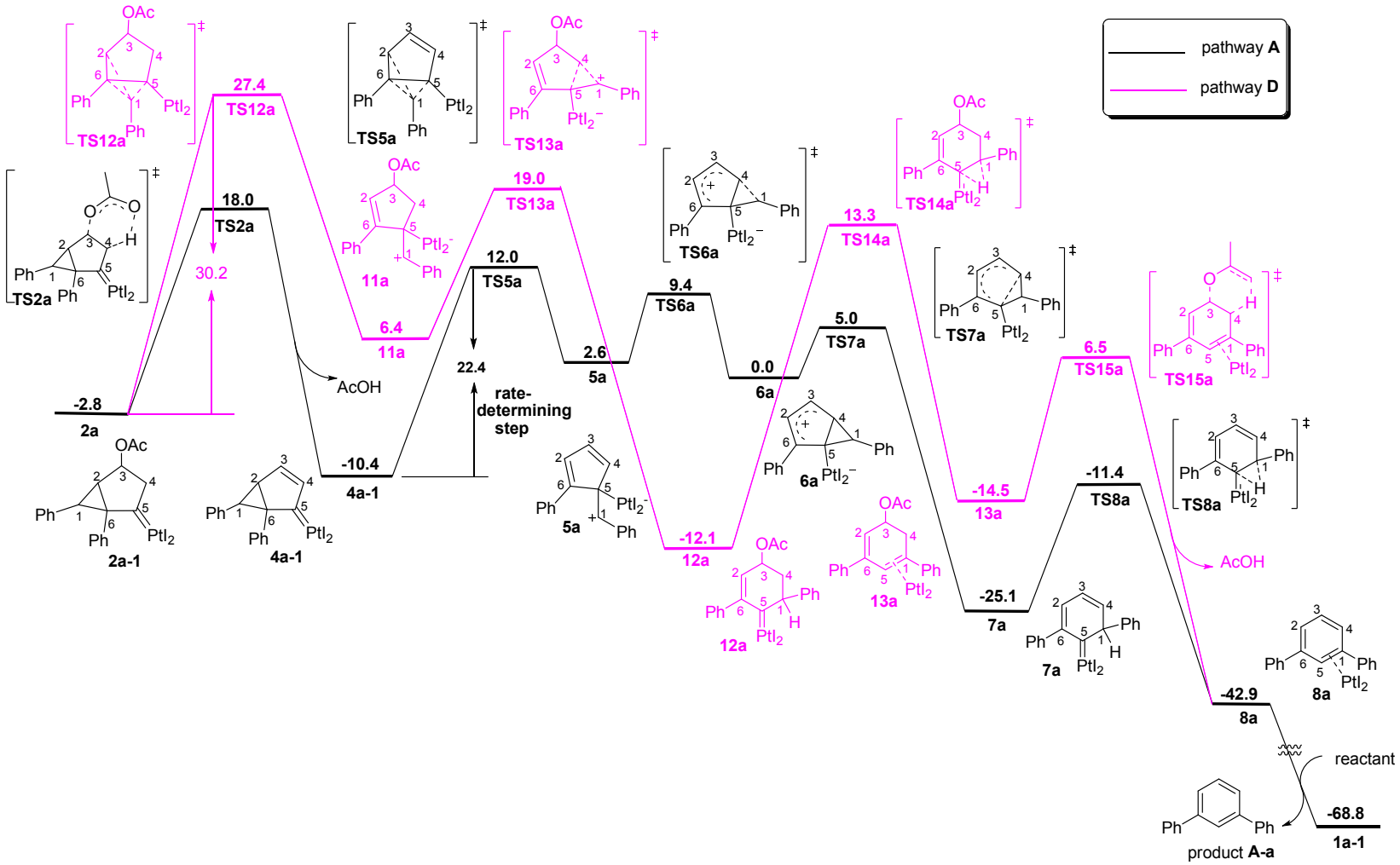
The calculation result of IRC (intrinsic reaction coordinate) confirms the connection of **TS5a** to the intermediates **4a** and **5a** on the energy profile in Figure S2.




***Scheme S2.*** Gibbs free energy profiles of the $PtI_2$-catalyzed cyclization of ACE **b**. Energies are in kcal/mol and calculated using B3LYP/SDD-6-311+G(d,p)/SMD(toluene)//B3LYP/SDD-6-31G(d)method with DFT-D3(BJ) dispersion correction.

The reaction initiates from the $PtI_2$-ACE π complex **1b-1**. The cyclopropanation of **1b-1** requires an overall activation free energy of 21.9 kcal/mol (from **1b-1** to **TS1b**). Next, acid elimination takes pace with an energy barrier of 20.3 kcal/mol (**TS2b**) to afford intermediate **4b-1**. We also considered pathway **C**, in which acid elimination occurs prior to cyclopropanation with a very high energy barrier of 39.1 kcal/mol (from **1b-1** to **TS3b**). Thus pathway **C** should be ruled out from the favored pathways. Then shift of elayl group from **4b-1** via transition state **TS5b** leads to the zwitterion-characterized intermediate **5b**. This step is the rate-determining step with an energy barrier of 24.5 kcal/mol, which is higher than that of each of the other steps in pathways **A** and **B**. Subsequent cyclopropanation and ring expansion take place from the intermediate **5b** via two distinct pathways: cyclopropanation by bonding between atom C1 and atom C4 forms the intermediate **6b**, which then isomerizes to carbene **7b** by ring expansion (pathway **A**, in blue line), or concerted bonding and ring expansion by simultaneous formation of C1-C6 bond and rupture of C6-C5 bond lead to carbene **9b** (pathway **B**, in black line). The computed activation barrier of bonding C1 to C4 (**TS6b**) is 4.8 kcal/mol higher than that for bonding C1 to C6 (**TS9b**), indicating the formation of carbene **9b** is kinetically favoured over the formation of carbene **7b**. Moreover, the computed potential energy profile indicates the formation of C1-C4 or C1-C6 bond to form carbene **7b** or **9b** is irreversible and thus is the regioselectivity-determining step. Thus the favored pathway (**B**) will lead to the major product, 2-methylbiphenyl. This prediction is consistent with the experimental observation. 1,2-hydrogen shift via **TS8b** leads to the formation of the product complex **8b**. The free energy barrier for this step is 11.8 kcal/mol. Ligands exchange of **8b** to release product **A-b**, the 3-methylbiphenyl, is highly exothermic. Similarly, 1,2-hydrogen shift via **TS10b** affords product complex **10b**, requiring 16.3 kcal/mol free energy of activation. Then the exchange of ligands produces product **B-b**, the 2-methylbiphenyl.

The above results indicated that, different from the case of ACE **a**, the preferred pathway for cyclization of ACE **b** is pathway **B** (black line), which involves cyclopropanation, acid elimination, elayl migration, concerted cyclopropanation and ring expansion (i.e. simultaneous formation of C1-C6 bond and rupture of C5-C6 bond) of the zwitterion-characterized intermediate, and 1,2-hydrogen shift to form the 2-methylbiphenyl product. The elayl migration is found to be the rate-determining step of the catalytic cycle. The concerted bonding and ring expansion of the zwitterion-characterized intermediate is the regioselectivity-determining step.




***Scheme S3.*** Gibbs free energy profile of pathway **D**, in which elimination of acetic acid takes place at the last aromatization step of the $PtI_2$-catalyzed cyclization of ACE **a**. For comparison, the Gibbs free energy profile of the most favored pathway (pathway **A**) is also shown.

We have also considered another possible pathway, pathway **D**, that leads to the major product *m*-terphenyl. In pathway **D**, elimination of acetic acid takes place at the last aromatization step. The energy barrier of the rate-determining benzal migration of pathway **D** is 30.2 kcal/mol, and much higher than that of the rate-determining step of pathway **A**. Thus, Pathway **D** should be ruled out from the favored pathway. This result also implies that elimination of acetic acid should take place at an early stage (**TS2a** in pathway **A**) instead of the last aromatization step.

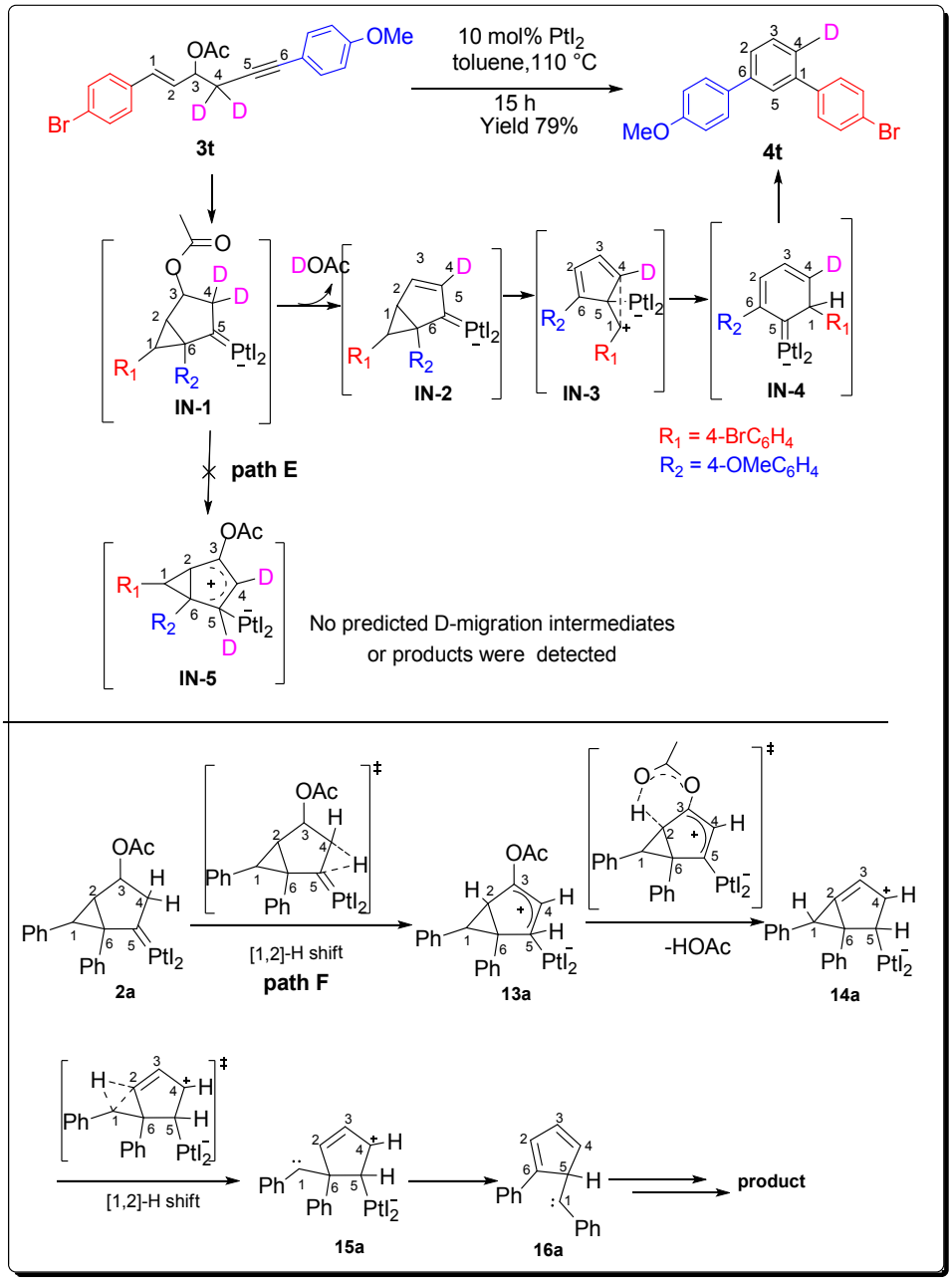
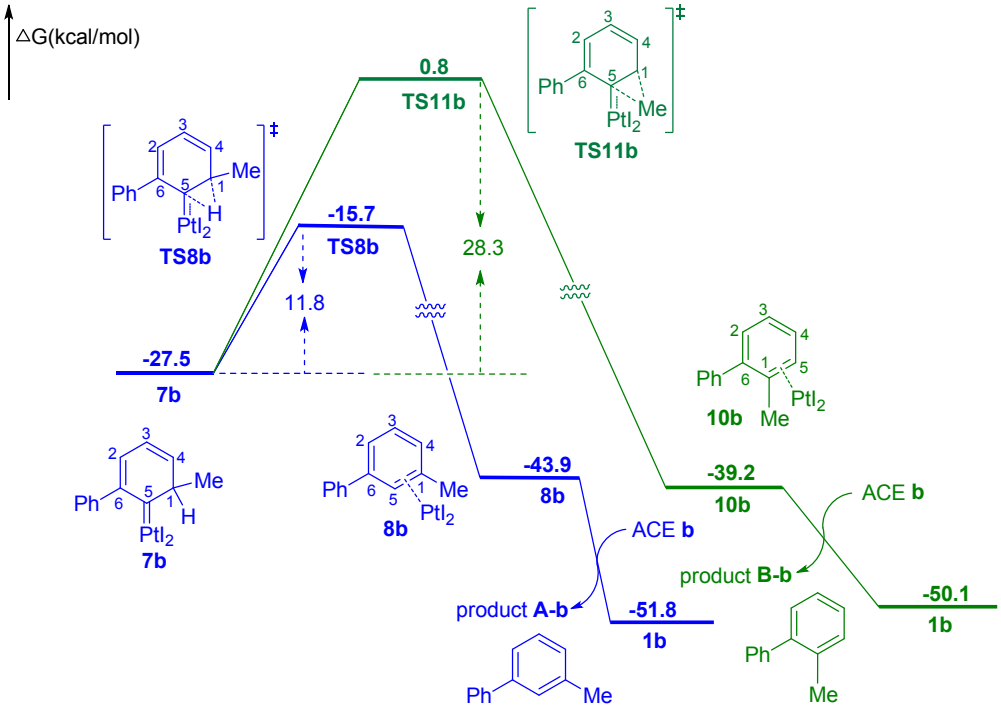


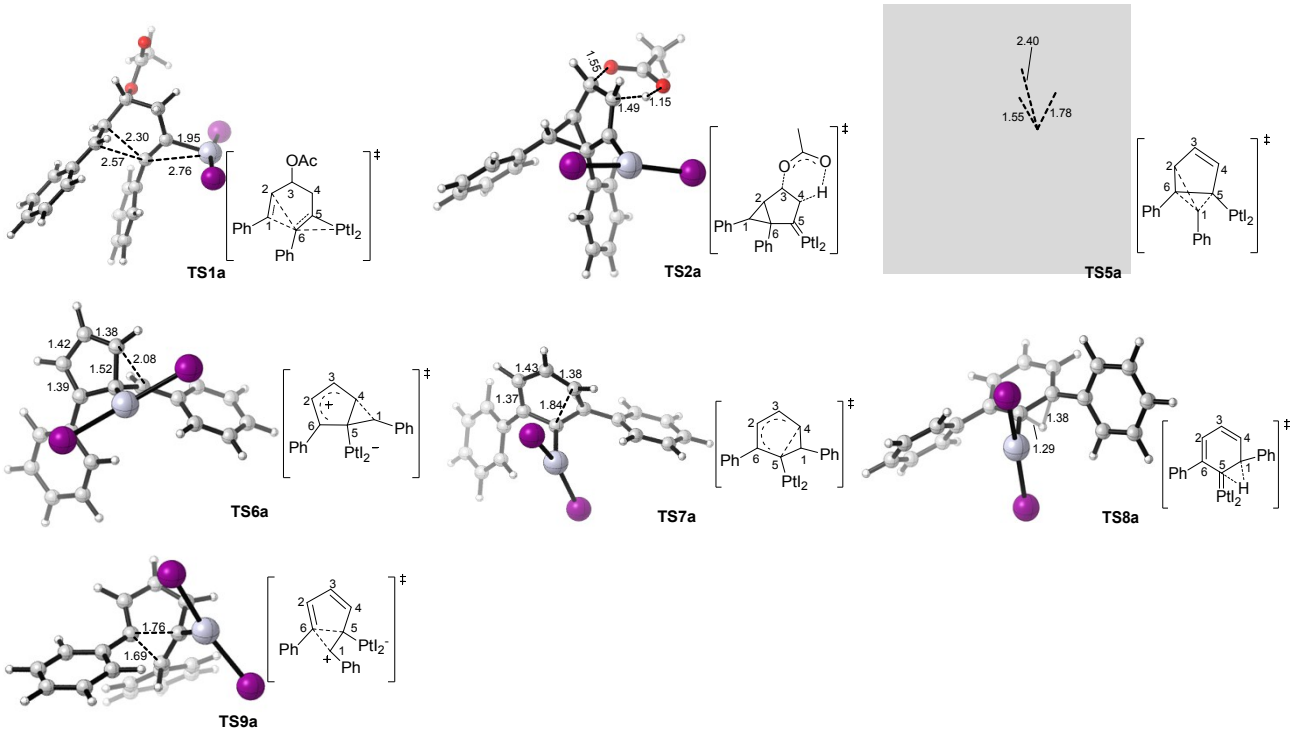

**Figure S3**. Other possible pathways **E** and **F** that involves one [1,2]-*H* shift prior to acid elimination.

Actually, we had considered other possible 1,2-*H* migration (Path E and F in Figure S3). And we designed the deuterated labeling experiment using **3t** as substrate. It was found that only one deuterium atom exists in the newly formed central benzene ring that is adjacent to the *p*-bromophenyl group in the *m*-terphenyls **4t**. This experiment indicated that the elimination of DOAc and the following benzyl carbon cation migration occurred instead of the D-migration predicted. Moreover, from the deuterated experiment we could see that no [1,2]-H shift occurred in our protocol. In addition, the possibility of another pathway involving the [1,2]-*H* shift process (from C4 to C5) followed by further transformations was also considered. The result shows that an intermediate **15a** with quite high energy would be generated in this pathway. Therefore, we deduce that this pathway is not preferred.

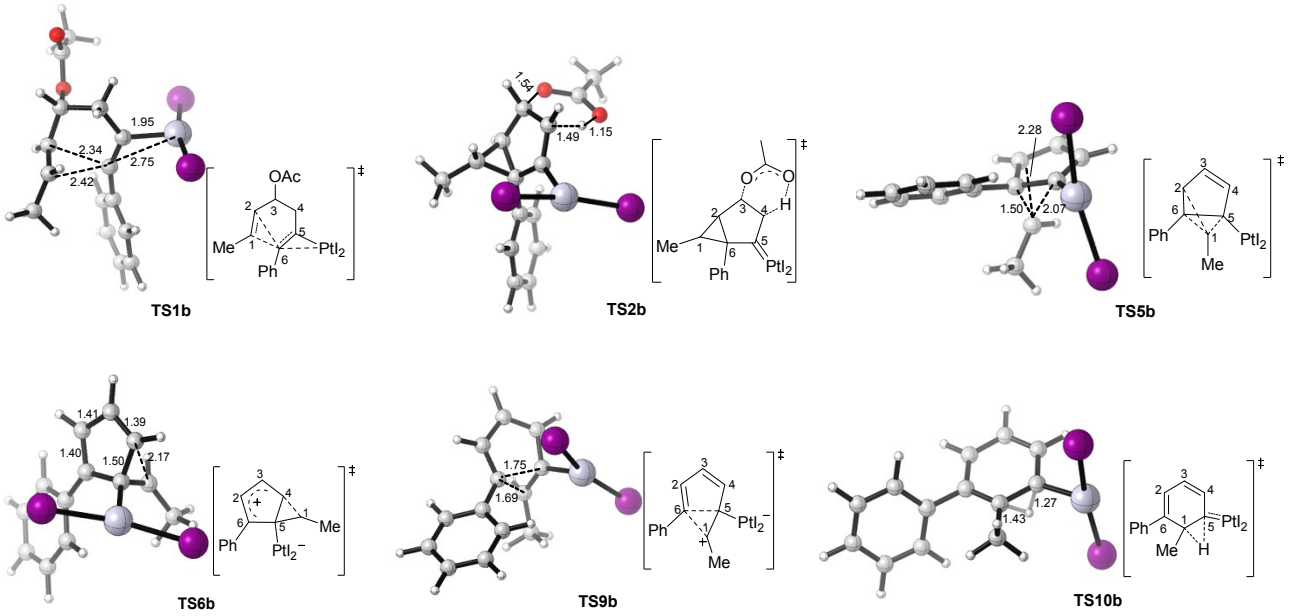



***Scheme S4***. Gibbs free energy profiles of 1,2-methyl shift (in green line) and 1,2-hydrogen shift (in blue line) from **7b**. Energies (in kcal/mol) are relative to **1b-1** in Scheme S2 and calculated using B3LYP/SDD-6-311+G(d,p)/SMD(toluene)//B3LYP/SDD-6-31G(d) method with DFT-D3(BJ) dispersion correction.

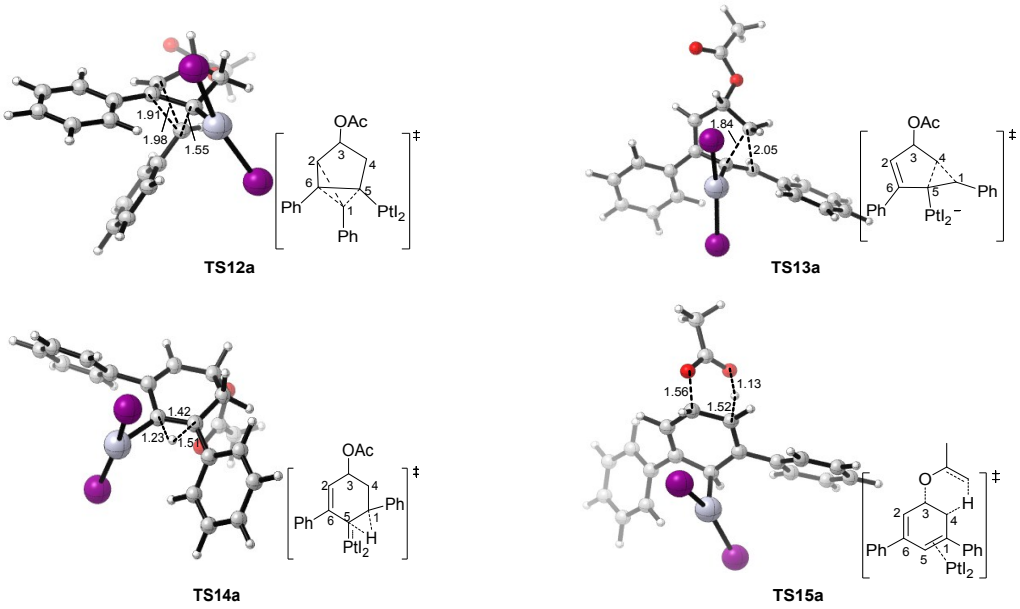
The activation barrier leading to the product **B-b** (**TS11b**, $\Delta G^{\neq}$= 28.3 kcal/mol) is much higher than that leading to the product **A-b** (**TS8b**, $\Delta G^{\neq}$= 11.8 kcal/mol), and also higher than that of the rate-determining elayl migration step (see Scheme S2). This implies that product **B-b** can not be produced through 1,2-methyl shift from **7b**.




