Substituent Effects on the *Z/E*-Selectivity in Cross-Metathesis of Conjugated Enynes

Byungman Kang, Ji Min Lee, Jaesik Kwak, Yoon Sup Lee* and Sukbok Chang*

Center for Molecular Design and Synthesis (CMDS), Department of Chemistry and School of Molecular Science (BK21), Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea

Supporting Information

Table of Contents

General	S3
Representative experimental procedure of enyne metathesis.	S3
Experimental Procedure of CM of 4-hexen-2-ynyl benzoate and allyl trimethylsilane with Catalyst 3.	S4
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-4-Hepten-2-ynyl] benzyl ether (1)	S4
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-6-Nonen-4-ynyl] benzyl ether (2)	S4
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-12-pentadecen-10-ynyl] benzyl ether (3)	S5
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-6-Trimethylsilyl-4-hexen-2-ynyl] benzyl ether (4)	S5
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-8-Trimethylsilyl-6-octen-4-ynyl] benzyl ether (5)	S6
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-4-Hepten-2-ynyl] benzoate (6)	S6
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-6-Nonen-4-ynyl] benzoate (7)	S6
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-12-Pentadecen-10-ynyl] benzoate (8)	S7
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-6-Trimethylsilyl-4-hexen-2-ynyl] benzoate (9)	S7
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-8-Trimethylsilyl-6-octen-4-ynyl] benzoate (10)	S7
¹H NMR, ¹³C NMR and HRMS (EI) of <i>N</i>-Ethyl-<i>N</i>-[(<i>Z</i>)-4-hepten-2-ynyl] benzamide (11)	S8
¹H NMR, ¹³C NMR and HRMS (EI) of <i>N</i>-Ethyl-<i>N</i>-[(<i>Z</i>)-4-hepten-2-ynyl] <i>p</i>-toluenesulfonamide (12)	S8
¹H NMR, ¹³C NMR and HRMS (EI) of <i>N</i>-Ethyl-<i>N</i>-[6-trimethylsilyl-(<i>Z</i>)-4-hexen-2-ynyl] <i>p</i>-toluenesulfonamide (13)	S8
¹H NMR, ¹³C NMR and HRMS (EI) of [(<i>Z</i>)-5-octen-3-ynyl] tosylate (15)	S9
Calculated energies (in hartree) of chelation and non-chelation metallacyclobutane intermediates of the reaction derived from Scheme 3 in the text.	S10

¹ H NMR and ¹³ C NMR Spectrums of [(Z)-4-Hepten-2-ynyl] benzyl ether (1)	S11
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-6-Nonen-4-ynyl] benzyl ether (2)	S12
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-12-pentadecen-10-ynyl] benzyl ether (3)	S13
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-6-Trimethylsilyl-4-hexen-2-ynyl] benzyl ether (4)	S14
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-8-Trimethylsilyl-6-octen-4-ynyl] benzyl ether (5)	S15
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-4-Hepten-2-ynyl] benzoate (6)	S16
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-6-Nonen-4-ynyl] benzoate (7)	S17
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-12-Pentadecen-10-ynyl] benzoate (8)	S18
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-6-Trimethylsilyl-4-hexen-2-ynyl] benzoate (9)	S19
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-8-Trimethylsilyl-6-octen-4-ynyl] benzoate (10)	S20
¹ H NMR and ¹³ C NMR Spectrums of <i>N</i> -Ethyl- <i>N</i> -[(Z)-4-hepten-2-ynyl] benzamide (11)	S21
¹ H NMR and ¹³ C NMR Spectrums of <i>N</i> -Ethyl- <i>N</i> -[(Z)-4-hepten-2-ynyl] <i>p</i> -toluenesulfonamide (12)	S22
¹ H NMR and ¹³ C NMR Spectrums of <i>N</i> -Ethyl- <i>N</i> -[6-trimethylsilyl-(Z)-4-hexen-2-ynyl] <i>p</i> -toluenesulfonamide (13)	S23
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-7-decen-5-ynyl] tosylate (14)	S24
¹ H NMR and ¹³ C NMR Spectrums of [(Z)-5-octen-3-ynyl] tosylate (15)	S25
Notes and References	S26

General. Chemical shift are reported in delta (δ) units, parts per million (ppm) downfield from tetramethylsilane, or in ppm relative to the singlet at 7.26 ppm of chloroform-*d*1. Splitting patterns are designated as follows: s; singlet, d; doublet, t; triplet, q; quartet, m; multiplet, td; doublet of triplet, dt; triplet of doublet, qd; doublet of quintet, b; broad. Catalyst (H₂IMes)(3-Br-Py)₂(Cl)₂Ru=CHPh (**3**) was prepared starting from (H₂IMes)(PCy₃)(Cl)₂Ru=CH Ph (**2**) according to the reported procedure.¹