***Scheme S5.*** 3D structures of some selected transition states involved in $PtI_2$-catalyzed cyclization of ACE **a**.




***Scheme S6.*** 3D structures of some selected transition states involved in $PtI_2$-catalyzed cyclization of ACE **b.**




***Scheme S7.*** 3D structures of some selected transition states involved in pathway **D** of $PtI_2$-catalyzed cyclization of ACE **a**

***Table S3.*** The B3LYP/SDD-6-31G(d) computed energies, enthalpies, free energies of all stationary points discussed in the text and in the supporting information

| | B3LYP/SDD-6-31G(d) | | | | |
|---|---|---|---|---|---|
| | E | H | G | G(qh) | G(D3(BJ)) |
| ACE **a** | -923.343198 | -922.996773 | -923.074307 | -923.064942 | -923.143762 |
| **AcOH** | -229.077610 | -229.010061 | -229.043019 | -229.042453 | -229.049454 |
| product **A-a** | -694.348851 | -694.071267 | -694.127178 | -694.125360 | -694.196985 |
| product **B-a** | -694.342593 | -694.065261 | -694.121163 | -694.119375 | -694.194844 |
| **1a-1** | -1065.674241 | -1065.319000 | -1065.410049 | -1065.400802 | -1065.519827 |
| **1a-2** | -1065.654109 | -1065.299021 | -1065.396797 | -1065.382414 | -1065.491722 |
| **2a-1** | -1065.686997 | -1065.331226 | -1065.421885 | -1065.410958 | -1065.528693 |
| **3a-1** | -836.559387 | -836.275282 | -836.359227 | -836.348485 | -836.443853 |
| **4a-1** | -836.589320 | -836.304184 | -836.381453 | -836.373554 | -836.475590 |
| **5a** | -836.558651 | -836.274459 | -836.351250 | -836.345077 | -836.453739 |
| **6a** | -836.569377 | -836.284409 | -836.361070 | -836.354460 | -836.458616 |
| **7a** | -836.606409 | -836.321441 | -836.398698 | -836.391133 | -836.497433 |

| | | | | | |
|---|---|---|---|---|---|
| **8a** | -836.644292 | -836.358019 | -836.435248 | -836.427594 | -836.525771 |
| **9a** | -836.613752 | -836.328010 | -836.405785 | -836.397895 | -836.501649 |
| **10a** | -836.631787 | -836.345877 | -836.421568 | -836.415770 | -836.525774 |
| **11a** | -1065.659952 | -1065.304376 | -1065.394249 | -1065.384676 | -1065.514405 |
| **12a** | -1065.695391 | -1065.339067 | -1065.42908 | -1065.418696 | -1065.543568 |
| **13a** | -1065.699223 | -1065.343195 | -1065.432457 | -1065.422761 | -1065.545986 |
| **TS1a** | -1065.643166 | -1065.289440 | -1065.381701 | -1065.370582 | -1065.489607 |
| **TS2a** | -1065.644814 | -1065.294313 | -1065.383691 | -1065.372756 | -1065.492826 |
| **TS3a** | -1065.612773 | -1065.263864 | -1065.357444 | -1065.345530 | -1065.455439 |
| **TS4a** | -836.536894 | -836.254401 | -836.335513 | -836.326066 | -836.427256 |
| **TS5a** | -836.546695 | -836.263371 | -836.338911 | -836.332551 | -836.439551 |
| **TS6a** | -836.551195 | -836.267828 | -836.342894 | -836.336953 | -836.442657 |
| **TS7a** | -836.560566 | -836.277258 | -836.352847 | -836.346473 | -836.450406 |
| **TS8a** | -836.578456 | -836.297530 | -836.373202 | -836.366823 | -836.472735 |
| **TS9a** | -836.548079 | -836.265242 | -836.341886 | -836.334899 | -836.439329 |
| **TS10a** | -836.577615 | -836.296723 | -836.373489 | -836.366395 | -836.470308 |
| **TS11a** | -836.5714389 | -836.287582 | -836.362832 | -836.3568836 | -836.463088 |
| **TS12a** | -1065.630173 | -1065.275883 | -1065.362666 | -1065.354807 | -1065.481106 |
| **TS13a** | -1065.638941 | -1065.285183 | -1065.374883 | -1065.36507 | -1065.489961 |
| **TS14a** | -1065.644148 | -1065.292576 | -1065.380655 | -1065.371888 | -1065.501063 |
| **TS15a** | -1065.653814 | -1065.30282 | -1065.391332 | -1065.381862 | -1065.508511 |
| | | | | | |
| ACE **b** | -731.607908 | -731.317698 | -731.385798 | -731.3800842 | -731.437677 |
| product **A-b** | -502.613695 | -502.392402 | -502.441717 | -502.440259 | -502.490730 |
| product **B-b** | -502.609575 | -502.388320 | -502.436639 | -502.435839 | -502.487973 |
| **1b-1** | -873.940482 | -873.641566 | -873.724150 | -873.717425 | -873.816352 |
| **1b-2** | -873.917035 | -873.618406 | -873.707977 | -873.696211 | -873.785719 |
| **2b-1** | -873.954854 | -873.655166 | -873.737954 | -873.728995 | -873.825610 |
| **3b-1** | -644.824137 | -644.596408 | -644.671267 | -644.664067 | -644.740986 |

| | | | | | |
|---|---|---|---|---|---|
| **4b-1** | -644.856655 | -644.627761 | -644.697281 | -644.691247 | -644.772503 |
| **5b** | -644.820772 | -644.592965 | -644.661757 | -644.657407 | -644.742102 |
| **6b** | -644.838179 | -644.609419 | -644.678383 | -644.673335 | -644.756775 |
| **7b** | -644.878544 | -644.649493 | -644.718401 | -644.713198 | -644.797605 |
| **8b** | -644.910388 | -644.680576 | -644.750192 | -644.744714 | -644.823871 |
| **9b** | -644.887031 | -644.657016 | -644.726800 | -644.720931 | -644.800632 |
| **10b** | -644.903776 | -644.673817 | -644.743917 | -644.737790 | -644.817009 |
| **TS1b** | -873.904881 | -873.607646 | -873.691511 | -873.683159 | -873.781501 |
| **TS2b** | -873.913836 | -873.619383 | -873.701269 | -873.691897 | -873.791234 |
| **TS3b** | -873.876286 | -873.583759 | -873.669035 | -873.659680 | -873.752123 |
| **TS4b** | -644.797966 | -644.571932 | -644.643888 | -644.637784 | -644.719285 |
| **TS5b** | -644.808566 | -644.582114 | -644.650114 | -644.645643 | -644.729796 |
| **TS6b** | -644.807623 | -644.581419 | -644.649364 | -644.644879 | -644.730049 |
| **TS7b** | -644.832963 | -644.605693 | -644.673607 | -644.668906 | -644.752237 |
| **TS8b** | -644.852845 | -644.628035 | -644.696143 | -644.691446 | -644.775343 |
| **TS9b** | -644.817577 | -644.590919 | -644.658741 | -644.654323 | -644.739120 |
| **TS10b** | -644.852804 | -644.627901 | -644.697073 | -644.691781 | -644.770828 |
| **TS11b** | -644.829584 | -644.601982 | -644.669888 | -644.665037 | -644.750697 |

E is the electronic energy without zero-point energy (ZPE) correction; H and G are the enthalpy and free energy at 298 K, respectively. G(qh) is the Gibbs free energy computed from Truhlar's quasiharmonic approximation. G(D3(BJ)) =G(qh)+$E_{disp}$, where $E_{disp}$ refers to B3LYP-D3(BJ) dispersion energy correction. The unit of all the energies in this table is Hartree.

***Table S4.*** The B3LYP /SDD-6-311+G(d,p)/SMD(toluene)//B3LYP/SDD-6-31G(d) computed energies, enthalpies, free energies of all stationary points discussed in the text and in the supporting information

| | B3LYP /SDD-6-311+G(d,p)/SMD(toluene)//B3LYP/SDD-6-31G(d) | | | | |
|---|---|---|---|---|---|
| | E | H | G | G(qh) | G(D3(BJ)) |
| ACE **a** | -923.634498 | -923.288073 | -923.365607 | -923.356242 | -923.435062 |
| **AcOH** | -229.171121 | -229.103573 | -229.136530 | -229.135965 | -229.142965 |
| product **A-a** | -694.553605 | -694.276273 | -694.332175 | -694.330387 | -694.405856 |

| | | | | | |
|---|---|---|---|---|---|
| product **B-a** | -694.546864 | -694.269280 | -694.325191 | -694.323373 | -694.394999 |
| **1a-1** | -1065.956690 | -1065.601448 | -1065.692498 | -1065.683251 | -1065.802275 |
| **1a-2** | -1065.938754 | -1065.583665 | -1065.681442 | -1065.667059 | -1065.776367 |
| **2a-1** | -1065.964995 | -1065.609224 | -1065.699883 | -1065.688956 | -1065.806691 |
| **3a-1** | -836.764791 | -836.480686 | -836.564631 | -836.553889 | -836.649256 |
| **4a-1** | -836.789565 | -836.504429 | -836.581698 | -836.573799 | -836.675834 |
| **5a** | -836.760151 | -836.475959 | -836.552750 | -836.546577 | -836.655240 |
| **6a** | -836.770144 | -836.485176 | -836.561837 | -836.555227 | -836.659383 |
| **7a** | -836.808348 | -836.523380 | -836.600637 | -836.593072 | -836.699372 |
| **8a** | -836.846123 | -836.559849 | -836.637078 | -836.629424 | -836.727601 |
| **9a** | -836.815814 | -836.530072 | -836.607847 | -836.599958 | -836.703712 |
| **10a** | -836.831667 | -836.545757 | -836.621448 | -836.615650 | -836.725654 |
| **11a** | -1065.937602 | -1065.582026 | -1065.671900 | -1065.662326 | -1065.792055 |
| **12a** | -1065.973312 | -1065.616988 | -1065.707001 | -1065.696617 | -1065.821489 |
| **13a** | -1065.978526 | -1065.622497 | -1065.71176 | -1065.702064 | -1065.825289 |
| **TS1a** | -1065.925642 | -1065.571915 | -1065.664177 | -1065.653058 | -1065.772082 |
| **TS2a** | -1065.925523 | -1065.575022 | -1065.664401 | -1065.653465 | -1065.773535 |
| **TS3a** | -1065.897847 | -1065.548938 | -1065.642518 | -1065.630603 | -1065.740512 |
| **TS4a** | -836.743021 | -836.460528 | -836.541640 | -836.532192 | -836.633383 |
| **TS5a** | -836.747333 | -836.464009 | -836.539549 | -836.533189 | -836.640189 |
| **TS6a** | -836.752902 | -836.469535 | -836.544601 | -836.538660 | -836.644365 |
| **TS7a** | -836.761453 | -836.478146 | -836.553735 | -836.547360 | -836.651293 |
| **TS8a** | -836.783147 | -836.502221 | -836.577893 | -836.571514 | -836.677425 |
| **TS9a** | -836.749889 | -836.467052 | -836.543696 | -836.536709 | -836.641139 |
| **TS10a** | -836.783161 | -836.502269 | -836.579035 | -836.571941 | -836.675855 |
| **TS11a** | -836.7735663 | -836.489709 | -836.564959 | -836.559011 | -836.665216 |
| **TS12a** | -1065.907595 | -1065.553305 | -1065.640088 | -1065.63223 | -1065.758528 |
| **TS13a** | -1065.920884 | -1065.567127 | -1065.656826 | -1065.647013 | -1065.771905 |
| **TS14a** | -1065.92413 | -1065.572559 | -1065.660637 | -1065.65187 | -1065.781044 |

| | | | | | |
|---|---|---|---|---|---|
| **TS15a** | -1065.937206 | -1065.586212 | -1065.674725 | -1065.665254 | -1065.791903 |
| | | | | | |
| ACE **b** | -731.843979 | -731.553769 | -731.621869 | -731.616155 | -731.673748 |
| product **A-b** | -502.764558 | -502.543265 | -502.592580 | -502.591122 | -502.641593 |
| product **B-b** | -502.760484 | -502.539229 | -502.587548 | -502.586748 | -502.638882 |
| **1b-1** | -874.169246 | -873.870330 | -873.952915 | -873.946189 | -874.045117 |
| **1b-2** | -874.148269 | -873.849641 | -873.939212 | -873.927445 | -874.016954 |
| **2b-1** | -874.179301 | -873.879614 | -873.962401 | -873.953442 | -874.050057 |
| **3b-1** | -644.975629 | -644.747900 | -644.822759 | -644.815560 | -644.892479 |
| **4b-1** | -645.003391 | -644.774498 | -644.844018 | -644.837983 | -644.919239 |
| **5b** | -644.969592 | -644.741785 | -644.810577 | -644.806227 | -644.890923 |
| **6b** | -644.985917 | -644.757157 | -644.826121 | -644.821073 | -644.904513 |
| **7b** | -645.026996 | -644.797944 | -644.866853 | -644.861650 | -644.946057 |
| **8b** | -645.058728 | -644.828915 | -644.898531 | -644.893054 | -644.972211 |
| **9b** | -645.035505 | -644.805489 | -644.875274 | -644.869405 | -644.949106 |
| **10b** | -645.051378 | -644.821419 | -644.891518 | -644.885392 | -644.964611 |
| **TS1b** | -874.133720 | -873.836485 | -873.920350 | -873.911998 | -874.010340 |
| **TS2b** | -874.140408 | -873.845955 | -873.927842 | -873.918469 | -874.017807 |
| **TS3b** | -874.107013 | -873.814486 | -873.899762 | -873.890407 | -873.982851 |
| **TS4b** | -644.950601 | -644.724567 | -644.796523 | -644.790419 | -644.871920 |
| **TS5b** | -644.958989 | -644.732537 | -644.800537 | -644.796066 | -644.880218 |
| **TS6b** | -644.957824 | -644.731621 | -644.799566 | -644.795080 | -644.880250 |
| **TS7b** | -644.980570 | -644.753300 | -644.821213 | -644.816512 | -644.899843 |
| **TS8b** | -645.004639 | -644.779829 | -644.847937 | -644.843240 | -644.927137 |
| **TS9b** | -644.966352 | -644.739695 | -644.807516 | -644.803099 | -644.887895 |
| **TS10b** | -645.005115 | -644.780211 | -644.849384 | -644.844092 | -644.923138 |
| **TS11b** | -644.979877 | -644.752275 | -644.820181 | -644.815331 | -644.900991 |

E is the electronic energy without zero-point energy (ZPE) correction; H and G are the enthalpy and free energy at 298 K, respectively. G(qh) is the Gibbs free energy computed from Truhlar's quasiharmonic approximation. G(D3(BJ)) =G(qh)+$E_{disp}$, where $E_{disp}$ refers to

B3LYP-D3(BJ) dispersion energy correction. The unit of all the energies in this table is Hartree.

### *References*


(1) (a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648. (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785.

(2) M. J. Frisch, et al. *Gaussian 09, revision B.01*; Gaussian, Inc.: Wallingford, CT, **2010**.

(3) K. Fukui, *Acc. Chem. Res.* **1981**, *14*, 363.

(4) D. Andrae, U. Haussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990**, *77*, 123.

(5) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378.

(6) S. Grimme, S. Ehrlich, L. J. Goerigk, *Comput. Chem.* **2011**, *32*, 1456.

(7) S. Grimme, *DFTD3, V2.0 Rev 1*; University Münster: Münster, Germany, **2010**.

(8) R. F. Ribeiro, A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2011**, *115*, 14556.

(9) C. Y. Legault, CYLview, 1.0b; Université de Sherbrooke: Sherbrooke, Québec, Canada, 2009 (http://www.cylview.org)

## The Cartesian Coordinates of the stationary points discussed in the text and in the supporting information

For transition state structures, one imaginary frequency was observed and given below. For all minimum structures, no imaginary frequency was observed.

**ACE a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.56061300 | 1.09069800 | -0.96975200 |
| C | -1.96978800 | 0.37043100 | 0.08333900 |
| H | -1.85505000 | 0.81858900 | -1.98240500 |
| H | -1.63046000 | 0.67977900 | 1.06899500 |
| C | -2.83452600 | -0.81959400 | 0.06508500 |
| C | -3.06727800 | -1.49961700 | 1.27385900 |
| C | -3.44633200 | -1.32058100 | -1.09972200 |
| C | -3.87082400 | -2.63827200 | 1.32165600 |
| H | -2.60603500 | -1.12665300 | 2.18555200 |
| C | -4.24916900 | -2.45670300 | -1.05407500 |
| H | -3.29810900 | -0.81516300 | -2.04978500 |
| C | -4.46552500 | -3.12323800 | 0.15634200 |
| H | -4.03245500 | -3.14514400 | 2.26941700 |
| H | -4.71145400 | -2.82415800 | -1.96660800 |
| C | -0.66727400 | 2.29596700 | -0.91098200 |
| H | -1.17570400 | 3.16861800 | -1.33889600 |
| O | -0.36425600 | 2.59080000 | 0.46711000 |
| C | -0.02998700 | 3.87042700 | 0.76647800 |
| O | 0.02938800 | 4.76198100 | -0.05226100 |
| C | 0.64575100 | 2.10848400 | -1.71748400 |
| H | 1.19143200 | 3.05916400 | -1.69445400 |
| H | 0.36765600 | 1.93755100 | -2.76763600 |
| C | 1.48656400 | 1.01640400 | -1.23459200 |
| C | 2.16833500 | 0.10107500 | -0.82550400 |
| C | 2.95611700 | -0.98928000 | -0.34234600 |
| C | 4.36271900 | -0.94451300 | -0.39893900 |
| C | 2.33291200 | -2.13102800 | 0.19916200 |
| C | 5.12133000 | -2.01349200 | 0.07284900 |
| H | 4.84739200 | -0.06682300 | -0.81568200 |
| C | 3.09891900 | -3.19500500 | 0.66968900 |
| H | 1.24871300 | -2.16825800 | 0.24350300 |
| C | 4.49393700 | -3.14123600 | 0.60842800 |
| H | 6.20593100 | -1.96624200 | 0.02247100 |
| H | 2.60539800 | -4.06983900 | 1.08465800 |
| H | -5.09376000 | -4.00921700 | 0.18836600 |
| H | 5.08860300 | -3.97332600 | 0.97558300 |
| C | 0.25420000 | 4.01302900 | 2.24279300 |
| H | 0.51296100 | 5.04893300 | 2.46429800 |
| H | -0.62220200 | 3.71379000 | 2.82704700 |
| H | 1.07926700 | 3.35241700 | 2.52908000 |

**AcOH**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.39746600 | -0.10997000 | 0.00000600 |
| H | 1.68544800 | -0.69065000 | 0.88258100 |
| H | 1.68543100 | -0.69283500 | -0.88111300 |

| | | | |
|---|---|---|---|
| H | 1.91738200 | 0.84813400 | -0.00109500 |
| C | -0.09243800 | 0.12560800 | -0.00015200 |
| O | -0.64546700 | 1.20210000 | 0.00003500 |
| O | -0.77886000 | -1.04658800 | 0.00000700 |
| H | -1.72381700 | -0.80257000 | 0.00017400 |

**product A-a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.21000200 | 2.11387500 | 0.41781900 |
| C | -1.22716400 | 0.73392800 | 0.15447700 |
| H | -2.14712400 | 2.64749800 | 0.54764800 |
| H | -0.00010100 | -0.99001800 | -0.23019200 |
| C | -2.51160900 | 0.00151300 | 0.00392600 |
| C | -3.60574700 | 0.59077300 | -0.65267000 |
| C | -2.66741500 | -1.29853100 | 0.51463400 |
| C | -4.81189900 | -0.09460100 | -0.79363400 |
| H | -3.49973100 | 1.58476300 | -1.07837800 |
| C | -3.87273700 | -1.98528100 | 0.37306000 |
| H | -1.84339500 | -1.76337200 | 1.04883800 |
| C | -4.95098300 | -1.38622100 | -0.28151500 |
| H | -5.64162000 | 0.37833800 | -1.31258000 |
| H | -3.97228200 | -2.98703700 | 0.78293900 |
| C | 0.00011200 | 2.79339100 | 0.54682900 |
| H | 0.00014800 | 3.85764600 | 0.76755100 |
| C | 1.21014100 | 2.11377700 | 0.41791000 |
| H | 2.14733000 | 2.64720900 | 0.54807400 |
| C | 1.22714500 | 0.73386300 | 0.15432400 |
| C | -0.00004100 | 0.06538600 | 0.02599000 |
| C | 2.51157000 | 0.00140900 | 0.00388300 |
| C | 3.60581200 | 0.59083600 | -0.65239400 |
| C | 2.66725100 | -1.29878000 | 0.51423700 |
| C | 4.81198700 | -0.09450200 | -0.79332200 |
| H | 3.49983400 | 1.58493300 | -1.07787400 |
| C | 3.87259900 | -1.98549500 | 0.37269600 |
| H | 1.84311700 | -1.76377800 | 1.04812200 |
| C | 4.95097000 | -1.38625600 | -0.28151100 |
| H | 5.64180900 | 0.37855200 | -1.31200400 |
| H | 3.97205200 | -2.98736900 | 0.78230600 |
| H | -5.89056000 | -1.92092800 | -0.39144900 |
| H | 5.89057000 | -1.92092800 | -0.39142900 |

**product B-a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.38221200 | 2.43441200 | -0.02948300 |
| C | -1.38272900 | 2.43410600 | 0.02951000 |
| H | 2.46746000 | 2.43153500 | -0.08263700 |
| H | -2.46798000 | 2.43096200 | 0.08262100 |
| C | -1.53046900 | -0.04218400 | 0.10099400 |
| C | -2.61283800 | -0.22922300 | -0.77468100 |
| C | -1.28938100 | -1.02080700 | 1.07971900 |
| C | -3.42480900 | -1.36049400 | -0.68129400 |
| H | -2.80781400 | 0.51378000 | -1.54372300 |
| C | -2.10315100 | -2.14860800 | 1.17672900 |
| H | -0.46325700 | -0.88999000 | 1.77173800 |
| C | -3.17320600 | -2.32465100 | 0.29593100 |
| H | -4.25229500 | -1.48836000 | -1.37446000 |
| H | -1.90268300 | -2.89049100 | 1.94536300 |
| C | 0.69675400 | 3.64704900 | -0.01143900 |
| H | 1.24885400 | 4.58295400 | -0.02544400 |
| C | -0.69754600 | 3.64689400 | 0.01144500 |

| | | | |
|---|---|---|---|
| H | -1.24984700 | 4.58267800 | 0.02541100 |
| C | -0.70858000 | 1.20087500 | 0.02167100 |
| C | 0.70835200 | 1.20102800 | -0.02161000 |
| C | 1.53052100 | -0.04187100 | -0.10100200 |
| C | 2.61281200 | -0.22883100 | 0.77479700 |
| C | 1.28970000 | -1.02045200 | -1.07982300 |
| C | 3.42499400 | -1.35994900 | 0.68138400 |
| H | 2.80755100 | 0.51409000 | 1.54397500 |
| C | 2.10368600 | -2.14809900 | -1.17686200 |
| H | 0.46360000 | -0.88974600 | -1.77190300 |
| C | 3.17367400 | -2.32404600 | -0.29597400 |
| H | 4.25240100 | -1.48774000 | 1.37465800 |
| H | 1.90342800 | -2.88992500 | -1.94560800 |
| H | 3.80557300 | -3.20496100 | -0.37160700 |
| H | -3.80495700 | -3.20567800 | 0.37153900 |

**1a-1**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -1.96494900 | 0.55299900 | -0.13666300 |
| C | -1.51917500 | 0.00806600 | -1.34896900 |
| H | -2.63260200 | -0.04130200 | 0.47983400 |
| H | -1.02947800 | 0.67816300 | -2.05064800 |
| C | -1.87599100 | -1.28811400 | -1.93747700 |
| C | -1.24928600 | -1.65949500 | -3.14286800 |
| C | -2.84615800 | -2.14892300 | -1.39141200 |
| C | -1.56423100 | -2.85936600 | -3.77400900 |
| H | -0.50691200 | -0.99639700 | -3.58145500 |
| C | -3.16431400 | -3.34577700 | -2.02718800 |
| H | -3.35544700 | -1.88245100 | -0.47248300 |
| C | -2.52305500 | -3.70802800 | -3.21513500 |
| H | -1.06732500 | -3.13021900 | -4.70123900 |
| H | -3.91660700 | -3.99861700 | -1.59400600 |
| C | -2.04858700 | 2.03909000 | 0.16502900 |
| H | -2.06327500 | 2.17571200 | 1.24868100 |
| O | -3.32010600 | 2.49322200 | -0.35826600 |
| C | -3.83969800 | 3.61771100 | 0.21286200 |
| O | -3.26050500 | 4.25905100 | 1.05960600 |
| C | -0.88699900 | 2.87939200 | -0.41936600 |
| H | -0.74649900 | 3.77073900 | 0.19904400 |
| H | -1.14817700 | 3.21866400 | -1.43025000 |
| C | 0.33988300 | 2.06210000 | -0.48282700 |
| C | 1.33799900 | 1.47619500 | -0.94733400 |
| C | 2.56718300 | 1.20473000 | -1.63966100 |
| C | 2.91210600 | -0.09560600 | -2.05011400 |
| C | 3.42360100 | 2.28095000 | -1.94559500 |
| C | 4.08930700 | -0.31055600 | -2.76142600 |
| H | 2.26342200 | -0.92555500 | -1.78944300 |
| C | 4.59677800 | 2.05403800 | -2.65982900 |
| H | 3.16505700 | 3.28118700 | -1.61239000 |
| C | 4.93230700 | 0.76059400 | -3.06923500 |
| H | 4.35309600 | -1.31833200 | -3.06867300 |
| H | 5.25457400 | 2.88742900 | -2.88930900 |
| Pt | 0.13084000 | 0.02761800 | 0.37633800 |
| I | 2.34083400 | 0.01133800 | 1.92170500 |
| I | -0.74948300 | -2.13327100 | 1.71336900 |
| H | 5.85227600 | 0.58724700 | -3.62037200 |
| H | -2.77525500 | -4.64378600 | -3.70610700 |
| C | -5.20404500 | 3.92356400 | -0.35390200 |
| H | -5.16236000 | 3.96776400 | -1.44666900 |
| H | -5.90443200 | 3.12517400 | -0.08577700 |

| | | | |
|---|---|---|---|
| H | -5.55835600 | 4.87327100 | 0.04798000 |

**1a-2**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.85026100 | 1.63816600 | 0.04171900 |
| C | -3.06821400 | 0.41635300 | -0.46961000 |
| H | -3.60019600 | 2.12675600 | 0.65889400 |
| H | -2.29757300 | -0.04539600 | -1.08544200 |
| C | -4.26166600 | -0.42420000 | -0.28365400 |
| C | -4.28945500 | -1.69178600 | -0.89325400 |
| C | -5.37891200 | -0.02792900 | 0.47617600 |
| C | -5.39113600 | -2.53532400 | -0.75149100 |
| H | -3.43537900 | -2.01374500 | -1.48490700 |
| C | -6.47842400 | -0.86926500 | 0.61681200 |
| H | -5.38894300 | 0.94426400 | 0.96009900 |
| C | -6.49052000 | -2.12715700 | 0.00445700 |
| H | -5.38922700 | -3.50951100 | -1.23278000 |
| H | -7.33138100 | -0.54377300 | 1.20641900 |
| C | -1.61606000 | 2.47454000 | -0.16363300 |
| H | -1.28721800 | 2.87160300 | 0.80232100 |
| O | -1.92987000 | 3.62239700 | -1.00982800 |
| C | -2.50187800 | 4.69088100 | -0.39722000 |
| O | -2.77720900 | 4.72032600 | 0.78212400 |
| C | -0.43243200 | 1.79931100 | -0.87822600 |
| H | 0.32702600 | 2.56127400 | -1.08537600 |
| H | -0.74681500 | 1.39753000 | -1.84799800 |
| C | 0.17931400 | 0.72617000 | -0.06650000 |
| C | 0.29962500 | 0.03220500 | 0.98886900 |
| C | 0.10145700 | -0.57955400 | 2.26594700 |
| C | 0.99013100 | -0.31766800 | 3.32993100 |
| C | -1.00303500 | -1.43501400 | 2.46453700 |
| C | 0.76332200 | -0.89383300 | 4.57498000 |
| H | 1.84815600 | 0.32509700 | 3.15998000 |
| C | -1.22101800 | -1.99857300 | 3.71748300 |
| H | -1.67633500 | -1.63886400 | 1.63881500 |
| C | -0.34012900 | -1.73138700 | 4.77036300 |
| H | 1.44718500 | -0.69290600 | 5.39417100 |
| H | -2.07523200 | -2.65082800 | 3.87237100 |
| Pt | 1.79609000 | -0.45354200 | -0.53323500 |
| I | 3.67762200 | 1.24350000 | 0.29847700 |
| I | 0.43158500 | -2.40348900 | -1.73736800 |
| H | -0.51107400 | -2.18084100 | 5.74461000 |
| H | -7.35123300 | -2.78069200 | 0.11697000 |
| C | -2.73941900 | 5.80691900 | -1.38642500 |
| H | -1.79472700 | 6.10788200 | -1.85088100 |
| H | -3.40181600 | 5.46214300 | -2.18732000 |
| H | -3.18932700 | 6.65682100 | -0.87231800 |

**2a-1**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.12826100 | 1.38206600 | 0.44208000 |
| C | -2.37599100 | 0.15421700 | -0.33959400 |
| H | -2.75062200 | 1.60982000 | 1.29986300 |
| H | -2.16384400 | 0.20678700 | -1.40357800 |
| C | -3.35679400 | -0.90319600 | 0.00438300 |
| C | -3.56876600 | -1.93229400 | -0.92894300 |
| C | -4.09702900 | -0.91119400 | 1.19748900 |
| C | -4.49946000 | -2.93901500 | -0.68100900 |
| H | -2.99547200 | -1.93998300 | -1.85293100 |
| C | -5.02795800 | -1.91868600 | 1.44413900 |

| | | | |
|---|---|---|---|
| H | -3.95051600 | -0.13259200 | 1.93892600 |
| C | -5.23254200 | -2.93476800 | 0.50772500 |
| H | -4.65122400 | -3.72529500 | -1.41500300 |
| H | -5.59554600 | -1.90847600 | 2.37032300 |
| C | -1.54205000 | 2.54928300 | -0.34368000 |
| H | -1.27777200 | 3.35472400 | 0.34666900 |
| O | -2.42896800 | 3.07792700 | -1.34623500 |
| C | -3.47946900 | 3.81000900 | -0.88166500 |
| O | -3.69411400 | 3.98061100 | 0.29750700 |
| C | -0.29576800 | 1.97553300 | -1.05037600 |
| H | 0.54336900 | 2.67516400 | -1.08213900 |
| H | -0.51399600 | 1.70579300 | -2.09310000 |
| C | 0.06411800 | 0.73271900 | -0.26992800 |
| C | -1.02707100 | 0.31166300 | 0.57981200 |
| C | -0.84345600 | -0.55915800 | 1.78203200 |
| C | -0.90974000 | 0.00399900 | 3.06274500 |
| C | -0.56675000 | -1.92686400 | 1.64799600 |
| C | -0.70139200 | -0.78634700 | 4.19443600 |
| H | -1.11092700 | 1.06610900 | 3.17602400 |
| C | -0.35644200 | -2.71422400 | 2.77966800 |
| H | -0.51189100 | -2.37134400 | 0.65922900 |
| C | -0.42328300 | -2.14676900 | 4.05436300 |
| H | -0.74952800 | -0.33594000 | 5.18188800 |
| H | -0.14106200 | -3.77272500 | 2.66390300 |
| Pt | 1.72348400 | -0.07991400 | -0.44047000 |
| I | 3.16535300 | 1.26063600 | 1.33880600 |
| I | 1.13854500 | -1.77604600 | -2.41095900 |
| H | -0.25805000 | -2.76236800 | 4.93428100 |
| H | -5.95900400 | -3.71840000 | 0.70385100 |
| C | -4.29747500 | 4.36057700 | -2.02285400 |
| H | -3.68854900 | 5.04649200 | -2.62158000 |
| H | -4.62094700 | 3.54995900 | -2.68354300 |
| H | -5.16462300 | 4.88869600 | -1.62543500 |

**3a-1**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.55160600 | -1.12399000 | 2.46825600 |
| C | -3.07449100 | -0.12542500 | 1.71077100 |
| H | -3.19305200 | -1.95234600 | 2.76333700 |
| H | -2.47580400 | 0.76952700 | 1.55798800 |
| C | -4.41941700 | -0.07966600 | 1.14139100 |
| C | -4.92903500 | 1.15740700 | 0.69900600 |
| C | -5.23605800 | -1.22174200 | 1.01268800 |
| C | -6.21308200 | 1.25617100 | 0.16806000 |
| H | -4.30786900 | 2.04590600 | 0.78189000 |
| C | -6.51719200 | -1.12196300 | 0.48046700 |
| H | -4.85559600 | -2.19390600 | 1.31137500 |
| C | -7.01298100 | 0.11675900 | 0.05913600 |
| H | -6.58943300 | 2.22092500 | -0.16070800 |
| H | -7.13048300 | -2.01353700 | 0.38412400 |
| C | -1.21756600 | -1.15831700 | 3.01502700 |
| H | -1.10358900 | -1.72155500 | 3.94023100 |
| C | -0.06958800 | -0.60133300 | 2.52583000 |
| H | 0.84625600 | -0.71043000 | 3.10180600 |
| C | 0.08365900 | 0.05434000 | 1.28378400 |
| C | 0.05311900 | 0.83300300 | 0.27700900 |
| C | -0.39505300 | 1.97572000 | -0.48341100 |
| C | -1.64476200 | 1.94483200 | -1.13130800 |
| C | 0.41591300 | 3.12320600 | -0.57610000 |
| C | -2.08537600 | 3.06201700 | -1.83681400 |

| | | | |
|---|---|---|---|
| H | -2.24942800 | 1.04535100 | -1.08511300 |
| C | -0.03604600 | 4.23263400 | -1.28508800 |
| H | 1.38948800 | 3.12678300 | -0.09600600 |
| C | -1.28473800 | 4.20529900 | -1.91369800 |
| H | -3.04958100 | 3.03520300 | -2.33613700 |
| H | 0.58930400 | 5.11800700 | -1.35245900 |
| Pt | 1.57127200 | -0.50873200 | -0.19331600 |
| I | 0.08873500 | -2.11877500 | -1.71032000 |
| I | 3.60973700 | 0.73154000 | 1.01991400 |
| H | -1.62933200 | 5.07145200 | -2.47176200 |
| H | -8.01327600 | 0.18951000 | -0.35843700 |

**4a-1**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 1.75741800 | 0.87764500 | 2.32148600 |
| C | 2.31829700 | -0.19104300 | 1.36517700 |
| H | 2.40243200 | 1.71140200 | 2.57817200 |
| H | 2.01196500 | -1.20662600 | 1.59955000 |
| C | 3.64558200 | -0.10533900 | 0.71781400 |
| C | 4.23905300 | -1.30280000 | 0.27954900 |
| C | 4.34968700 | 1.09876500 | 0.53831800 |
| C | 5.49549800 | -1.29912300 | -0.32268000 |
| H | 3.70402300 | -2.24014400 | 0.40884900 |
| C | 5.60711700 | 1.10008700 | -0.06091800 |
| H | 3.91496500 | 2.04080300 | 0.85632300 |
| C | 6.18437300 | -0.09666500 | -0.49371400 |
| H | 5.93553000 | -2.23444000 | -0.65646400 |
| H | 6.13745600 | 2.03915600 | -0.19147900 |
| C | 0.80731700 | 0.30639500 | 3.29556700 |
| H | 1.02173000 | 0.20960100 | 4.35577100 |
| C | -0.30430900 | -0.17269200 | 2.66759800 |
| H | -1.12842000 | -0.70230400 | 3.12758900 |
| C | -0.18484400 | 0.05420400 | 1.24889100 |
| C | 1.10281300 | 0.75178500 | 0.97346200 |
| C | 1.23469900 | 1.74518100 | -0.14139400 |
| C | 1.15771400 | 3.11718900 | 0.12783600 |
| C | 1.39166800 | 1.31259400 | -1.46510500 |
| C | 1.23692100 | 4.04636300 | -0.91142900 |
| H | 1.02200300 | 3.45995900 | 1.15045900 |
| C | 1.46809200 | 2.24199600 | -2.50206300 |
| H | 1.44949700 | 0.24983300 | -1.67929300 |
| C | 1.39154600 | 3.60968800 | -2.22804300 |
| H | 1.17023300 | 5.10817600 | -0.69127400 |
| H | 1.58798600 | 1.89618400 | -3.52492000 |
| Pt | -1.41977500 | -0.53343100 | -0.01833000 |
| I | -3.22282300 | 1.40855900 | 0.04928500 |
| I | -0.25819200 | -2.83366000 | -0.69771200 |
| H | 1.44995600 | 4.33169700 | -3.03785400 |
| H | 7.16503600 | -0.09071400 | -0.96119000 |

**5a**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 1.16636900 | 1.41932400 | 2.71797600 |
| C | 1.01296200 | -1.28510200 | 1.33996100 |
| H | 1.81456600 | 2.18523600 | 3.13193200 |
| H | 1.22767600 | -1.58061200 | 2.36814500 |
| C | 1.71335300 | -2.02871000 | 0.34867400 |
| C | 1.50895100 | -1.87015800 | -1.04603900 |
| C | 2.69228000 | -2.95728400 | 0.79443600 |
| C | 2.27250500 | -2.59626000 | -1.94901100 |

| | | | |
|---|---|---|---|
| H | 0.72073200 | -1.20831800 | -1.38849500 |
| C | 3.44473400 | -3.68409000 | -0.11396500 |
| H | 2.84937200 | -3.08781900 | 1.86200200 |
| C | 3.23567400 | -3.50154500 | -1.48787600 |
| H | 2.10669900 | -2.47549600 | -3.01506000 |
| H | 4.18995100 | -4.39186600 | 0.23571700 |
| C | -0.02582500 | 0.94599700 | 3.34710700 |
| H | -0.37540800 | 1.25768400 | 4.32459500 |
| C | -0.63082100 | 0.04313200 | 2.51935900 |
| H | -1.49063900 | -0.57903400 | 2.72931200 |
| C | 0.15133600 | -0.09186800 | 1.24714000 |
| C | 1.33908200 | 0.87284100 | 1.45181300 |
| C | 2.47764100 | 1.17137500 | 0.56755200 |
| C | 3.75011800 | 1.37627300 | 1.13902300 |
| C | 2.34899500 | 1.28632900 | -0.82839700 |
| C | 4.84879400 | 1.69900100 | 0.34801400 |
| H | 3.87660400 | 1.26428700 | 2.21264000 |
| C | 3.45406600 | 1.60448000 | -1.61920000 |
| H | 1.37269600 | 1.17414900 | -1.28332200 |
| C | 4.70464300 | 1.81365200 | -1.03770800 |
| H | 5.81934500 | 1.85390100 | 0.81151400 |
| H | 3.32842000 | 1.70384500 | -2.69385300 |
| Pt | -1.25422900 | 0.19960600 | -0.18724800 |
| I | -1.16986100 | 2.81727000 | -0.65105600 |
| I | -2.10898900 | -2.34517300 | -0.05205200 |
| H | 5.56097700 | 2.06674400 | -1.65679000 |
| H | 3.81874900 | -4.07746100 | -2.20137400 |

**6a**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -1.80602300 | 0.53509000 | 2.86704500 |
| C | 1.03308500 | 0.48966500 | 2.05255900 |
| H | -2.61025100 | 0.99011800 | 3.43065500 |
| H | 0.85505400 | 1.34886400 | 2.69678900 |
| C | 2.46231200 | 0.25928500 | 1.78249000 |
| C | 2.94855000 | -0.85138600 | 1.06797300 |
| C | 3.38661300 | 1.17453300 | 2.31955700 |
| C | 4.31724800 | -1.03859100 | 0.90589900 |
| H | 2.25153700 | -1.55016300 | 0.61526800 |
| C | 4.75641600 | 0.99192200 | 2.14562300 |
| H | 3.02385200 | 2.03489800 | 2.87725100 |
| C | 5.22538600 | -0.11880000 | 1.44094100 |
| H | 4.67736700 | -1.89710800 | 0.34669700 |
| H | 5.45521700 | 1.71173000 | 2.56219600 |
| C | -0.95740600 | -0.43451400 | 3.35696200 |
| H | -1.03043900 | -0.88567100 | 4.34217700 |
| C | 0.06861500 | -0.74093600 | 2.38867900 |
| H | 0.55260700 | -1.70763600 | 2.33600700 |
| C | -0.19650100 | 0.10365300 | 1.18105300 |
| C | -1.37238700 | 0.94528000 | 1.57849800 |
| C | -1.91789500 | 2.08840900 | 0.87562800 |
| C | -3.17162300 | 2.62576300 | 1.25885000 |
| C | -1.21879300 | 2.70244000 | -0.18749200 |
| C | -3.70379900 | 3.72396300 | 0.59782000 |
| H | -3.74543000 | 2.15804700 | 2.05154500 |
| C | -1.74545400 | 3.81749500 | -0.82798800 |
| H | -0.26769500 | 2.29822300 | -0.51045900 |
| C | -2.98919700 | 4.32767200 | -0.44378800 |
| H | -4.67551700 | 4.11123700 | 0.88923600 |
| H | -1.19028600 | 4.27796600 | -1.63950800 |

| | | | |
|---|---|---|---|
| Pt | -0.17656800 | -0.65300300 | -0.67336400 |
| I | 1.61955800 | 0.75955600 | -2.06918000 |
| I | -2.05588700 | -2.46680500 | -0.08146100 |
| H | -3.40625900 | 5.18889500 | -0.95840600 |
| H | 6.29310500 | -0.26666100 | 1.30500200 |

**7a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.09292500 | 0.62071800 | 3.29298800 |
| C | -1.32584100 | -0.04299200 | 1.95588900 |
| H | 2.01264200 | 0.84115300 | 3.82988800 |
| H | -1.52683300 | -1.13638400 | 1.97197200 |
| C | -2.51756500 | 0.60128300 | 1.23573900 |
| C | -2.58321800 | 1.99573100 | 1.11890600 |
| C | -3.56932400 | -0.18056700 | 0.74801900 |
| C | -3.68191600 | 2.59800600 | 0.50724100 |
| H | -1.76848200 | 2.61088300 | 1.49218900 |
| C | -4.66926000 | 0.42459200 | 0.13685200 |
| H | -3.52132200 | -1.26331900 | 0.82684300 |
| C | -4.72766800 | 1.81361000 | 0.01483700 |
| H | -3.71830200 | 3.67959600 | 0.41291300 |
| H | -5.47718400 | -0.19283500 | -0.24570600 |
| C | -0.13894700 | 0.68735200 | 4.01676900 |
| H | -0.12076200 | 0.97242000 | 5.06426300 |
| C | -1.29551400 | 0.37044800 | 3.39319900 |
| H | -2.24851000 | 0.38328700 | 3.91453000 |
| C | 0.00090300 | 0.01742700 | 1.22464700 |
| C | 1.20458900 | 0.27837800 | 1.95169500 |
| C | 2.56230600 | 0.25717500 | 1.33417200 |
| C | 3.40633100 | 1.36944000 | 1.47681700 |
| C | 3.04061300 | -0.87727900 | 0.65927700 |
| C | 4.69692100 | 1.35439900 | 0.94782000 |
| H | 3.03913500 | 2.26149000 | 1.97784000 |
| C | 4.33474900 | -0.89214400 | 0.13886600 |
| H | 2.40579000 | -1.75045200 | 0.55234900 |
| C | 5.16442200 | 0.22255800 | 0.27771800 |
| H | 5.33178900 | 2.22977500 | 1.05257100 |
| H | 4.69328700 | -1.77916600 | -0.37580200 |
| Pt | -0.00272800 | -0.32493300 | -0.62878700 |
| I | -0.54109700 | -2.93866000 | -0.46772400 |
| I | 0.43842100 | 2.03839800 | -1.74771200 |
| H | 6.16898700 | 0.20987300 | -0.13595700 |
| H | -5.58267400 | 2.28354300 | -0.46308300 |

**8a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.26182000 | 0.91253900 | 1.64110700 |
| C | 1.31133200 | 1.92710300 | 0.63265900 |
| H | 2.18617300 | 0.51643700 | 2.04422100 |
| H | 0.14346400 | 3.31825200 | -0.52217500 |
| C | 2.60932700 | 2.38685000 | 0.10188900 |
| C | 3.74774500 | 2.45322600 | 0.92687300 |
| C | 2.73256700 | 2.77851300 | -1.24478400 |
| C | 4.96459700 | 2.90780400 | 0.42455300 |
| H | 3.67292500 | 2.17953100 | 1.97487800 |
| C | 3.95297200 | 3.22182000 | -1.74760900 |
| H | 1.87635100 | 2.69559200 | -1.90717600 |
| C | 5.07189000 | 3.29181400 | -0.91403300 |
| H | 5.82929700 | 2.96406000 | 1.07951400 |
| H | 4.03338400 | 3.50332100 | -2.79357900 |

| | | | |
|---|---|---|---|
| C | 0.02712000 | 0.55168700 | 2.24798100 |
| H | 0.00085500 | -0.03989600 | 3.15730800 |
| C | -1.17164900 | 1.00221900 | 1.62889800 |
| H | -2.12648500 | 0.67969000 | 2.02634600 |
| C | -1.13654100 | 2.02142800 | 0.62210300 |
| C | 0.10828300 | 2.48997700 | 0.17561900 |
| C | -2.39212300 | 2.57789000 | 0.08201600 |
| C | -3.53003900 | 2.72644300 | 0.89705900 |
| C | -2.47387900 | 2.98094500 | -1.26451300 |
| C | -4.70514100 | 3.27145700 | 0.38523800 |
| H | -3.48589300 | 2.44483600 | 1.94473100 |
| C | -3.65330700 | 3.51482000 | -1.77682900 |
| H | -1.62021500 | 2.83667000 | -1.91958200 |
| C | -4.77141400 | 3.66587100 | -0.95296700 |
| H | -5.56930000 | 3.38993500 | 1.03255400 |
| H | -3.70305700 | 3.80404700 | -2.82261100 |
| Pt | -0.02687300 | -0.75236400 | 0.50335100 |
| I | -1.99741700 | -2.23742700 | -0.45435200 |
| I | 1.78618500 | -2.39324000 | -0.50956700 |
| H | 6.02339800 | 3.63899200 | -1.30669700 |
| H | -5.69085300 | 4.08385500 | -1.35298700 |

**9a**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.38716800 | -0.40714800 | 2.61588000 |
| C | -1.35691100 | -0.00452900 | 0.38171500 |
| H | -3.24106700 | -0.49208400 | 3.28004900 |
| H | -1.41184600 | 0.97280500 | -0.11966500 |
| C | -1.40142800 | -1.07081000 | -0.73657200 |
| C | -1.46758800 | -2.42908600 | -0.40710600 |
| C | -1.35925500 | -0.68700900 | -2.08009600 |
| C | -1.49419600 | -3.39387900 | -1.41380800 |
| H | -1.49196900 | -2.73621600 | 0.63525300 |
| C | -1.38897900 | -1.65480000 | -3.08597200 |
| H | -1.28996800 | 0.36496900 | -2.34220800 |
| C | -1.45655300 | -3.00898500 | -2.75578300 |
| H | -1.54086800 | -4.44622300 | -1.14814300 |
| H | -1.35488900 | -1.34637900 | -4.12714600 |
| C | -1.08202500 | -0.52389300 | 3.16992300 |
| H | -0.99514700 | -0.74609900 | 4.23137800 |
| C | 0.07711200 | -0.32893900 | 2.43984900 |
| H | 1.04541800 | -0.39582400 | 2.92124600 |
| C | -0.00789900 | -0.02288500 | 1.06902300 |
| C | -2.56731200 | -0.13193300 | 1.28698000 |
| C | -3.91025500 | 0.03737200 | 0.70811000 |
| C | -5.00302700 | -0.69475800 | 1.21619700 |
| C | -4.14687400 | 0.94260000 | -0.34548000 |
| C | -6.28177400 | -0.52353700 | 0.69533000 |
| H | -4.83822700 | -1.42846200 | 1.99929800 |
| C | -5.42978700 | 1.11968800 | -0.85729900 |
| H | -3.33396100 | 1.53808000 | -0.74774700 |
| C | -6.50116700 | 0.38774800 | -0.34116500 |
| H | -7.10707100 | -1.10752500 | 1.09251200 |
| H | -5.59268600 | 1.83434600 | -1.65874900 |
| Pt | 1.54869700 | 0.39651200 | 0.08250700 |
| I | 2.87943000 | -1.89841000 | 0.21191200 |
| I | 0.93793800 | 2.92986100 | -0.50483400 |
| H | -7.50001500 | 0.52372900 | -0.74586400 |
| H | -1.47602200 | -3.76123700 | -3.53924900 |

**10a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.75467900 | 2.10598400 | 0.78532800 |
| C | -0.91463200 | 0.99499800 | 2.52758700 |
| H | -3.45824600 | 2.55514400 | 0.09136100 |
| H | -0.27105100 | 0.55499000 | 3.27859200 |
| C | -1.02938600 | -1.26980000 | 1.45352500 |
| C | -1.79168500 | -2.30322300 | 0.83968600 |
| C | 0.22335400 | -1.64180100 | 2.05261700 |
| C | -1.31177200 | -3.59590100 | 0.77585000 |
| H | -2.76842400 | -2.07825800 | 0.43590600 |
| C | 0.69610100 | -2.97231200 | 1.95060100 |
| H | 0.73313300 | -1.00127300 | 2.76269500 |
| C | -0.04907900 | -3.93553800 | 1.30549900 |
| H | -1.92298400 | -4.36364000 | 0.30973600 |
| H | 1.64842000 | -3.22100500 | 2.40785500 |
| C | -2.19723600 | 2.89104400 | 1.80216700 |
| H | -2.49015900 | 3.93228200 | 1.89946900 |
| C | -1.27292700 | 2.33462700 | 2.67456000 |
| H | -0.83270200 | 2.92327000 | 3.47291000 |
| C | -1.44906900 | 0.16897700 | 1.49186500 |
| C | -2.40765100 | 0.76999500 | 0.59007600 |
| C | -3.05254200 | 0.08731400 | -0.57372100 |
| C | -4.44726100 | -0.07866800 | -0.58391100 |
| C | -2.31298300 | -0.31953400 | -1.69650200 |
| C | -5.08594100 | -0.66385200 | -1.67897700 |
| H | -5.02992600 | 0.24139400 | 0.27618300 |
| C | -2.95548600 | -0.89637800 | -2.79184900 |
| H | -1.23688700 | -0.17283400 | -1.70855900 |
| C | -4.34099900 | -1.07591900 | -2.78524100 |
| H | -6.16483200 | -0.79315000 | -1.66668300 |
| H | -2.36919700 | -1.19963600 | -3.65480300 |
| Pt | 0.62190400 | 0.04433700 | 0.40886000 |
| I | 1.21033500 | 2.36681600 | -0.70219600 |
| I | 2.54249900 | -1.19611100 | -0.92464800 |
| H | -4.83732300 | -1.52720100 | -3.63999200 |
| H | 0.31472500 | -4.95587700 | 1.23203200 |

**11a**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.64730600 | 1.25911000 | 1.94985100 |
| C | 1.22937600 | -1.05742500 | -0.34147700 |
| H | 2.19302500 | 2.13048100 | 2.29399300 |
| H | 1.89243600 | -1.75151700 | 0.17346700 |
| C | 1.72676200 | -0.65291900 | -1.64824800 |
| C | 0.97715000 | 0.11079900 | -2.56664900 |
| C | 3.03473200 | -1.05081900 | -1.99925300 |
| C | 1.53581800 | 0.49336000 | -3.77921800 |
| H | -0.05016800 | 0.36440500 | -2.32630800 |
| C | 3.59474600 | -0.65570300 | -3.21001300 |
| H | 3.61198100 | -1.65807700 | -1.30649000 |
| C | 2.84505800 | 0.11701900 | -4.10119600 |
| H | 0.95037700 | 1.08132600 | -4.47932100 |
| H | 4.60726100 | -0.95580800 | -3.46306900 |
| C | 1.56436400 | 0.00261000 | 2.76395700 |
| C | 0.46060200 | -0.79047500 | 2.06106900 |
| H | 0.62745200 | -1.87023100 | 2.09494200 |
| C | 0.40120400 | -0.23319300 | 0.61044600 |
| C | 1.02623700 | 1.17427400 | 0.75403600 |
| C | 1.13700300 | 2.25577300 | -0.25775300 |

| | | | |
|---|---|---|---|
| C | 2.40783300 | 2.80886600 | -0.50632000 |
| C | 0.03346300 | 2.79481100 | -0.93954200 |
| C | 2.57117700 | 3.85995600 | -1.40667600 |
| H | 3.27421000 | 2.39430000 | 0.00121200 |
| C | 0.19764400 | 3.85214300 | -1.83494700 |
| H | -0.95747000 | 2.40248600 | -0.75045600 |
| C | 1.46441600 | 4.38715800 | -2.07561900 |
| H | 3.56331600 | 4.26580900 | -1.58558600 |
| H | -0.67351900 | 4.26201200 | -2.33909600 |
| Pt | -1.54537900 | -0.46279500 | -0.00833100 |
| I | -3.06700500 | 1.43369200 | 1.01084900 |
| I | -0.58390100 | -2.88370700 | -0.84620900 |
| H | 1.58834600 | 5.20946400 | -2.77526900 |
| H | 3.27504700 | 0.41508200 | -5.05343000 |
| H | -0.48792800 | -0.58624000 | 2.56321600 |
| H | 1.38041200 | 0.17725600 | 3.82579400 |
| O | 2.80889500 | -0.77056800 | 2.66069700 |
| C | 3.84408500 | -0.33825300 | 3.42271600 |
| O | 3.79441800 | 0.64757600 | 4.12480100 |
| C | 5.03929000 | -1.25286700 | 3.27891200 |
| H | 4.78815500 | -2.25703200 | 3.63705300 |
| H | 5.32637300 | -1.34288700 | 2.22616200 |
| H | 5.87214700 | -0.85342900 | 3.85860700 |

**12a**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.92038100 | 0.65035500 | -0.72914000 |
| C | -1.15173000 | -1.58898000 | -0.41136000 |
| H | -3.66116000 | 1.44543400 | -0.73195200 |
| H | -1.65936600 | -1.82724300 | 0.53887800 |
| C | -0.08961300 | -2.65579200 | -0.63558600 |
| C | 0.71191100 | -2.66460800 | -1.78591100 |
| C | 0.04192100 | -3.70131600 | 0.28602300 |
| C | 1.63495000 | -3.68885300 | -1.99796000 |
| H | 0.63281900 | -1.86285200 | -2.51421100 |
| C | 0.96389100 | -4.72776300 | 0.07453800 |
| H | -0.57382700 | -3.70829700 | 1.18211800 |
| C | 1.76448800 | -4.72313500 | -1.06826700 |
| H | 2.25482800 | -3.67478200 | -2.89012300 |
| H | 1.05609500 | -5.52706900 | 0.80465100 |
| C | -3.38535800 | -0.68666100 | -1.22911900 |
| H | -4.02678400 | -0.54840600 | -2.10432600 |
| C | -2.23043800 | -1.62722300 | -1.52366700 |
| H | -1.77638300 | -1.33956000 | -2.47891800 |
| C | -0.68523400 | -0.16058600 | -0.19865900 |
| C | -1.67301400 | 0.91648100 | -0.24895100 |
| C | -1.35137700 | 2.31602500 | 0.16843800 |
| C | -1.55231800 | 3.36838900 | -0.73752800 |
| C | -0.91280800 | 2.61030300 | 1.46870100 |
| C | -1.30645500 | 4.68782900 | -0.35707400 |
| H | -1.87941900 | 3.14872800 | -1.75010500 |
| C | -0.67617100 | 3.93146800 | 1.84848300 |
| H | -0.76198400 | 1.80968900 | 2.18518500 |
| C | -0.86745700 | 4.97220400 | 0.93704300 |
| H | -1.45330800 | 5.49054300 | -1.07419800 |
| H | -0.34123500 | 4.14499900 | 2.85961000 |
| Pt | 1.09916900 | 0.20923000 | 0.16278400 |
| I | 1.39171300 | -0.55447600 | 2.69302000 |
| I | 2.00752100 | 1.23793800 | -2.11267900 |
| H | -0.67453700 | 5.99937700 | 1.23395500 |

| | | | |
|---|---|---|---|
| H | 2.48434700 | -5.51983400 | -1.23446100 |
| H | -2.60113900 | -2.65064400 | -1.63188900 |
| O | -4.20034600 | -1.30964100 | -0.18795700 |
| C | -5.49175400 | -0.88637200 | -0.10170400 |
| O | -5.95355800 | -0.01689700 | -0.80626500 |
| C | -6.23299400 | -1.64373500 | 0.97242200 |
| H | -6.19542800 | -2.71938600 | 0.77242300 |
| H | -5.75819000 | -1.47479700 | 1.94471100 |
| H | -7.26901600 | -1.30523800 | 1.00289800 |

**13a**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.53137300 | 1.35335200 | 1.16275600 |
| C | -1.70125700 | 0.37206900 | 1.58735300 |
| H | -3.60471100 | 1.26888100 | 1.29999900 |
| H | 0.39209800 | 0.10992500 | 2.21097600 |
| C | -2.21648900 | -0.88656900 | 2.18803400 |
| C | -3.36863800 | -1.49613400 | 1.66200700 |
| C | -1.58311000 | -1.48853200 | 3.28764600 |
| C | -3.87773800 | -2.66416400 | 2.22689900 |
| H | -3.84617500 | -1.06603700 | 0.78619900 |
| C | -2.09501100 | -2.65617800 | 3.85325300 |
| H | -0.69576100 | -1.03733200 | 3.72250200 |
| C | -3.24388800 | -3.24804100 | 3.32580700 |
| H | -4.76229500 | -3.12665300 | 1.79773400 |
| H | -1.59334400 | -3.10301000 | 4.70715100 |
| C | -2.00466400 | 2.64793100 | 0.61007800 |
| H | -1.82722900 | 3.33960500 | 1.44519200 |
| O | -2.97798000 | 3.37604500 | -0.17457200 |
| C | -3.56757900 | 2.74716100 | -1.22697200 |
| O | -3.33394500 | 1.60262500 | -1.54576000 |
| C | -0.68804900 | 2.45797300 | -0.15545200 |
| H | -0.25490600 | 3.42809900 | -0.41057400 |
| H | -0.92897900 | 1.94944900 | -1.10352300 |
| C | 0.30405800 | 1.63012900 | 0.67770400 |
| C | -0.24017800 | 0.57574300 | 1.46253900 |
| C | 1.64426300 | 2.21886300 | 0.94371100 |
| C | 2.36111200 | 2.84589600 | -0.09200300 |
| C | 2.20969000 | 2.19316100 | 2.22904300 |
| C | 3.61110100 | 3.40960200 | 0.14700400 |
| H | 1.94956300 | 2.86363600 | -1.09740600 |
| C | 3.45816200 | 2.76687000 | 2.46951000 |
| H | 1.66532100 | 1.73897800 | 3.05120400 |
| C | 4.16472100 | 3.37285000 | 1.42993200 |
| H | 4.15611000 | 3.87476600 | -0.66950700 |
| H | 3.87529400 | 2.74303500 | 3.47235200 |
| Pt | 0.27795000 | -0.24855600 | -0.47772400 |
| I | 0.04104100 | -1.58862500 | -2.73362300 |
| I | 2.42094500 | -1.50128600 | 0.42265800 |
| H | -3.63691600 | -4.16208300 | 3.76213400 |
| H | 5.13824400 | 3.81705000 | 1.61728400 |
| C | -4.53434900 | 3.67401200 | -1.92384000 |
| H | -3.99394200 | 4.52982000 | -2.34239900 |
| H | -5.04141800 | 3.13214200 | -2.72271000 |
| H | -5.26562000 | 4.06709500 | -1.21045000 |

**TS1a**

Imaginary frequency: -250.54 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 1.80746200 | 2.01989300 | -1.08583700 |

| | | | |
|---|---|---|---|
| C | 2.67277700 | 1.04236600 | -1.49600400 |
| H | 2.09398700 | 2.74485900 | -0.32984100 |
| H | 2.35543700 | 0.39997500 | -2.31641600 |
| C | 3.99441000 | 0.74807000 | -0.96613000 |
| C | 4.69926600 | -0.35114200 | -1.49912000 |
| C | 4.60520000 | 1.50914900 | 0.05279100 |
| C | 5.96920700 | -0.67943400 | -1.03382300 |
| H | 4.23912700 | -0.94625700 | -2.28402800 |
| C | 5.87220100 | 1.17699800 | 0.51822800 |
| H | 4.08878000 | 2.36373700 | 0.47768000 |
| C | 6.55829700 | 0.08379500 | -0.02293500 |
| H | 6.49816700 | -1.52810600 | -1.45729100 |
| H | 6.33104600 | 1.77216600 | 1.30236400 |
| C | 0.52385000 | 2.30795500 | -1.82030100 |
| H | 0.70647600 | 2.71228200 | -2.82226700 |
| O | -0.15133300 | 3.31404600 | -1.04279700 |
| C | -1.09616700 | 4.04991200 | -1.69801700 |
| O | -1.32503000 | 3.92544100 | -2.87982000 |
| C | -0.33675600 | 1.03348000 | -1.91271600 |
| H | -1.37752600 | 1.29733100 | -2.10642500 |
| H | -0.02158600 | 0.39341200 | -2.74742600 |
| C | -0.18563300 | 0.27540000 | -0.61968700 |
| C | 0.85073300 | 0.35516900 | 0.17384200 |
| C | 1.62668000 | 0.04050400 | 1.32288000 |
| C | 1.64500100 | 0.92358700 | 2.42768900 |
| C | 2.37092200 | -1.16058600 | 1.38163600 |
| C | 2.37887500 | 0.60327400 | 3.56356000 |
| H | 1.05679900 | 1.83476400 | 2.38228500 |
| C | 3.09787200 | -1.47291400 | 2.52502200 |
| H | 2.33392000 | -1.84344700 | 0.53960200 |
| C | 3.10437700 | -0.59315200 | 3.61245800 |
| H | 2.37815800 | 1.27520700 | 4.41668900 |
| H | 3.65413200 | -2.40417200 | 2.57391300 |
| Pt | -1.60787600 | -0.89145700 | 0.03701600 |
| I | -2.94690900 | 0.94057300 | 1.44076100 |
| I | -0.68699700 | -3.06211900 | -1.22418100 |
| H | 3.67065200 | -0.84368700 | 4.50541000 |
| H | 7.54995100 | -0.16885800 | 0.34167700 |
| C | -1.79550000 | 4.98595500 | -0.74736800 |
| H | -1.07139600 | 5.53018000 | -0.13387700 |
| H | -2.42710100 | 4.39852500 | -0.07051800 |
| H | -2.41523500 | 5.68211300 | -1.31357500 |

**TS2a**

Imaginary frequency: -897.83 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.53656200 | 1.83030000 | 1.28628800 |
| C | -2.22551300 | 0.51400900 | 1.05178300 |
| H | -2.06732500 | 2.74734700 | 1.05343700 |
| H | -2.00316500 | -0.27358700 | 1.76884500 |
| C | -3.60149000 | 0.40701700 | 0.48539000 |
| C | -4.29388500 | -0.80019500 | 0.67082500 |
| C | -4.24052800 | 1.44557200 | -0.20905700 |
| C | -5.58935300 | -0.96422700 | 0.18188300 |
| H | -3.80616000 | -1.61682800 | 1.19717400 |
| C | -5.53601500 | 1.28115300 | -0.69849100 |
| H | -3.72815000 | 2.38659900 | -0.38398300 |
| C | -6.21662800 | 0.07767600 | -0.50333800 |
| H | -6.10691600 | -1.90677900 | 0.33754400 |
| H | -6.01361500 | 2.09705700 | -1.23425300 |

| | | | |
|---|---|---|---|
| C | -0.55824100 | 1.83627800 | 2.43624500 |
| H | -1.00675300 | 1.67689700 | 3.41801800 |
| O | -0.07174200 | 3.29128600 | 2.62117000 |
| C | 1.08581800 | 3.70249600 | 2.21432000 |
| O | 1.95449800 | 2.95743800 | 1.67517200 |
| C | 0.51999700 | 0.85778900 | 2.04060300 |
| H | 1.10922600 | 0.33145800 | 2.78759000 |
| H | 1.50813700 | 1.90287800 | 1.64354800 |
| C | 0.23325000 | 0.29439100 | 0.79060300 |
| C | -0.98881900 | 0.91814600 | 0.18881500 |
| C | -1.10613100 | 1.19090900 | -1.27926000 |
| C | -0.91341800 | 2.48297600 | -1.78204200 |
| C | -1.38399700 | 0.14725000 | -2.17292500 |
| C | -0.99331800 | 2.73259800 | -3.15360700 |
| H | -0.69190100 | 3.29935300 | -1.09834200 |
| C | -1.46075100 | 0.39524000 | -3.54280300 |
| H | -1.53185900 | -0.85782200 | -1.79047500 |
| C | -1.26618600 | 1.68743400 | -4.03688100 |
| H | -0.83771900 | 3.74019700 | -3.52964700 |
| H | -1.67386200 | -0.42303500 | -4.22496100 |
| Pt | 1.22078200 | -1.10531000 | -0.01934400 |
| I | -0.27591700 | -3.13726600 | 0.86064000 |
| I | 3.16037900 | 0.37464800 | -1.09253600 |
| H | -1.32610300 | 1.87790900 | -5.10494700 |
| H | -7.22652900 | -0.04709400 | -0.88422500 |
| C | 1.38002500 | 5.15773600 | 2.39848100 |
| H | 0.63411700 | 5.62703100 | 3.04062500 |
| H | 2.38365400 | 5.27282000 | 2.81681500 |
| H | 1.37584700 | 5.64142600 | 1.41479900 |

**TS3a**

Imaginary frequency: -1208.73 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -3.16469800 | -0.97660600 | -0.83486800 |
| C | -4.43513200 | -1.01345100 | -1.26876600 |
| H | -2.86713500 | -0.40542400 | 0.04115500 |
| H | -4.65289800 | -1.60857000 | -2.15703100 |
| C | -5.59867100 | -0.32794900 | -0.69362800 |
| C | -6.85122100 | -0.49523200 | -1.31031200 |
| C | -5.52145200 | 0.49191800 | 0.44842400 |
| C | -7.99036300 | 0.13136400 | -0.80737900 |
| H | -6.92788100 | -1.12446600 | -2.19420900 |
| C | -6.65849500 | 1.11635000 | 0.95126100 |
| H | -4.56862700 | 0.64400500 | 0.94655200 |
| C | -7.89753600 | 0.93979200 | 0.32618500 |
| H | -8.94789100 | -0.01151200 | -1.30043600 |
| H | -6.57938100 | 1.74480300 | 1.83394800 |
| C | -2.05648200 | -1.66319200 | -1.55400100 |
| H | -2.42791300 | -2.20239700 | -2.43044900 |
| O | -1.56522400 | -2.75258400 | -0.63601900 |
| C | -0.39921300 | -3.31070000 | -0.83159900 |
| O | 0.40201100 | -2.92041200 | -1.72079500 |
| C | -0.89650900 | -0.75380900 | -1.99682200 |
| H | -0.92453100 | -0.48815600 | -3.05840800 |
| H | 0.02294700 | -1.78428800 | -2.01007700 |
| C | -0.31505900 | 0.12844900 | -1.13637300 |
| C | 0.29382200 | 0.89973400 | -0.29114500 |
| C | -0.09033400 | 2.23724700 | 0.19378300 |
| C | -0.84179800 | 3.08503000 | -0.64165700 |
| C | 0.26838400 | 2.68125000 | 1.47718600 |

| | | | |
|---|---|---|---|
| C | -1.23768700 | 4.34297700 | -0.19456200 |
| H | -1.09639000 | 2.75802200 | -1.64583000 |
| C | -0.13278400 | 3.94140400 | 1.91788400 |
| H | 0.85515300 | 2.03289600 | 2.11808100 |
| C | -0.88549200 | 4.77436700 | 1.08712300 |
| H | -1.81254200 | 4.99053800 | -0.85084500 |
| H | 0.14969700 | 4.27400700 | 2.91274700 |
| Pt | 1.94740700 | -0.05759800 | 0.24159400 |
| I | 3.41204200 | 0.79074300 | -1.80452900 |
| I | 0.99839800 | -1.22299000 | 2.46602700 |
| C | -0.04822800 | -4.42679300 | 0.09215800 |
| H | 0.64075200 | -5.11317600 | -0.40375200 |
| H | 0.46112900 | -3.98099900 | 0.95786800 |
| H | -0.94511400 | -4.94205900 | 0.43998600 |
| H | -1.18861800 | 5.75895900 | 1.43254900 |
| H | -8.78243700 | 1.43055500 | 0.72164400 |

**TS4a**

Imaginary frequency: -282.08 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 2.03711000 | -0.68262100 | -2.27577100 |
| C | 2.95372400 | 0.29004200 | -1.96048700 |
| H | 2.24194800 | -1.73143500 | -2.05962700 |
| H | 2.70097400 | 1.30722100 | -2.25831600 |
| C | 4.21088600 | 0.14193100 | -1.25281200 |
| C | 4.91464600 | 1.30888800 | -0.88559500 |
| C | 4.76720700 | -1.11242300 | -0.92042200 |
| C | 6.12511000 | 1.22866500 | -0.20491500 |
| H | 4.49779600 | 2.28003100 | -1.14013900 |
| C | 5.97665100 | -1.18962300 | -0.23982900 |
| H | 4.25949800 | -2.02615900 | -1.21239200 |
| C | 6.65782200 | -0.02155900 | 0.12103100 |
| H | 6.65354000 | 2.13653100 | 0.07056600 |
| H | 6.39614600 | -2.16079100 | 0.00602600 |
| C | 0.88702800 | -0.36663600 | -3.15341800 |
| H | 1.00476200 | -0.39504300 | -4.23414000 |
| C | -0.26073200 | -0.01758700 | -2.55109300 |
| H | -1.16948300 | 0.25405000 | -3.07365900 |
| C | -0.22874300 | -0.04183800 | -1.08845100 |
| C | 0.86716300 | -0.28974900 | -0.39896700 |
| C | 1.60620500 | -0.42069400 | 0.80891500 |
| C | 1.99560500 | -1.69864500 | 1.27266600 |
| C | 1.93341500 | 0.72295600 | 1.57525900 |
| C | 2.67871600 | -1.82699000 | 2.47678200 |
| H | 1.72347400 | -2.57506700 | 0.69309300 |
| C | 2.61167400 | 0.58228600 | 2.78021100 |
| H | 1.60968300 | 1.69864200 | 1.22744700 |
| C | 2.98677100 | -0.68896300 | 3.22965100 |
| H | 2.96070300 | -2.81182000 | 2.83725800 |
| H | 2.84210400 | 1.46061000 | 3.37578500 |
| Pt | -1.83661600 | 0.13294400 | 0.00869500 |
| I | -2.45923900 | -2.45914500 | 0.05139500 |
| I | -1.68990900 | 2.79066400 | 0.25559000 |
| H | 3.51303100 | -0.79368400 | 4.17452100 |
| H | 7.60512400 | -0.08785800 | 0.64866600 |

**TS5a**

Imaginary frequency: -140.63$cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -0.10171800 | 2.42714100 | 2.45952600 |

| | | | |
|---|---|---|---|
| C | 1.42676300 | 0.80048900 | 1.58187600 |
| H | 0.24534500 | 3.40907100 | 2.76219700 |
| H | 1.55659600 | 0.68801200 | 2.65217000 |
| C | 2.59787900 | 0.43843200 | 0.80795000 |
| C | 2.69132400 | 0.52263000 | -0.59913800 |
| C | 3.72965900 | 0.00402500 | 1.53667800 |
| C | 3.88384700 | 0.20939000 | -1.24052600 |
| H | 1.82789500 | 0.81181100 | -1.18339000 |
| C | 4.91722900 | -0.31186200 | 0.88990200 |
| H | 3.66489200 | -0.08013800 | 2.61860300 |
| C | 4.99694000 | -0.20448600 | -0.50276600 |
| H | 3.94070400 | 0.27043000 | -2.32294900 |
| H | 5.77705200 | -0.64365400 | 1.46412200 |
| C | -0.83456600 | 1.54146900 | 3.21191700 |
| H | -1.22259100 | 1.71293400 | 4.20904300 |
| C | -0.91178600 | 0.32072300 | 2.50240700 |
| H | -1.36689500 | -0.59031100 | 2.87335400 |
| C | -0.27638000 | 0.41095700 | 1.21918700 |
| C | 0.31068100 | 1.79509300 | 1.17656600 |
| C | 0.51614700 | 2.71070700 | -0.00603300 |
| C | 1.56550400 | 3.64134900 | 0.04680700 |
| C | -0.34236900 | 2.70978600 | -1.10993900 |
| C | 1.75644800 | 4.55350800 | -0.98963100 |
| H | 2.24532400 | 3.64470400 | 0.89589100 |
| C | -0.14420400 | 3.62208200 | -2.15016500 |
| H | -1.16005600 | 2.00094200 | -1.15759300 |
| C | 0.90109600 | 4.54433200 | -2.09433000 |
| H | 2.57527800 | 5.26578400 | -0.93661600 |
| H | -0.81722500 | 3.60893800 | -3.00285800 |
| Pt | -0.83272100 | -0.87769300 | -0.16336700 |
| I | -3.29827300 | 0.19272300 | -0.18195900 |
| I | 1.04577900 | -2.73709600 | -0.43413600 |
| H | 1.04998700 | 5.25227800 | -2.90498600 |
| H | 5.92319700 | -0.45355700 | -1.01310700 |

**TS6a**

Imaginary frequency: -65.33 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.70254500 | 0.86962600 | 2.77197300 |
| C | 0.55974100 | 1.87794200 | 0.98948700 |
| H | -2.60311200 | 1.07901100 | 3.33682500 |
| H | 0.17121500 | 2.58504100 | 1.72230800 |
| C | 1.56630100 | 2.42527400 | 0.13327300 |
| C | 1.87902500 | 1.88801900 | -1.13952300 |
| C | 2.20680600 | 3.62411700 | 0.54617500 |
| C | 2.80292100 | 2.52734600 | -1.95821000 |
| H | 1.37303000 | 0.98874400 | -1.47172400 |
| C | 3.14916200 | 4.23706000 | -0.26285200 |
| H | 1.95895800 | 4.04967400 | 1.51533700 |
| C | 3.44633500 | 3.68796100 | -1.51907500 |
| H | 3.02995400 | 2.11430300 | -2.93603600 |
| H | 3.64723000 | 5.14317400 | 0.06825200 |
| C | -0.46793100 | 0.50801100 | 3.36431500 |
| H | -0.31536900 | 0.34332200 | 4.42619300 |
| C | 0.49826600 | 0.34335500 | 2.38660300 |
| H | 1.51700800 | 0.00536300 | 2.50450300 |
| C | -0.14510000 | 0.57627200 | 1.03484700 |
| C | -1.57730500 | 0.96661400 | 1.39089300 |
| C | -2.53765100 | 1.58571400 | 0.47251000 |
| C | -3.76938900 | 2.07937500 | 0.94827500 |

| | | | |
|---|---|---|---|
| C | -2.25329100 | 1.72939600 | -0.90015800 |
| C | -4.68172000 | 2.68104600 | 0.08639800 |
| H | -4.02290300 | 1.98964100 | 1.99962500 |
| C | -3.15854400 | 2.34751900 | -1.75682600 |
| H | -1.32906600 | 1.32673300 | -1.29919300 |
| C | -4.37929100 | 2.82245300 | -1.26998500 |
| H | -5.62826000 | 3.04507900 | 0.47596000 |
| H | -2.91766000 | 2.44224500 | -2.81179400 |
| Pt | 0.24419200 | -1.05553600 | -0.10810400 |
| I | -2.20552500 | -1.95631900 | -0.59438800 |
| I | 2.92949300 | -1.26845900 | 0.08674200 |
| H | -5.08981600 | 3.29512900 | -1.94224800 |
| H | 4.17678500 | 4.17493700 | -2.15936000 |

**TS7a**

Imaginary frequency: -334.87 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.06398900 | 0.17543000 | 2.56219800 |
| C | 0.75957900 | 0.77911100 | 1.93541200 |
| H | -3.03079500 | 0.33133500 | 3.02659600 |
| H | 0.39358400 | 1.61805700 | 2.53623100 |
| C | 2.24346300 | 0.83255700 | 1.75207300 |
| C | 2.98159600 | -0.17794900 | 1.11829700 |
| C | 2.92321800 | 1.94016300 | 2.27882800 |
| C | 4.36759700 | -0.07507300 | 1.01256300 |
| H | 2.47307000 | -1.03599400 | 0.68853700 |
| C | 4.30894500 | 2.04744400 | 2.16327200 |
| H | 2.36258800 | 2.72641600 | 2.77932000 |
| C | 5.03524800 | 1.03702700 | 1.53152600 |
| H | 4.92533800 | -0.86293400 | 0.51447600 |
| H | 4.81826000 | 2.91619200 | 2.57078200 |
| C | -1.06714300 | -0.71078100 | 3.08250300 |
| H | -1.30640100 | -1.52400900 | 3.76337300 |
| C | 0.19451900 | -0.57747700 | 2.55176600 |
| H | 0.92719400 | -1.37452500 | 2.58324300 |
| C | -0.25576300 | 0.30134100 | 1.00473600 |
| C | -1.64536100 | 0.78996600 | 1.41415500 |
| C | -2.31925500 | 1.91232300 | 0.75940300 |
| C | -3.13829000 | 2.77343200 | 1.52473400 |
| C | -2.19942500 | 2.15605500 | -0.62302800 |
| C | -3.81769000 | 3.82723400 | 0.92593200 |
| H | -3.21508600 | 2.62545300 | 2.59765400 |
| C | -2.88331200 | 3.21432100 | -1.21842500 |
| H | -1.59114500 | 1.49794000 | -1.23120800 |
| C | -3.69350800 | 4.05126500 | -0.45004500 |
| H | -4.43707200 | 4.48265000 | 1.53169100 |
| H | -2.78214200 | 3.37926000 | -2.28706400 |
| Pt | -0.03784500 | -0.72834300 | -0.60986600 |
| I | 1.27272700 | 0.93761100 | -2.21574800 |
| I | -1.21348400 | -3.00816400 | 0.10280000 |
| H | -4.22328700 | 4.87714300 | -0.91661000 |
| H | 6.11531800 | 1.11472900 | 1.44335700 |

**TS8a**

Imaginary frequency: -855.05 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 1.22192400 | 0.22166200 | 3.33450300 |
| C | -1.15495700 | -0.41455100 | 1.95802700 |
| H | 2.12477600 | 0.47589300 | 3.88120400 |
| H | -0.19668300 | -1.29339000 | 1.50416400 |

| | | | |
|---|---|---|---|
| C | -2.47012200 | -0.70266400 | 1.30663700 |
| C | -3.54935600 | 0.13283500 | 1.62970800 |
| C | -2.67141900 | -1.78543400 | 0.43956700 |
| C | -4.80761400 | -0.09928000 | 1.07447700 |
| H | -3.39762100 | 0.98230200 | 2.28956900 |
| C | -3.93449600 | -2.01792300 | -0.10368400 |
| H | -1.84822000 | -2.44495800 | 0.18409000 |
| C | -5.00332300 | -1.17519100 | 0.20752700 |
| H | -5.63099400 | 0.56613200 | 1.31727400 |
| H | -4.07859700 | -2.86113000 | -0.77290700 |
| C | 0.04916800 | -0.08663900 | 4.05169700 |
| H | 0.07038900 | -0.08253100 | 5.13769100 |
| C | -1.11134100 | -0.40136800 | 3.38726600 |
| H | -2.01932500 | -0.65562400 | 3.92293500 |
| C | 0.04962000 | -0.06921100 | 1.19437500 |
| C | 1.26665300 | 0.23991000 | 1.94750600 |
| C | 2.55874000 | 0.56226800 | 1.29126400 |
| C | 3.70912800 | -0.14672900 | 1.67926900 |
| C | 2.68074800 | 1.58948800 | 0.34029200 |
| C | 4.94804500 | 0.14553400 | 1.11157000 |
| H | 3.62411700 | -0.95461800 | 2.40102400 |
| C | 3.92645000 | 1.89103300 | -0.20936100 |
| H | 1.80988500 | 2.16500100 | 0.04904000 |
| C | 5.05983700 | 1.16725200 | 0.16638900 |
| H | 5.82285800 | -0.42802500 | 1.40450900 |
| H | 4.00715500 | 2.69548300 | -0.93483300 |
| Pt | -0.00865400 | 0.04803600 | -0.75458700 |
| I | 1.06555500 | -2.38386200 | -1.12505200 |
| I | -1.14594400 | 2.45444000 | -0.94796900 |
| H | 6.02563000 | 1.39831900 | -0.27440000 |
| H | -5.98383300 | -1.35624400 | -0.22360300 |

**TS9a**

Imaginary frequency: -323.93cm$^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.04371400 | 1.96058000 | -1.74083300 |
| C | 1.75081800 | 0.13954700 | 0.12358700 |
| H | 0.96344300 | 3.01246700 | -2.00263600 |
| H | 1.61532400 | 0.16444900 | 1.20253000 |
| C | 3.15505000 | -0.11789900 | -0.32063900 |
| C | 4.17307600 | 0.78900100 | 0.01381100 |
| C | 3.48559500 | -1.30585400 | -0.98822900 |
| C | 5.49347000 | 0.52332700 | -0.33804500 |
| H | 3.92415900 | 1.70453300 | 0.54400100 |
| C | 4.81261900 | -1.57257600 | -1.33355400 |
| H | 2.71369400 | -2.04011500 | -1.19652000 |
| C | 5.81565800 | -0.65747800 | -1.01623300 |
| H | 6.27411600 | 1.23299700 | -0.07889800 |
| H | 5.05853900 | -2.49901000 | -1.84452300 |
| C | 1.00168400 | 0.91900700 | -2.72816600 |
| H | 1.14656500 | 1.08253500 | -3.78939700 |
| C | 0.77284700 | -0.27278100 | -2.12771000 |
| H | 0.78814400 | -1.25115200 | -2.59177200 |
| C | 0.57370100 | -0.12729700 | -0.65087500 |
| C | 1.00293200 | 1.55935100 | -0.41456800 |
| C | 0.75460300 | 2.50849400 | 0.70743800 |
| C | 1.42001500 | 3.74629000 | 0.69936900 |
| C | -0.09433600 | 2.20448100 | 1.78350800 |
| C | 1.22767000 | 4.66431000 | 1.73163400 |
| H | 2.10320000 | 3.98624600 | -0.11158200 |

| | | | |
|---|---|---|---|
| C | -0.27866000 | 3.12305000 | 2.81635000 |
| H | -0.63476800 | 1.26212600 | 1.79009800 |
| C | 0.37765700 | 4.35535200 | 2.79474900 |
| H | 1.75043900 | 5.61646700 | 1.70714600 |
| H | -0.94956300 | 2.87555000 | 3.63407000 |
| Pt | -1.16529700 | -0.75053900 | -0.03812800 |
| I | -0.20201800 | -2.84216000 | 1.29631900 |
| I | -2.81430100 | 1.04137300 | -1.12034600 |
| H | 0.22854300 | 5.06851100 | 3.60048100 |
| H | 6.84752800 | -0.86525600 | -1.28516700 |

**TS10a**

Imaginary frequency: -871.33cm$^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.28093500 | -0.23401800 | -2.73419700 |
| C | -1.32960100 | -0.20937900 | -0.49104000 |
| H | -3.15011900 | -0.27997200 | -3.38366500 |
| H | -0.43587400 | -1.31571000 | -0.76816100 |
| C | -1.48437600 | -0.08218100 | 0.99096500 |
| C | -2.05749900 | 1.09597000 | 1.49044300 |
| C | -1.06788900 | -1.08071800 | 1.88080400 |
| C | -2.20253400 | 1.27303500 | 2.86544800 |
| H | -2.37321100 | 1.87749400 | 0.80665200 |
| C | -1.22481300 | -0.90095600 | 3.25521700 |
| H | -0.61133600 | -1.99270900 | 1.50776300 |
| C | -1.78922300 | 0.27549900 | 3.75052400 |
| H | -2.63539900 | 2.19490100 | 3.24266300 |
| H | -0.89835500 | -1.68192900 | 3.93572500 |
| C | -0.99489400 | -0.19795900 | -3.31410100 |
| H | -0.89598100 | -0.18707300 | -4.39562200 |
| C | 0.12430800 | -0.20336200 | -2.52045900 |
| H | 1.11950100 | -0.19654700 | -2.94833200 |
| C | 0.00966500 | -0.18800000 | -1.08042700 |
| C | -2.48149900 | -0.26214100 | -1.36127500 |
| C | -3.87396000 | -0.32806900 | -0.83806800 |
| C | -4.84220100 | 0.55604800 | -1.34216400 |
| C | -4.26488400 | -1.29517700 | 0.10244100 |
| C | -6.16755700 | 0.47820600 | -0.91467300 |
| H | -4.54895800 | 1.32240500 | -2.05491800 |
| C | -5.59141200 | -1.37642200 | 0.52098900 |
| H | -3.53283600 | -1.99025600 | 0.50043400 |
| C | -6.54615500 | -0.48999200 | 0.01645300 |
| H | -6.90103800 | 1.17733500 | -1.30626400 |
| H | -5.87960100 | -2.13580000 | 1.24227800 |
| Pt | 1.64766000 | 0.10940200 | -0.05736800 |
| I | 1.50801100 | 2.76397400 | -0.01596700 |
| I | 2.26747200 | -2.50305300 | 0.03980700 |
| H | -7.57817400 | -0.55261100 | 0.34977500 |
| H | -1.90399200 | 0.41601000 | 4.82158200 |

**TS11a**

Imaginary frequency: -351.59 cm$^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 2.39758000 | 0.70489200 | 2.31078800 |
| C | 1.42843600 | 0.30201200 | 0.14012400 |
| H | 3.25367200 | 0.76525300 | 2.97689700 |
| H | 1.56530500 | -0.12379000 | -0.84344900 |
| C | 0.42268900 | 1.80327600 | -0.29650100 |
| C | 0.73015300 | 3.03237000 | 0.31544300 |
| C | 0.05107500 | 1.77254000 | -1.65651800 |

| | | | |
|---|---|---|---|
| C | 0.63173200 | 4.21028100 | -0.41385700 |
| H | 1.02805800 | 3.06451100 | 1.35680000 |
| C | -0.03898600 | 2.95794900 | -2.37724300 |
| H | -0.20136100 | 0.82496100 | -2.12012600 |
| C | 0.24536600 | 4.17827900 | -1.75903800 |
| H | 0.85043900 | 5.15807200 | 0.06886800 |
| H | -0.34358800 | 2.92753700 | -3.41872200 |
| C | 1.08467900 | 0.82994000 | 2.86652200 |
| H | 0.98401700 | 1.00037400 | 3.93491700 |
| C | -0.03035500 | 0.72117700 | 2.08780400 |
| H | -1.02403400 | 0.82683000 | 2.50653600 |
| C | 0.08438600 | 0.41469300 | 0.65987400 |
| C | 2.60240900 | 0.47048300 | 0.97006500 |
| C | 3.95236100 | 0.33264000 | 0.37721800 |
| C | 5.00522700 | 1.15788700 | 0.81021100 |
| C | 4.21380800 | -0.62537700 | -0.61908900 |
| C | 6.28157500 | 1.02859200 | 0.26578600 |
| H | 4.81439800 | 1.92199700 | 1.55895700 |
| C | 5.49225000 | -0.75389300 | -1.15952900 |
| H | 3.42738000 | -1.30095600 | -0.94506300 |
| C | 6.52946900 | 0.07222600 | -0.72121500 |
| H | 7.08046000 | 1.68132200 | 0.60660300 |
| H | 5.67887900 | -1.50817200 | -1.91863100 |
| Pt | -1.38792100 | -0.72828200 | -0.01868400 |
| I | -3.37714700 | 1.05044400 | 0.15262400 |
| I | 0.11210500 | -2.92152400 | -0.33458600 |
| H | 7.52420400 | -0.02842900 | -1.14606100 |
| H | 0.16411600 | 5.10394200 | -2.32131500 |

**TS12a**

Imaginary frequency: -253.76 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.22495900 | 1.13362900 | -1.06957400 |
| C | -1.64154500 | -0.36355500 | 0.08470300 |
| H | -3.14284800 | 1.67612700 | -0.87180100 |
| H | -2.26326200 | -1.04196700 | -0.50091900 |
| C | -2.01514800 | -0.35039900 | 1.51641200 |
| C | -1.08150900 | -0.28195100 | 2.56246400 |
| C | -3.38171800 | -0.47099900 | 1.83167500 |
| C | -1.51085900 | -0.31971100 | 3.88904200 |
| H | -0.02319600 | -0.25693300 | 2.33376100 |
| C | -3.80743700 | -0.49871100 | 3.15596100 |
| H | -4.11262300 | -0.53925800 | 1.02899800 |
| C | -2.86961800 | -0.42020300 | 4.18987800 |
| H | -0.77606900 | -0.28346200 | 4.68802100 |
| H | -4.86604300 | -0.58854600 | 3.38205300 |
| C | -2.01595800 | 0.37615700 | -2.36543800 |
| C | -0.63511500 | -0.28758900 | -2.13725700 |
| H | 0.13267700 | 0.15861600 | -2.77134900 |
| C | -0.32831200 | 0.00662700 | -0.64578400 |
| C | -0.99867500 | 1.36079600 | -0.40926800 |
| C | -0.75225900 | 2.42330300 | 0.55034500 |
| C | -1.62478300 | 3.53550700 | 0.58814100 |
| C | 0.36712700 | 2.41030700 | 1.40698100 |
| C | -1.38980700 | 4.58884100 | 1.46168700 |
| H | -2.47169200 | 3.58863600 | -0.08825800 |
| C | 0.59532600 | 3.46781700 | 2.28272200 |
| H | 1.05744600 | 1.57620500 | 1.36397300 |
| C | -0.28041600 | 4.55449700 | 2.31451300 |
| H | -2.06283700 | 5.44084500 | 1.47421700 |

| | | | |
|---|---|---|---|
| H | 1.46512300 | 3.44627300 | 2.93214000 |
| Pt | 1.49212000 | -0.60447400 | -0.14349300 |
| I | 2.84550600 | 1.44187800 | -1.22216400 |
| I | 0.79815000 | -3.03387300 | 0.72807100 |
| H | -0.09508700 | 5.38181600 | 2.99405500 |
| H | -3.19787000 | -0.45021800 | 5.22513000 |
| H | -0.67086400 | -1.36171500 | -2.33032800 |
| H | -2.03696000 | 1.07951200 | -3.20307100 |
| O | -3.01272300 | -0.63857900 | -2.61312900 |
| C | -4.24695300 | -0.19567400 | -2.99053600 |
| O | -4.54014200 | 0.97836100 | -3.03079000 |
| C | -5.14651600 | -1.35126100 | -3.34873600 |
| H | -4.78691400 | -1.82345100 | -4.26975000 |
| H | -5.12718900 | -2.11362400 | -2.56410100 |
| H | -6.16317500 | -0.98695600 | -3.49960600 |

**TS13a**

Imaginary frequency: -302.18 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.18689700 | 1.38458900 | 0.88809600 |
| C | 0.26568200 | -0.43513400 | 1.94420900 |
| H | -2.86354000 | 2.23004100 | 0.93419000 |
| H | -0.04903700 | 0.12178100 | 2.82849600 |
| C | 1.02947200 | -1.63285000 | 2.24761200 |
| C | 1.49110400 | -2.54699700 | 1.27667300 |
| C | 1.30388300 | -1.88320700 | 3.61041600 |
| C | 2.21252400 | -3.66953500 | 1.66679700 |
| H | 1.29242100 | -2.35658100 | 0.22608100 |
| C | 2.04048100 | -2.99837300 | 3.99201500 |
| H | 0.94502200 | -1.18739200 | 4.36523700 |
| C | 2.49353600 | -3.89437500 | 3.01875100 |
| H | 2.56741300 | -4.36591600 | 0.91327300 |
| H | 2.25778000 | -3.17306300 | 5.04135200 |
| C | -2.72065100 | -0.01035700 | 0.88866800 |
| H | -3.20569700 | -0.25239500 | -0.06457300 |
| C | -1.54598100 | -0.95986400 | 1.14064100 |
| H | -1.38808400 | -1.75685600 | 0.42004500 |
| C | -0.14159100 | 0.15313600 | 0.71631600 |
| C | -0.85119300 | 1.48875100 | 0.78388200 |
| C | -0.13166500 | 2.78010800 | 0.70266900 |
| C | -0.66840000 | 3.82729400 | -0.06652300 |
| C | 1.04728200 | 3.01084200 | 1.42862000 |
| C | -0.04991000 | 5.07568000 | -0.09429500 |
| H | -1.56021400 | 3.64811400 | -0.66006500 |
| C | 1.65982400 | 4.26294700 | 1.40598800 |
| H | 1.49296200 | 2.21259400 | 2.01352400 |
| C | 1.11387700 | 5.29852900 | 0.64540900 |
| H | -0.47261800 | 5.87161200 | -0.70108600 |
| H | 2.57045700 | 4.42466700 | 1.97577800 |
| Pt | 0.66253300 | -0.18942600 | -1.05106800 |
| I | 3.16551200 | 0.47733800 | -0.40838400 |
| I | -1.38113000 | -1.04415700 | -2.56023100 |
| H | 1.59851000 | 6.27061300 | 0.62053500 |
| H | 3.06606800 | -4.76922300 | 3.31415300 |
| H | -1.64979300 | -1.37927500 | 2.14318000 |
| O | -3.67118100 | -0.24562200 | 1.96185800 |
| C | -4.93878800 | 0.20464900 | 1.74620100 |
| O | -5.26707800 | 0.81777000 | 0.75687500 |
| C | -5.84141700 | -0.17300300 | 2.89610800 |
| H | -6.82775800 | 0.26440100 | 2.73873900 |

| | | | |
|---|---|---|---|
| H | -5.92773700 | -1.26310600 | 2.96023000 |
| H | -5.42063900 | 0.17924500 | 3.84325200 |

**TS14a**

Imaginary frequency: -714.60 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 0.93750300 | 2.21968400 | -2.13167200 |
| C | -1.41706200 | 1.09644400 | -0.86335000 |
| H | 1.80929900 | 2.61639000 | -2.64440000 |
| H | -0.37232700 | 1.50404000 | 0.15282700 |
| C | -2.64302800 | 0.73058900 | -0.12666000 |
| C | -3.86405500 | 0.68920700 | -0.82960300 |
| C | -2.64587100 | 0.44050700 | 1.25142000 |
| C | -5.04127200 | 0.32096000 | -0.18406600 |
| H | -3.89264300 | 0.89589500 | -1.89440300 |
| C | -3.83377500 | 0.10959400 | 1.89694500 |
| H | -1.72872000 | 0.49947100 | 1.82492700 |
| C | -5.03115900 | 0.03389200 | 1.18245500 |
| H | -5.96608100 | 0.26103300 | -0.75015400 |
| H | -3.81757200 | -0.09440800 | 2.96335700 |
| C | -0.34328700 | 2.96887800 | -2.30553800 |
| H | -0.44001100 | 3.28387100 | -3.34684000 |
| C | -1.57254200 | 2.12303300 | -1.96231200 |
| H | -1.80049700 | 1.52946100 | -2.86165400 |
| C | -0.12201600 | 0.56663800 | -0.60510500 |
| C | 1.05442500 | 1.09117800 | -1.40404100 |
| C | 2.39215700 | 0.43509400 | -1.31760800 |
| C | 3.48449200 | 1.17244700 | -0.83640200 |
| C | 2.60363800 | -0.87541500 | -1.77471400 |
| C | 4.76046000 | 0.60932200 | -0.79832400 |
| H | 3.32451700 | 2.18069300 | -0.46520700 |
| C | 3.88279200 | -1.43087500 | -1.74589000 |
| H | 1.77274700 | -1.45650600 | -2.15946700 |
| C | 4.96265300 | -0.69412300 | -1.25375600 |
| H | 5.59256300 | 1.18824800 | -0.40717400 |
| H | 4.03255200 | -2.44401600 | -2.10863800 |
| Pt | 0.15455800 | -1.06273400 | 0.46617100 |
| I | 1.28844900 | 0.06326200 | 2.61541800 |
| I | -1.00756100 | -2.69319600 | -1.30881900 |
| H | 5.95558400 | -1.13458700 | -1.22453500 |
| H | -5.95226700 | -0.24169400 | 1.68807700 |
| H | -2.43346200 | 2.76854900 | -1.77630900 |
| O | -0.31556500 | 4.28171800 | -1.64544500 |
| C | -0.29257400 | 4.37598700 | -0.30246900 |
| O | -0.38928200 | 3.42962700 | 0.45702700 |
| C | -0.13050700 | 5.80860800 | 0.14037600 |
| H | -0.80708100 | 6.46437900 | -0.41476300 |
| H | -0.31985400 | 5.88032100 | 1.21174900 |
| H | 0.89353200 | 6.13793600 | -0.06930800 |

**TS15a**

Imaginary frequency: -765.32 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 2.59219600 | 0.73806600 | 0.12077500 |
| C | 1.47509400 | 1.15368300 | -0.51712900 |
| H | 3.35203600 | 1.44808900 | 0.43257000 |
| H | -0.19472900 | 0.46430000 | -1.70412200 |
| C | 1.34116100 | 2.56822900 | -0.95487700 |
| C | 2.45539400 | 3.24263900 | -1.48611700 |
| C | 0.12186800 | 3.25993500 | -0.85947000 |

| | | | |
|---|---|---|---|
| C | 2.35936100 | 4.57069200 | -1.89665200 |
| H | 3.39666200 | 2.71134400 | -1.59918800 |
| C | 0.02944200 | 4.59073600 | -1.26759400 |
| H | -0.74801400 | 2.76105000 | -0.44558800 |
| C | 1.14457000 | 5.25107000 | -1.78619700 |
| H | 3.23046200 | 5.07087500 | -2.31155100 |
| H | -0.92036100 | 5.11009600 | -1.17625800 |
| C | 2.77664100 | -0.66898900 | 0.55264200 |
| H | 2.74914600 | -0.79016000 | 1.64334600 |
| O | 4.28074900 | -1.00524400 | 0.30367700 |
| C | 4.67903100 | -1.39097300 | -0.85815600 |
| O | 3.88806800 | -1.66727300 | -1.81610200 |
| C | 1.91198500 | -1.65531200 | -0.17244000 |
| H | 2.02067700 | -2.70218000 | 0.11042400 |
| H | 2.84367200 | -1.67108000 | -1.37710200 |
| C | 0.71091600 | -1.24501900 | -0.74219700 |
| C | 0.37191200 | 0.18855100 | -0.81502100 |
| C | -0.16154800 | -2.26460200 | -1.37685900 |
| C | -0.43138100 | -3.47770700 | -0.71967600 |
| C | -0.68465000 | -2.05825600 | -2.66368500 |
| C | -1.20870100 | -4.45672800 | -1.33384200 |
| H | -0.07138300 | -3.62967300 | 0.29369800 |
| C | -1.44601100 | -3.04774100 | -3.28252400 |
| H | -0.49064100 | -1.12841700 | -3.18907700 |
| C | -1.71347800 | -4.24712200 | -2.61938000 |
| H | -1.42830200 | -5.37944500 | -0.80428500 |
| H | -1.83805100 | -2.87609000 | -4.28080200 |
| Pt | -0.99898300 | 0.14109200 | 0.74922800 |
| I | 0.18729600 | -0.29281400 | 3.13023600 |
| I | -3.06443000 | 0.61430400 | -0.88151000 |
| H | 1.06721900 | 6.28620700 | -2.10755800 |
| H | -2.31962500 | -5.01088300 | -3.09842300 |
| C | 6.15422100 | -1.50853200 | -1.06948100 |
| H | 6.68492700 | -1.43543800 | -0.11968500 |
| H | 6.37880800 | -2.45302600 | -1.57203900 |
| H | 6.47759900 | -0.69525400 | -1.72997400 |

**ACE b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -1.65040000 | 1.44060100 | -0.34645400 |
| C | -2.57859600 | 2.39759100 | -0.28783600 |
| H | -0.61304700 | 1.69694200 | -0.55828400 |
| H | -3.60809900 | 2.11827200 | -0.07165100 |
| C | -1.87819200 | -0.03040600 | -0.13826200 |
| H | -1.66094100 | -0.58967900 | -1.05464900 |
| O | -3.26622700 | -0.24566600 | 0.20098300 |
| C | -3.81105600 | -1.44117300 | -0.13834200 |
| O | -3.19888900 | -2.33617000 | -0.67814000 |
| C | -1.00176700 | -0.62160900 | 0.99922800 |
| H | -1.27206000 | -1.67854500 | 1.11259700 |
| H | -1.26151600 | -0.10948800 | 1.93470600 |
| C | 0.43006900 | -0.50647000 | 0.73336300 |
| C | 1.61496400 | -0.41191600 | 0.49092000 |
| C | 3.01313100 | -0.30768300 | 0.21075500 |
| C | 3.78740700 | 0.71547700 | 0.79213800 |
| C | 3.64015800 | -1.22762100 | -0.65246900 |
| C | 5.14931900 | 0.81228500 | 0.51611200 |
| H | 3.30859000 | 1.42639300 | 1.45864800 |
| C | 5.00241200 | -1.12360000 | -0.92396400 |
| H | 3.04731800 | -2.01803500 | -1.10247100 |

| | | | |
|---|---|---|---|
| C | 5.76147700 | -0.10513200 | -0.34183100 |
| H | 5.73498600 | 1.60619700 | 0.97186900 |
| H | 5.47337500 | -1.83990100 | -1.59184200 |
| H | 6.82401400 | -0.02685600 | -0.55539500 |
| C | -5.27201400 | -1.48630300 | 0.24530200 |
| H | -5.39443000 | -1.24705500 | 1.30640400 |
| H | -5.83096400 | -0.73665000 | -0.32531600 |
| H | -5.67131400 | -2.47926900 | 0.03607100 |
| C | -2.30901100 | 3.85955400 | -0.50311400 |
| H | -1.25072200 | 4.05047000 | -0.71072800 |
| H | -2.89679900 | 4.25108100 | -1.34456900 |
| H | -2.59486100 | 4.44923600 | 0.37858700 |

**product A-b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 3.15053400 | 0.71290400 | -0.15160700 |
| C | 2.65573300 | -0.56672100 | 0.13460100 |
| H | 4.22511800 | 0.87755900 | -0.18923800 |
| H | 0.87635300 | -1.73739600 | 0.40953300 |
| C | 2.27582400 | 1.77313600 | -0.38888000 |
| H | 2.67077800 | 2.75921300 | -0.61985600 |
| C | 0.89686700 | 1.57288400 | -0.34768800 |
| H | 0.22311400 | 2.39728900 | -0.56330600 |
| C | 0.37119400 | 0.30092500 | -0.06816300 |
| C | 1.26984800 | -0.75264200 | 0.16852400 |
| C | -1.09669700 | 0.07317900 | -0.02614400 |
| C | -1.96042400 | 1.03406300 | 0.52742900 |
| C | -1.66176500 | -1.10784400 | -0.53741800 |
| C | -3.33807600 | 0.82224400 | 0.56863600 |
| H | -1.54348700 | 1.94319100 | 0.95187800 |
| C | -3.03919100 | -1.32122200 | -0.49558500 |
| H | -1.01631300 | -1.85281700 | -0.99438800 |
| C | -3.88422800 | -0.35700300 | 0.05773600 |
| H | -3.98510200 | 1.57653600 | 1.00900900 |
| H | -3.45370200 | -2.23909100 | -0.90455400 |
| H | -4.95768700 | -0.52282200 | 0.09009900 |
| C | 3.59696700 | -1.71144600 | 0.43436400 |
| H | 3.90034400 | -1.71145800 | 1.48998800 |
| H | 3.12894100 | -2.68022800 | 0.23041100 |
| H | 4.51213900 | -1.64471400 | -0.16440800 |

**product B-b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -3.47222900 | -0.46031200 | -0.12353400 |
| C | -2.87392000 | 0.76011500 | 0.18701300 |
| H | -4.55562200 | -0.54443600 | -0.14476200 |
| C | -2.67116300 | -1.56900600 | -0.39526200 |
| H | -3.11975000 | -2.52904100 | -0.63629300 |
| C | -1.28470600 | -1.43661100 | -0.35806200 |
| H | -0.65446600 | -2.29370400 | -0.58040200 |
| C | -0.66998700 | -0.20853700 | -0.06035900 |
| C | -1.48121700 | 0.91463400 | 0.22462600 |
| C | 0.82108800 | -0.15163800 | -0.04051000 |
| C | 1.55024300 | -1.05331900 | 0.75290800 |
| C | 1.53597900 | 0.76017400 | -0.83453800 |
| C | 2.94543600 | -1.03974900 | 0.75894500 |
| H | 1.01259600 | -1.76019700 | 1.37936400 |
| C | 2.93101100 | 0.77326100 | -0.83209500 |
| H | 0.99371400 | 1.44938500 | -1.47561900 |
| C | 3.64170200 | -0.12545000 | -0.03375300 |

| | | | |
|---|---|---|---|
| H | 3.48817600 | -1.74238200 | 1.38608900 |
| H | 3.46328800 | 1.48264400 | -1.46062100 |
| H | 4.72836100 | -0.11400800 | -0.03082300 |
| C | -0.90362900 | 2.26354000 | 0.59812100 |
| H | -0.64667900 | 2.86056900 | -0.28645500 |
| H | -1.62985500 | 2.84383000 | 1.17692000 |
| H | 0.00935400 | 2.16607800 | 1.19307800 |
| H | -3.50075900 | 1.61865400 | 0.41852000 |

**1b-1**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 2.15335500 | 0.16035400 | 0.71385900 |
| C | 1.39209700 | 0.44705200 | 1.85199400 |
| H | 2.71760300 | -0.76909000 | 0.70478600 |
| H | 1.03781700 | 1.46664200 | 1.98962300 |
| C | 2.63066600 | 1.16991100 | -0.31381000 |
| H | 2.80669800 | 0.65223900 | -1.25980500 |
| O | 3.90146100 | 1.66844700 | 0.16580400 |
| C | 4.74609400 | 2.17383600 | -0.77944700 |
| O | 4.44492600 | 2.28173600 | -1.94605800 |
| C | 1.64529500 | 2.33562600 | -0.56819200 |
| H | 1.80078900 | 2.71959500 | -1.58064400 |
| H | 1.85546900 | 3.15565000 | 0.13054600 |
| C | 0.25538100 | 1.87634200 | -0.37259800 |
| C | -0.91111900 | 1.84094400 | 0.06454300 |
| C | -2.25134400 | 2.18781600 | 0.44123700 |
| C | -2.91769100 | 1.52470300 | 1.48779000 |
| C | -2.89252500 | 3.24650100 | -0.23180400 |
| C | -4.19946500 | 1.92124400 | 1.85719100 |
| H | -2.43125000 | 0.69191400 | 1.98545500 |
| C | -4.17322900 | 3.63705700 | 0.14932700 |
| H | -2.38403400 | 3.74511500 | -1.05087000 |
| C | -4.82899300 | 2.97700600 | 1.19199200 |
| H | -4.71149200 | 1.39999700 | 2.66067900 |
| H | -4.66362400 | 4.45199100 | -0.37524200 |
| Pt | 0.05968900 | -0.27830100 | 0.11638900 |
| I | -1.91823300 | -0.91854000 | -1.60366000 |
| I | 0.53022500 | -2.90869800 | 0.46440700 |
| H | -5.83140100 | 3.28011300 | 1.48068600 |
| C | 6.06893600 | 2.55711600 | -0.16396300 |
| H | 5.91438700 | 3.21579700 | 0.69622100 |
| H | 6.58146800 | 1.65967000 | 0.19929700 |
| H | 6.68631900 | 3.05373300 | -0.91303700 |
| C | 1.38274100 | -0.39055200 | 3.10106000 |
| H | 0.38487100 | -0.42498400 | 3.55006700 |
| H | 1.71566400 | -1.41304200 | 2.91638800 |
| H | 2.05712300 | 0.07461500 | 3.83486100 |

**1b-2**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 3.56761700 | 1.25016600 | 0.05356900 |
| C | 2.90843300 | 2.32779600 | -0.38255300 |
| H | 4.47714800 | 1.37528800 | 0.63973100 |
| H | 1.99466000 | 2.21356100 | -0.96581400 |
| C | 3.20204300 | -0.18971500 | -0.18994400 |
| H | 3.22044700 | -0.73558300 | 0.75868700 |
| O | 4.20245000 | -0.80698500 | -1.05430000 |
| C | 5.31640200 | -1.29275000 | -0.44771800 |
| O | 5.51690700 | -1.22362100 | 0.74484300 |
| C | 1.86952000 | -0.45062500 | -0.91502900 |

| | | | |
|---|---|---|---|
| H | 1.82775600 | -1.51139300 | -1.18571900 |
| H | 1.82183600 | 0.11616900 | -1.85182900 |
| C | 0.69821000 | -0.12762200 | -0.07671000 |
| C | 0.11262100 | 0.30541800 | 0.96270300 |
| C | -0.15051200 | 0.79501100 | 2.28226900 |
| C | 0.29512400 | 0.05423400 | 3.39675900 |
| C | -0.83181100 | 2.01423400 | 2.47598300 |
| C | 0.08405400 | 0.54486300 | 4.68161200 |
| H | 0.80076700 | -0.89315700 | 3.24065400 |
| C | -1.04515900 | 2.48743300 | 3.76635800 |
| H | -1.19061600 | 2.56548100 | 1.61240800 |
| C | -0.58650500 | 1.75745100 | 4.86800200 |
| H | 0.43431200 | -0.02275100 | 5.53854500 |
| H | -1.57147700 | 3.42559400 | 3.91510900 |
| Pt | -1.29882600 | -0.31841500 | -0.55804700 |
| I | -1.57009000 | -2.83356400 | 0.26392700 |
| I | -1.58662800 | 2.04843900 | -1.76562600 |
| H | -0.75795900 | 2.13107100 | 5.87361800 |
| C | 6.24630300 | -1.91296900 | -1.46331900 |
| H | 5.73221800 | -2.70939500 | -2.01108700 |
| H | 6.55495100 | -1.15977700 | -2.19588400 |
| H | 7.12239700 | -2.31557900 | -0.95397600 |
| C | 3.33012300 | 3.74461400 | -0.11994300 |
| H | 4.25374600 | 3.79173800 | 0.46606300 |
| H | 3.49191800 | 4.28396500 | -1.06263500 |
| H | 2.54877200 | 4.29236900 | 0.42322300 |

**2b-1**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.81130600 | 0.43975000 | 0.51000600 |
| C | -2.40981000 | -0.55190200 | 1.52654200 |
| H | -3.40753800 | 1.29496800 | 0.80992400 |
| H | -2.33535800 | -1.58909400 | 1.20825000 |
| C | -2.92653000 | -0.06164800 | -0.92230400 |
| H | -3.04755100 | 0.78759300 | -1.59996100 |
| O | -4.02129100 | -0.97343800 | -1.13345200 |
| C | -5.26174000 | -0.41175700 | -1.16301900 |
| O | -5.45725100 | 0.76644700 | -0.96519300 |
| C | -1.60856200 | -0.81490100 | -1.19258200 |
| H | -1.25112400 | -0.71468200 | -2.21989500 |
| H | -1.71932600 | -1.89255700 | -1.00401800 |
| C | -0.62494200 | -0.23803800 | -0.20254200 |
| C | -1.30474200 | 0.40977200 | 0.90479400 |
| C | -0.64223400 | 1.43369000 | 1.77674100 |
| C | -0.96558600 | 2.78992900 | 1.64717400 |
| C | 0.31828900 | 1.04607400 | 2.72245000 |
| C | -0.33757200 | 3.74576000 | 2.44814400 |
| H | -1.70236100 | 3.10257000 | 0.91216500 |
| C | 0.94658700 | 2.00267900 | 3.51978100 |
| H | 0.58048400 | -0.00292100 | 2.82444800 |
| C | 0.62002400 | 3.35405800 | 3.38487100 |
| H | -0.59389200 | 4.79524000 | 2.33398500 |
| H | 1.69136000 | 1.69040100 | 4.24649500 |
| Pt | 1.20264100 | -0.34924400 | -0.47339200 |
| I | 1.65515300 | 1.79946000 | -1.96335500 |
| I | 1.69361400 | -2.63834500 | 0.79413200 |
| H | 1.11038400 | 4.09793000 | 4.00663700 |
| C | -6.31331600 | -1.44536800 | -1.48073500 |
| H | -6.16917200 | -1.81889600 | -2.50052200 |

| | | | |
|---|---|---|---|
| H | -6.22540400 | -2.30124800 | -0.80441500 |
| H | -7.30244500 | -0.99506800 | -1.39270500 |
| C | -2.76223900 | -0.37639000 | 2.98544500 |
| H | -2.83354200 | 0.67732600 | 3.26574100 |
| H | -3.73360700 | -0.84967000 | 3.17401800 |
| H | -2.02111500 | -0.85425600 | 3.63378300 |

**3b-1**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -2.91399100 | -0.84980500 | 2.81848900 |
| C | -3.39674500 | -0.13956100 | 1.77056900 |
| H | -3.61316800 | -1.48106600 | 3.36579700 |
| H | -2.74037800 | 0.54069800 | 1.23475800 |
| C | -1.56647900 | -0.86057100 | 3.33315000 |
| H | -1.45677800 | -1.36397200 | 4.29269300 |
| C | -0.39418100 | -0.36510600 | 2.81878000 |
| H | 0.51625000 | -0.51870700 | 3.39726800 |
| C | -0.22915400 | 0.29183600 | 1.59303000 |
| C | -0.04444700 | 1.06879500 | 0.59477800 |
| C | -0.09450700 | 2.42920300 | 0.09861400 |
| C | -0.04113100 | 2.71179500 | -1.27624900 |
| C | -0.20684600 | 3.48725200 | 1.02254200 |
| C | -0.10729100 | 4.03180300 | -1.71818000 |
| H | 0.04924900 | 1.89308300 | -1.98223600 |
| C | -0.27331500 | 4.80129900 | 0.57031700 |
| H | -0.23326400 | 3.27038100 | 2.08651400 |
| C | -0.22397000 | 5.07714600 | -0.79976200 |
| H | -0.06569800 | 4.24241900 | -2.78283000 |
| H | -0.35813700 | 5.61235600 | 1.28803800 |
| Pt | 0.51813600 | -0.66010100 | -0.31768400 |
| I | -1.77284900 | -1.19619300 | -1.57115600 |
| I | 3.07765100 | -0.59899600 | 0.41501500 |
| H | -0.27222200 | 6.10489800 | -1.14844800 |
| C | -4.81529600 | -0.19576000 | 1.30614200 |
| H | -5.28045600 | 0.79831500 | 1.36237000 |
| H | -4.85604700 | -0.49867500 | 0.25217700 |
| H | -5.41436800 | -0.89682300 | 1.89540700 |

**4b-1**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 2.14024600 | -1.49549000 | 2.22732800 |
| C | 1.58891500 | -2.52725500 | 1.23345600 |
| H | 3.20168000 | -1.53023500 | 2.45322700 |
| H | 0.60565100 | -2.92281500 | 1.47756200 |
| C | 1.14814200 | -1.06966000 | 3.23320300 |
| H | 1.22239100 | -1.31445600 | 4.28897500 |
| C | 0.09509800 | -0.43098100 | 2.64830200 |
| H | -0.80090300 | -0.07661900 | 3.14106100 |
| C | 0.31075400 | -0.36533100 | 1.22406300 |
| C | 1.62032300 | -1.00566500 | 0.89516400 |
| C | 2.49189900 | -0.49875800 | -0.21755500 |
| C | 3.61110000 | 0.29405200 | 0.06322100 |
| C | 2.17437300 | -0.78694400 | -1.55282600 |
| C | 4.40286400 | 0.79255100 | -0.97324700 |
| H | 3.85843400 | 0.53299900 | 1.09414700 |
| C | 2.96573500 | -0.28749000 | -2.58703700 |
| H | 1.30155900 | -1.39254900 | -1.77866100 |
| C | 4.08139700 | 0.50272300 | -2.29998600 |
| H | 5.26548900 | 1.41125200 | -0.74200900 |
| H | 2.70847300 | -0.51483400 | -3.61777800 |

| | | | |
|---|---|---|---|
| Pt | -0.91554100 | 0.32913300 | 0.00842000 |
| I | -0.42792200 | 2.92938100 | 0.15702500 |
| I | -2.09395000 | -1.93545500 | -0.74895400 |
| H | 4.69528800 | 0.89284100 | -3.10703900 |
| C | 2.50521100 | -3.48831700 | 0.52100500 |
| H | 3.48320000 | -3.04703000 | 0.31110800 |
| H | 2.65036200 | -4.38550600 | 1.13494800 |
| H | 2.06341400 | -3.80416700 | -0.43064000 |
| H | 5.74667200 | -2.49639200 | -0.31107200 |
| H | 3.22388900 | -0.59389200 | -3.23231700 |
| Pt | -0.88061100 | 0.45301500 | -0.15522100 |
| I | 0.62852500 | 2.65791700 | -0.19337200 |
| I | -2.89673200 | -1.26775500 | -0.42275800 |
| H | 5.34676900 | -1.75894600 | -2.65601800 |
| C | 0.39920200 | -3.05587400 | 0.12157800 |
| H | 1.23913400 | -3.75668800 | 0.19487100 |
| H | -0.53061600 | -3.63016000 | 0.21451100 |
| H | 0.39662200 | -2.57478400 | -0.85656800 |

**5b**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 2.08284100 | -0.35568200 | 2.46795000 |
| C | 0.43410800 | -2.06988400 | 1.24287600 |
| H | 3.12314100 | -0.27158200 | 2.76920700 |
| H | 0.43090900 | -2.50032700 | 2.24540000 |
| C | 0.99450100 | 0.08113400 | 3.25074200 |
| H | 1.06271800 | 0.44956800 | 4.26713800 |
| C | -0.15895800 | -0.11305800 | 2.52211600 |
| H | -1.17908600 | -0.05679000 | 2.88307600 |
| C | 0.15791600 | -0.62724900 | 1.16642700 |
| C | 1.68450400 | -0.82937300 | 1.18787200 |
| C | 2.66863100 | -1.07455400 | 0.09342400 |
| C | 3.86549300 | -1.74171100 | 0.40643200 |
| C | 2.44789100 | -0.67085200 | -1.23167700 |
| C | 4.82651200 | -1.98189500 | -0.57385100 |
| H | 4.04137900 | -2.08703400 | 1.42283900 |
| C | 3.40853300 | -0.92127100 | -2.21310800 |
| H | 1.53393400 | -0.14612000 | -1.48632700 |
| C | 4.60002000 | -1.57150000 | -1.88955300 |

**6b**

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.82827300 | 0.04521000 | 1.77234600 |
| C | -0.02925800 | 0.47839400 | 2.66877500 |
| H | -3.88064200 | 0.29735500 | 1.77948600 |
| H | -0.63911600 | 1.24488700 | 3.14833800 |
| C | -2.23401600 | -0.84472300 | 2.64260400 |
| H | -2.77040400 | -1.43486200 | 3.38060300 |
| C | -0.80547700 | -0.88611900 | 2.44423400 |
| H | -0.21791100 | -1.77393700 | 2.64773800 |
| C | -0.50532500 | 0.04132600 | 1.29105400 |
| C | -1.83437900 | 0.66543000 | 0.97005500 |
| C | -2.06965000 | 1.81677000 | 0.12567300 |
| C | -3.39125800 | 2.25958200 | -0.13237300 |
| C | -0.99575900 | 2.53610500 | -0.44856900 |
| C | -3.62424100 | 3.36917600 | -0.93221200 |
| H | -4.23803200 | 1.71949100 | 0.27617100 |
| C | -1.23506700 | 3.65923000 | -1.23024800 |
| H | 0.02170000 | 2.20048800 | -0.28866000 |

| | | | |
|---|---|---|---|
| C | -2.54646300 | 4.07583200 | -1.47940200 |
| H | -4.64306000 | 3.68680400 | -1.13240300 |
| H | -0.39695400 | 4.19938900 | -1.65973300 |
| Pt | 0.63878900 | -0.57962400 | -0.23296500 |
| I | 2.74509700 | 1.07197700 | -0.26664500 |
| I | -1.07243100 | -2.52291100 | -0.91855300 |
| H | -2.73108600 | 4.94464800 | -2.10515100 |
| C | 1.39177400 | 0.41541300 | 3.15672600 |
| H | 1.90583500 | 1.35647700 | 2.93500200 |
| H | 1.40541100 | 0.26550600 | 4.24371500 |
| H | 1.95174600 | -0.38587700 | 2.66969800 |
| H | 0.29698500 | -2.17856200 | -1.42846300 |
| C | 3.59952500 | -2.08981900 | -2.24180600 |
| H | 5.19968500 | -1.62882300 | -0.86925600 |
| H | 1.80081800 | -2.50785000 | -3.35814200 |
| Pt | -0.47887200 | 0.52528900 | -0.23450800 |
| I | -2.69199500 | -0.70042300 | -1.08664600 |
| I | 1.37152900 | 2.41085000 | 0.02511900 |
| H | 4.25952400 | -2.23069400 | -3.09324000 |
| C | -1.48728000 | 0.77327000 | 2.84460100 |
| H | -2.18907500 | 0.67492600 | 3.67932800 |
| H | -0.63458600 | 1.37794000 | 3.16498000 |
| H | -1.98402500 | 1.28673000 | 2.01995300 |

**7b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 1.29761600 | -2.28627700 | 2.28976300 |
| C | -1.01233400 | -0.63519700 | 2.39601800 |
| H | 2.15731300 | -2.95139200 | 2.25410300 |
| H | -1.92068300 | -1.14893600 | 2.00593500 |
| C | 0.53950300 | -2.23176900 | 3.50107100 |
| H | 0.85195100 | -2.83651200 | 4.34688100 |
| C | -0.56348000 | -1.45253300 | 3.55984000 |
| H | -1.17949700 | -1.41228200 | 4.45487200 |
| C | -0.09916000 | -0.64972600 | 1.19459100 |
| C | 1.00562300 | -1.55697800 | 1.14487300 |
| C | 1.89027300 | -1.71245100 | -0.04581200 |
| C | 3.27939300 | -1.57385100 | 0.09840700 |
| C | 1.36712800 | -2.05122700 | -1.30392200 |
| C | 4.12793400 | -1.75592400 | -0.99356500 |
| H | 3.69384100 | -1.29201300 | 1.06286900 |
| C | 2.21933100 | -2.24046500 | -2.39194200 |

**8b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.21966200 | 2.42985700 | -0.90395700 |
| C | 0.53011200 | 2.83737200 | 0.24923100 |
| H | -1.13263300 | 2.96081900 | -1.15288000 |
| H | 2.34130800 | 2.56641100 | 1.36107500 |
| C | 0.33752300 | 1.51961600 | -1.84328800 |
| H | -0.10310800 | 1.38418900 | -2.82554300 |
| C | 1.50847800 | 0.80739800 | -1.46046900 |
| H | 1.90026500 | 0.03926300 | -2.11671900 |
| C | 2.24149700 | 1.17932900 | -0.29637900 |
| C | 1.75514700 | 2.23472500 | 0.51068100 |
| C | 3.49359100 | 0.48251100 | 0.05298300 |
| C | 4.36897200 | 0.01817700 | -0.94697500 |
| C | 3.84049900 | 0.27125400 | 1.40119600 |
| C | 5.55671300 | -0.62527700 | -0.60865500 |
| H | 4.13575800 | 0.19146100 | -1.99322300 |

| | | | |
|---|---|---|---|
| C | 5.02216400 | -0.38473800 | 1.73628800 |
| H | 3.15971600 | 0.58652500 | 2.18586900 |
| C | 5.88597400 | -0.83107900 | 0.73323100 |
| H | 6.22677600 | -0.96486100 | -1.39318800 |
| H | 5.26433400 | -0.55590100 | 2.78114500 |
| Pt | -0.58791500 | 0.16580500 | -0.39913600 |
| I | -0.47042900 | -2.43180300 | 0.08042000 |
| I | -3.07356000 | 0.29372300 | 0.49520900 |
| H | 6.80889500 | -1.34040200 | 0.99564500 |
| C | -0.03931700 | 3.89641700 | 1.14977900 |
| H | -0.98593300 | 3.54833200 | 1.58314900 |
| H | 0.64365600 | 4.14278200 | 1.96690100 |
| H | -0.26040200 | 4.81345500 | 0.58999700 |
| H | 4.94890400 | 2.35887600 | 0.87158700 |
| C | 5.54226700 | -0.79235400 | -1.30306500 |
| H | 3.50102000 | -1.29969400 | -0.89968800 |
| C | 6.58349200 | 0.11220900 | -1.08443800 |
| H | 7.16528800 | 1.95812300 | -0.12901800 |
| H | 5.70591500 | -1.67631500 | -1.91244400 |
| Pt | -1.38010200 | -0.24916600 | -0.00679900 |
| I | -0.69815200 | -2.82299800 | 0.12281000 |
| I | -2.74759700 | 1.97799000 | -0.49984400 |
| H | 7.55837200 | -0.05993200 | -1.53149300 |
| C | 1.37764100 | 1.30171700 | -1.33109100 |
| H | 0.51153600 | 0.98617900 | -1.91572900 |
| H | 1.24946400 | 2.35199600 | -1.05478200 |
| H | 2.28698700 | 1.19558000 | -1.92760800 |

**9b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | 2.63465400 | 1.37531400 | 1.93862200 |
| C | 0.20128800 | 0.48513300 | 0.72799100 |
| H | 3.52254800 | 1.66708800 | 2.48991700 |
| H | 1.58476100 | -0.62808600 | -0.40822800 |
| C | 1.36493600 | 1.54743800 | 2.55345600 |
| H | 1.32992300 | 2.01560100 | 3.53482200 |
| C | 0.17979600 | 1.10824500 | 1.98837000 |
| H | -0.75644800 | 1.22395200 | 2.52146000 |
| C | 1.49050300 | 0.40486500 | -0.04750900 |
| C | 2.74388400 | 0.78858300 | 0.70569300 |
| C | 4.05478600 | 0.55736400 | 0.07527700 |
| C | 5.11704300 | 1.46151400 | 0.28387700 |
| C | 4.28907100 | -0.57108900 | -0.73648600 |
| C | 6.36470300 | 1.24222800 | -0.29163800 |

**10b**

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.14362500 | -2.06694900 | 0.94845100 |
| C | -1.07113800 | -1.60407800 | 1.92771100 |
| H | 0.71121000 | -2.65775900 | 1.25949400 |
| C | -0.49668800 | -1.98694300 | -0.42897700 |
| H | 0.08743100 | -2.51306000 | -1.17651200 |
| C | -1.75892300 | -1.42880400 | -0.78388300 |
| H | -2.03653400 | -1.38085100 | -1.83227900 |
| C | -2.61624100 | -0.90572200 | 0.17230800 |
| C | -2.26719100 | -1.00537000 | 1.57521600 |
| C | -3.90352000 | -0.29988900 | -0.27188200 |
| C | -4.80937900 | -1.05653900 | -1.03293300 |
| C | -4.21978200 | 1.03781800 | 0.01762800 |
| C | -6.00409100 | -0.49435800 | -1.48396300 |

| | | | |
|---|---|---|---|
| H | -4.57926800 | -2.09467700 | -1.25750300 |
| C | -5.40944100 | 1.60143600 | -0.44242100 |
| H | -3.51837400 | 1.64744400 | 0.58015600 |
| C | -6.30718400 | 0.83616200 | -1.19029900 |
| H | -6.69712300 | -1.09706000 | -2.06452000 |
| H | -5.63142800 | 2.64173600 | -0.22130800 |
| Pt | 0.70417300 | -0.12705600 | 0.10564900 |
| I | 1.46068500 | 2.37761700 | 0.06932800 |
| I | 3.03900300 | -1.16238900 | -0.51664000 |
| H | -7.23540700 | 1.27574800 | -1.54452300 |
| C | -3.21148800 | -0.52712500 | 2.65085200 |
| H | -3.24072100 | 0.56724600 | 2.70824000 |
| H | -4.23694400 | -0.86073900 | 2.46034200 |
| H | -2.89922000 | -0.90012300 | 3.63050100 |
| H | -0.82045700 | -1.72244500 | 2.97800100 |

**TS1b**

Imaginary frequency: -240.21 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -1.38230000 | 2.70397000 | -1.50763900 |
| C | -0.16105700 | 3.09941200 | -1.96076900 |
| H | -1.94940700 | 3.34785200 | -0.83900700 |
| H | 0.35680500 | 2.47950000 | -2.69119700 |
| C | -2.06982300 | 1.45499600 | -1.98272100 |
| H | -2.47796400 | 1.57304900 | -2.99327300 |
| O | -3.16402100 | 1.23931900 | -1.07349000 |
| C | -4.18422200 | 0.45510100 | -1.53236600 |
| O | -4.21631600 | 0.01053600 | -2.65725900 |
| C | -1.09572200 | 0.26156600 | -1.94742600 |
| H | -1.65608200 | -0.67427100 | -1.94537700 |
| H | -0.45852500 | 0.23581400 | -2.84153800 |
| C | -0.22591800 | 0.38899900 | -0.72419000 |
| C | 0.10627400 | 1.51533800 | -0.14479100 |
| C | 0.75154300 | 2.29991100 | 0.85677300 |
| C | -0.00024000 | 2.89287000 | 1.89532800 |
| C | 2.15573400 | 2.46958500 | 0.83108000 |
| C | 0.63890000 | 3.63262400 | 2.88367600 |
| H | -1.07571900 | 2.74880600 | 1.91764800 |
| C | 2.78611500 | 3.19973300 | 1.83381600 |
| H | 2.73110200 | 1.98370400 | 0.04903700 |
| C | 2.03011300 | 3.78457900 | 2.85497700 |
| H | 0.05887600 | 4.07973100 | 3.68542900 |
| H | 3.86646100 | 3.30892500 | 1.82365500 |
| Pt | 0.50166000 | -1.19445600 | 0.15363800 |
| I | -1.50048900 | -1.61226900 | 1.86247600 |
| I | 2.71637100 | -1.24802700 | -1.34569700 |
| H | 2.52660100 | 4.35451500 | 3.63543600 |
| C | -5.20530400 | 0.22390800 | -0.44981900 |
| H | -5.47466400 | 1.16536300 | 0.03793800 |
| H | -4.77065500 | -0.43145100 | 0.31426100 |
| H | -6.08870200 | -0.25005500 | -0.87898800 |
| C | 0.49690100 | 4.39275700 | -1.60746800 |
| H | 1.50479000 | 4.22449800 | -1.20857400 |
| H | 0.61165600 | 5.00543500 | -2.51162100 |
| H | -0.07905700 | 4.96089700 | -0.87170900 |

**TS2b**

Imaginary frequency: -913.07 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -1.77887500 | 2.37533200 | -0.78395200 |

| | | | |
|---|---|---|---|
| C | -0.41979600 | 2.93786800 | -0.47711000 |
| H | -2.65333300 | 2.89478100 | -0.40388200 |
| H | 0.33491600 | 2.85430700 | -1.25812200 |
| C | -1.89339500 | 1.61625000 | -2.08316600 |
| H | -1.74282900 | 2.22067200 | -2.97925400 |
| O | -3.37739900 | 1.24688800 | -2.28186200 |
| C | -3.84360300 | 0.06309200 | -2.04359100 |
| O | -3.13518200 | -0.91706600 | -1.67392600 |
| C | -0.96657300 | 0.43365000 | -1.93364900 |
| H | -0.51703500 | -0.04759100 | -2.79891000 |
| H | -2.05034000 | -0.54190600 | -1.63173700 |
| C | -0.32631000 | 0.46800900 | -0.68928100 |
| C | -0.84163700 | 1.59573500 | 0.15216000 |
| C | -1.04701900 | 1.46372800 | 1.63186900 |
| C | -2.33077100 | 1.31271700 | 2.16909100 |
| C | 0.05457800 | 1.47979800 | 2.50031400 |
| C | -2.51568900 | 1.17788600 | 3.54668700 |
| H | -3.19288200 | 1.29564400 | 1.50669300 |
| C | -0.12927400 | 1.34367900 | 3.87598100 |
| H | 1.05469600 | 1.58838600 | 2.09147300 |
| C | -1.41425100 | 1.19242500 | 4.40303200 |
| H | -3.51850100 | 1.05769900 | 3.94772900 |
| H | 0.73345100 | 1.35396900 | 4.53635400 |
| Pt | 1.04761900 | -0.72192400 | -0.15076400 |
| I | 3.10978500 | 0.84943300 | -0.79977100 |
| I | -0.47523500 | -2.77613900 | 0.59970100 |
| H | -1.55540000 | 1.08515400 | 5.47502500 |
| C | -5.31666300 | -0.12374500 | -2.22671100 |
| H | -5.77889400 | 0.78340300 | -2.61655600 |
| H | -5.48845500 | -0.96542500 | -2.90459100 |
| H | -5.76054800 | -0.38681300 | -1.26041100 |
| C | -0.29033300 | 4.17880400 | 0.37913800 |
| H | -0.38325900 | 5.07562200 | -0.24491600 |
| H | -1.05763500 | 4.22034800 | 1.15774500 |
| H | 0.68893100 | 4.20732300 | 0.86808000 |

**TS3b**

Imaginary frequency: -1198.88 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -3.90134400 | 0.62351900 | -1.02322300 |
| C | -5.08466700 | 1.06374600 | -1.46130000 |
| H | -3.44966400 | 1.02621200 | -0.11800000 |
| H | -5.50123600 | 0.63324000 | -2.37411500 |
| C | -3.09953200 | -0.40600200 | -1.74629300 |
| H | -3.60673600 | -0.72995400 | -2.65983200 |
| O | -3.11184200 | -1.63120900 | -0.87067300 |
| C | -2.22397400 | -2.57756400 | -1.02773900 |
| O | -1.27737200 | -2.49482100 | -1.85340000 |
| C | -1.66071000 | 0.00341000 | -2.10522100 |
| H | -1.52601400 | 0.26923700 | -3.15862000 |
| H | -1.19158200 | -1.29374300 | -2.11437200 |
| C | -0.83664400 | 0.59048000 | -1.19183600 |
| C | -0.02817000 | 1.06395900 | -0.29647400 |
| C | 0.10565600 | 2.44445400 | 0.20095900 |
| C | -0.21129800 | 3.51858100 | -0.65178600 |
| C | 0.53324900 | 2.71253400 | 1.51171000 |
| C | -0.11614900 | 4.83079600 | -0.19580400 |
| H | -0.51446000 | 3.31743300 | -1.67540900 |
| C | 0.62446700 | 4.02894600 | 1.96120000 |
| H | 0.78647600 | 1.88638900 | 2.16667000 |

| | | | |
|---|---|---|---|
| C | 0.30077600 | 5.08986900 | 1.11257700 |
| H | -0.35759900 | 5.65173000 | -0.86543000 |
| H | 0.95522800 | 4.22455100 | 2.97728500 |
| Pt | 1.09052600 | -0.46250000 | 0.29797600 |
| I | 2.91010300 | -0.22602000 | -1.62121700 |
| I | -0.40208800 | -1.19330000 | 2.40640400 |
| C | -2.37431200 | -3.76372100 | -0.13712800 |
| H | -1.94973400 | -4.64515700 | -0.62126000 |
| H | -1.80297100 | -3.55409500 | 0.77780900 |
| H | -3.42051300 | -3.91973100 | 0.13137800 |
| H | 0.38155300 | 6.11441400 | 1.46524700 |
| C | -5.90683600 | 2.12806600 | -0.79891400 |
| H | -6.07257900 | 2.97415800 | -1.47869000 |
| H | -6.89855000 | 1.74120600 | -0.53067800 |
| H | -5.42678900 | 2.50488200 | 0.10922400 |

**TS4b**

Imaginary frequency: -276.54 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.49298000 | -0.25971900 | 2.65767800 |
| C | -3.20974400 | 0.82826200 | 2.24437200 |
| H | -2.92201300 | -1.25855500 | 2.56428700 |
| H | -2.77313500 | 1.81194500 | 2.41615100 |
| C | -1.21862700 | -0.08409800 | 3.38793700 |
| H | -1.20797100 | -0.08695800 | 4.47493700 |
| C | -0.12386200 | 0.12082700 | 2.63890300 |
| H | 0.86798500 | 0.29298900 | 3.03770300 |
| C | -0.33885100 | 0.07088400 | 1.19085900 |
| C | -1.53984700 | -0.03608300 | 0.64591900 |
| C | -2.37716500 | -0.13092400 | -0.50874600 |
| C | -2.99879100 | -1.35386300 | -0.84478400 |
| C | -2.56210400 | 0.99378400 | -1.34605800 |
| C | -3.77941500 | -1.44868100 | -1.99187700 |
| H | -2.83537400 | -2.22105700 | -0.21285800 |
| C | -3.33698000 | 0.88519700 | -2.49666800 |
| H | -2.05842200 | 1.92313200 | -1.09867100 |
| C | -3.94829400 | -0.33166000 | -2.81747500 |
| H | -4.24433200 | -2.39463100 | -2.25309600 |
| H | -3.45939700 | 1.74559300 | -3.14778200 |
| Pt | 1.14048800 | -0.00868800 | -0.07548200 |
| I | 1.33548200 | -2.66506400 | -0.14840900 |
| I | 1.38024600 | 2.63850600 | -0.35895900 |
| H | -4.55133400 | -0.41234800 | -3.71762500 |
| C | -4.56410500 | 0.79173000 | 1.62509200 |
| H | -4.56206700 | 1.31497100 | 0.66028100 |
| H | -4.92606200 | -0.22840600 | 1.47254400 |
| H | -5.27494800 | 1.32466900 | 2.27134300 |

**TS5b**

Imaginary frequency: -113.62 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 2.32340100 | -0.58070100 | 2.53498200 |
| C | 1.14976400 | -2.07374800 | 1.27656600 |
| H | 3.30560700 | -0.92904400 | 2.82724700 |
| H | 0.73349200 | -2.32955800 | 2.24228800 |
| C | 1.33704100 | -0.08102400 | 3.35275400 |
| H | 1.42226400 | 0.08619500 | 4.42063900 |
| C | 0.16657500 | 0.14072400 | 2.58937700 |
| H | -0.76275800 | 0.53883700 | 2.97861500 |
| C | 0.37072200 | -0.15972500 | 1.22209700 |

| | | | |
|---|---|---|---|
| C | 1.78695600 | -0.72407600 | 1.13999600 |
| C | 2.75240100 | -0.54733700 | -0.01751000 |
| C | 3.99198000 | -1.20606000 | 0.04369500 |
| C | 2.45896800 | 0.23636700 | -1.13690900 |
| C | 4.91751700 | -1.08094100 | -0.99042400 |
| H | 4.24266300 | -1.82551400 | 0.90214100 |
| C | 3.38879200 | 0.36023000 | -2.17340500 |
| H | 1.50816100 | 0.75107400 | -1.20155800 |
| C | 4.61738800 | -0.29461200 | -2.10549300 |
| H | 5.87154700 | -1.59652900 | -0.92371500 |
| H | 3.14327400 | 0.97716000 | -3.03303500 |
| Pt | -0.93484800 | 0.28827700 | -0.12913800 |
| I | -0.40708400 | 2.91059300 | -0.07180200 |
| I | -2.20738300 | -2.02308600 | -0.51287100 |
| H | 5.33764500 | -0.19463000 | -2.91261100 |
| C | 1.21867500 | -3.12394000 | 0.23731400 |
| H | 1.12765400 | -2.70495900 | -0.76827300 |
| H | 2.21471500 | -3.59544100 | 0.29617700 |
| H | 0.45963800 | -3.89201400 | 0.39427900 |

**TS6b**

Imaginary frequency: -173.92cm$^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -2.07518700 | 0.69054800 | 2.48667600 |
| C | -0.14127100 | 2.32921300 | 1.00051800 |
| H | -3.07949300 | 0.60083700 | 2.88493100 |
| H | -0.69703400 | 2.82955000 | 1.79098400 |
| C | -0.90521100 | 0.65233000 | 3.27391800 |
| H | -0.88748800 | 0.53861300 | 4.35249800 |
| C | 0.20875500 | 0.75518100 | 2.45439900 |
| H | 1.25209100 | 0.76841300 | 2.73742100 |
| C | -0.24444100 | 0.85297800 | 1.02999700 |
| C | -1.76404800 | 0.82138800 | 1.12629000 |
| C | -2.70700900 | 1.05797700 | 0.02735500 |
| C | -4.03430200 | 1.44329000 | 0.30472900 |
| C | -2.31764500 | 0.92488200 | -1.32069900 |
| C | -4.94237200 | 1.66944800 | -0.72533200 |
| H | -4.35659800 | 1.58007600 | 1.33259400 |
| C | -3.22544400 | 1.16725800 | -2.34876300 |
| H | -1.31038700 | 0.59176700 | -1.55252800 |
| C | -4.54105400 | 1.53422500 | -2.05704500 |
| H | -5.96201000 | 1.96011000 | -0.48882900 |
| H | -2.90709200 | 1.04970900 | -3.38060800 |
| Pt | 0.79336500 | -0.43623600 | -0.12210200 |
| I | -0.98737000 | -2.42190100 | -0.01331500 |
| I | 3.18706900 | 0.71914700 | -0.47333300 |
| H | -5.24999600 | 1.71138900 | -2.86092000 |
| C | 0.48744900 | 3.18749500 | -0.01340300 |
| H | 0.37984400 | 4.25080400 | 0.21039300 |
| H | 1.54361300 | 2.91662600 | -0.15555000 |
| H | 0.01873400 | 2.95716400 | -0.98586900 |

**TS7b**

Imaginary frequency: -312.36 cm$^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -0.91494400 | -2.84758700 | 1.11269100 |
| C | -0.50661500 | -0.27438500 | 2.52405400 |
| H | -1.39511400 | -3.79311900 | 0.88893900 |
| H | -1.43388200 | -0.67451400 | 2.94872100 |
| C | 0.23365300 | -2.72238300 | 1.95314700 |

| | | | |
|---|---|---|---|
| H | 0.89716900 | -3.55814200 | 2.16190500 |
| C | 0.54950200 | -1.44117100 | 2.35871500 |
| H | 1.55476200 | -1.16603800 | 2.65856100 |
| C | -0.37544000 | -0.52556000 | 1.10117100 |
| C | -1.31960500 | -1.62976000 | 0.63228300 |
| C | -2.57513700 | -1.35430100 | -0.06162800 |
| C | -3.67146500 | -2.23334900 | 0.09618700 |
| C | -2.73092100 | -0.23286400 | -0.90155900 |
| C | -4.86846000 | -2.00312400 | -0.56960800 |
| H | -3.58620200 | -3.08261500 | 0.76701400 |
| C | -3.93495600 | -0.00576100 | -1.56502300 |
| H | -1.89705000 | 0.44241900 | -1.05211400 |
| C | -5.00481400 | -0.88733700 | -1.40408100 |
| H | -5.70200000 | -2.68590000 | -0.43164000 |
| H | -4.03135600 | 0.86089600 | -2.21229300 |
| Pt | 0.74886000 | 0.40979500 | -0.16644700 |
| I | -0.23491200 | 2.88450400 | -0.07889700 |
| I | 2.37307700 | -1.56607800 | -0.90654200 |
| H | -5.94291700 | -0.70738500 | -1.92173100 |
| C | 0.01704100 | 0.94810100 | 3.24487000 |
| H | -0.70988800 | 1.76114100 | 3.16117100 |
| H | 0.16939400 | 0.72177600 | 4.30613200 |
| H | 0.95623900 | 1.29776600 | 2.80911800 |

**TS8b**

Imaginary frequency: -863.83 $cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | -1.44374900 | -1.48697600 | 2.80109300 |
| C | 0.53806500 | 0.49299900 | 2.50648100 |
| H | -2.20251200 | -2.25205400 | 2.93487900 |
| H | -0.57496500 | 0.97385400 | 1.88239600 |
| C | -0.81481600 | -0.93859400 | 3.93851400 |
| H | -1.10363600 | -1.28498000 | 4.92658800 |
| C | 0.14614300 | 0.03257200 | 3.80197400 |
| H | 0.63349700 | 0.46761000 | 4.66858700 |
| C | -0.08005200 | -0.09019600 | 1.31956300 |
| C | -1.12225200 | -1.09904000 | 1.50885300 |
| C | -1.87826800 | -1.69583000 | 0.37905400 |
| C | -3.28340400 | -1.67487300 | 0.42228700 |
| C | -1.24008700 | -2.31941000 | -0.70605400 |
| C | -4.03369000 | -2.24098800 | -0.60701700 |
| H | -3.78743000 | -1.18021400 | 1.24818200 |
| C | -1.99583500 | -2.90016800 | -1.72424400 |
| H | -0.15831800 | -2.37085400 | -0.74146100 |
| C | -3.39081600 | -2.85606000 | -1.68318600 |
| H | -5.11842500 | -2.19591200 | -0.56981700 |
| H | -1.48846300 | -3.38776500 | -2.55175500 |
| Pt | 0.53431500 | 0.45262300 | -0.45476800 |
| I | -1.32966300 | 2.36297300 | -0.65742300 |
| I | 2.68616600 | -1.12363400 | -0.60588700 |
| H | -3.97444200 | -3.29935400 | -2.48523600 |
| C | 1.65729300 | 1.49803100 | 2.38743000 |
| H | 1.77059000 | 2.06509000 | 3.31616700 |
| H | 2.58994900 | 0.96211600 | 2.17703800 |
| H | 1.49170300 | 2.18409500 | 1.55329400 |

**TS9b**

Imaginary frequency: -321.19$cm^{-1}$

| **ATOM** | **X** | **Y** | **Z** |
|---|---|---|---|
| C | 2.11528300 | -0.06708400 | 2.33296500 |

| | | | |
|---|---|---|---|
| C | 0.49645900 | -1.94409700 | 1.34712300 |
| H | 3.13249600 | 0.29992800 | 2.44671100 |
| H | 0.55064900 | -2.35050800 | 2.36189800 |
| C | 1.04491400 | 0.33276100 | 3.20442300 |
| H | 1.18877500 | 0.79701900 | 4.17291700 |
| C | -0.14299000 | 0.02144800 | 2.63227000 |
| H | -1.12617400 | 0.07109300 | 3.08715900 |
| C | 0.02151800 | -0.59265500 | 1.27676800 |
| C | 1.75418900 | -0.81842300 | 1.22502400 |
| C | 2.71311800 | -1.09680600 | 0.11717600 |
| C | 3.95064200 | -1.67090200 | 0.45461400 |
| C | 2.44322600 | -0.81258400 | -1.23011300 |
| C | 4.90371100 | -1.93818300 | -0.52789900 |
| H | 4.16265900 | -1.91704800 | 1.49237300 |
| C | 3.39643600 | -1.08907200 | -2.21071300 |
| H | 1.49922300 | -0.35336700 | -1.50214300 |
| C | 4.62805600 | -1.64857800 | -1.86532300 |
| H | 5.85629900 | -2.37898900 | -0.24736200 |
| H | 3.17566400 | -0.85221900 | -3.24765800 |
| Pt | -0.88801300 | 0.41491500 | -0.12090600 |
| I | -2.95513400 | -1.23104800 | -0.42339700 |
| I | 0.65168400 | 2.58626000 | -0.30606500 |
| H | 5.36788600 | -1.85748400 | -2.63293700 |
| C | 0.41324000 | -2.98669300 | 0.26641200 |
| H | 1.27968100 | -3.65482000 | 0.29940800 |
| H | -0.48913900 | -3.57915000 | 0.45323700 |
| H | 0.32308100 | -2.54885100 | -0.72779000 |

**TS10b**

Imaginary frequency: -846.16 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.20570800 | 3.32338000 | 0.97161100 |
| C | 1.27074300 | 1.19802700 | 1.96928000 |
| H | -0.76084300 | 4.17282400 | 0.58482100 |
| H | 1.92735600 | 0.38587100 | 2.25600000 |
| C | 0.82909500 | 3.56032300 | 1.91343500 |
| H | 1.03632100 | 4.58086500 | 2.22282300 |
| C | 1.56349600 | 2.51777600 | 2.41780000 |
| H | 2.36405300 | 2.67009200 | 3.13387900 |
| C | 0.28621500 | 0.92602000 | 0.96099600 |
| C | -0.50921400 | 2.06550400 | 0.47891700 |
| C | -1.63085500 | 1.93012100 | -0.48225500 |
| C | -2.86340300 | 2.53388300 | -0.17011600 |
| C | -1.49888100 | 1.26388900 | -1.71299200 |
| C | -3.93919200 | 2.45640900 | -1.05277400 |
| H | -2.98465300 | 3.04204800 | 0.78303000 |
| C | -2.57227900 | 1.20298000 | -2.60017000 |
| H | -0.54892900 | 0.81469000 | -1.98131100 |
| C | -3.79527900 | 1.79144500 | -2.27216500 |
| H | -4.88889800 | 2.91143000 | -0.78586600 |
| H | -2.45003000 | 0.69121300 | -3.55035800 |
| Pt | 0.45568300 | -0.75743600 | -0.03207100 |
| I | 2.79589500 | 0.03810400 | -1.06225800 |
| I | -1.68798700 | -2.22154400 | 0.59135700 |
| H | -4.63181800 | 1.73183700 | -2.96279100 |
| C | -0.48206700 | 0.60556700 | 2.73279300 |
| H | -1.33851700 | 0.14981400 | 2.24214700 |
| H | 0.01869600 | -0.13622600 | 3.35006100 |
| H | -0.72111800 | 1.53590900 | 3.24072800 |

**TS11b**

Imaginary frequency: -466.56 $cm^{-1}$

| ATOM | X | Y | Z |
|---|---|---|---|
| C | -0.20570800 | 3.32338000 | 0.97161100 |
| C | 1.27074300 | 1.19802700 | 1.96928000 |
| H | -0.76084300 | 4.17282400 | 0.58482100 |
| H | 1.92735600 | 0.38587100 | 2.25600000 |
| C | 0.82909500 | 3.56032300 | 1.91343500 |
| H | 1.03632100 | 4.58086500 | 2.22282300 |
| C | 1.56349600 | 2.51777600 | 2.41780000 |
| H | 2.36405300 | 2.67009200 | 3.13387900 |
| C | 0.28621500 | 0.92602000 | 0.96099600 |
| C | -0.50921400 | 2.06550400 | 0.47891700 |
| C | -1.63085500 | 1.93012100 | -0.48225500 |
| C | -2.86340300 | 2.53388300 | -0.17011600 |
| C | -1.49888100 | 1.26388900 | -1.71299200 |
| C | -3.93919200 | 2.45640900 | -1.05277400 |
| H | -2.98465300 | 3.04204800 | 0.78303000 |
| C | -2.57227900 | 1.20298000 | -2.60017000 |
| H | -0.54892900 | 0.81469000 | -1.98131100 |
| C | -3.79527900 | 1.79144500 | -2.27216500 |
| H | -4.88889800 | 2.91143000 | -0.78586600 |
| H | -2.45003000 | 0.69121300 | -3.55035800 |
| Pt | 0.45568300 | -0.75743600 | -0.03207100 |
| I | 2.79589500 | 0.03810400 | -1.06225800 |
| I | -1.68798700 | -2.22154400 | 0.59135700 |
| H | -4.63181800 | 1.73183700 | -2.96279100 |