Representative experimental procedure of enyne metathesis. To a solution of 7-octen-5-yn-1-yl *p*-toluenesulfonate (111 mg, 0.39 mmol) in benzene (1.0 mL) was added *trans*-3-hexene (0.15 mL, 1.1 mmol) followed by catalyst **3** (18 mg, 0.019 mmol) in benzene (1.5 mL). The reaction mixture was stirred for 5 h at 70 °C under nitrogen atmosphere. Then catalyst **3** (18 mg, 0.019 mmol) in benzene (1.5 mL) was added again and the mixture was stirred for another 5 h at the same temperature. After removal of organic solvent under reduced pressure, the residue was purified by a column chromatography on silica gel (ethyl acetate:hexane, 1/7) to afford the corresponding enyne as an analytically pure isomer, [(*Z*)-7-decen-5-ynyl] tosylate (**14**) (97 mg, 81 %): ¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, 2H, *J* = 8.3 Hz), 7.30 (d, 2H, *J* = 8.2 Hz), 5.77 (dt, 1H, *J* = 10.6, 7.3 Hz), 5.32 (d, 1H, *J* = 10.7 Hz), 4.02 (t, 2H, *J* = 6.2 Hz), 2.41 (s, 3H), 2.28 (td, 2H, *J* = 6.9, 2.1 Hz), 2.21 (qd, 2H, *J* = 7.5, 1.2 Hz), 1.71-1.78 (m, 2H), 1.49-1.56 (m, 2H), 0.95 (t, 3H, *J* = 7.1 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 144.7, 144.3, 132.9, 129.7, 127.7, 108.3, 92.9, 77.8, 69.9, 27.8, 24.5, 23.4, 21.5, 18.7, 13.3; HRMS (EI) calcd for C₁₇H₂₂O₃S [M⁺] 306.1290, found 306.1292.

Experimental Procedure of CM of 4-hexen-2-ynyl benzoate and allyl trimethylsilane with Catalyst 3. To a solution of 4-hexen-2-ynyl benzoate (74 mg, 0.39 mmol) in benzene (1.0 mL) was added allyl trimethylsilane (0.15 mL, 1.1 mmol) followed by catalyst **3** (18 mg, 0.019 mmol) in benzene (1.5 mL). The reaction mixture was stirred for 4.5 h at 70 °C under nitrogen atmosphere, and at 0.5, 2 and 4 h, 0.5 mL of reaction mixture was sampled each time and purified by short column. At 4.5 h, catalyst **3** (18 mg, 0.019 mmol) in benzene (1.5 mL) was added and 0.5 mL of reaction mixture was sampled at 2 h interval, purified by short column to determine the conversion (%) and *Z/E* ratio. The conversion (%) and *Z/E* ratio was determined via crude ¹H NMR by comparing the area of vinyl proton of *Z* & *E*- products with vinyl proton of the starting material.

[(*Z*)-4-Hepten-2-ynyl] benzyl ether (1): ¹H NMR (400 MHz, CDCl₃) δ 7.28-7.19 (m, 5H), 5.86 (dt, 1H, *J* = 10.7, 7.4 Hz), 5.40 (d, 1H, *J* = 10.7 Hz), 4.54 (s, 2H), 4.25 (d, 2H, *J* = 2.5 Hz), 2.26 (qd, 2H, *J* = 7.5, 1.1 Hz), 0.95 (t, 3H, *J* = 7.5 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 146.1, 137.5, 128.4, 128.1, 127.8, 107.8, 89.0, 83.2, 71.4, 57.9, 23.7, 13.3; HRMS (EI) calcd for C₁₄H₁₆O [*M*⁺] 200.1201, found 200.1203.

[(*Z*)-6-Nonen-4-ynyl] benzyl ether (2): ¹H NMR (400 MHz, CDCl₃) δ 7.31-7.33 (m, 4H), 7.24-7.27 (m, 1H), 5.80 (dt, 1H, *J* = 10.7, 7.2 Hz), 5.38 (dt, 1H, *J* = 10.6, 1.4 Hz), 4.51 (s, 2H), 3.58 (t, 2H, *J* = 6.2 Hz), 2.46 (td, 2H, *J* = 7.0, 2.1 Hz), 2.26 (qd, 2H, *J* = 7.5, 1.3 Hz), 1.80-

1.87 (m, 2H), 0.98 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 144.3, 138.5, 128.4, 127.6, 127.5, 108.6, 93.6, 77.2, 73.0, 68.9, 29.1, 23.4, 16.4, 13.4; HRMS (EI) calcd for $\text{C}_{16}\text{H}_{20}\text{O}$ [M^+] 228.1514, found 228.1518.

[(Z)-12-pentadecen-10-ynyl] benzyl ether (3): ^1H NMR (300 MHz, CDCl_3) δ 7.24-7.34 (m, 5H), 5.79 (dt, 1H, $J = 10.7, 7.2$ Hz), 5.40 (d, 1H $J = 10.9$ Hz), 4.49 (s, 2H), 3.46 (t, 2H, $J = 6.6$ Hz), 2.30 (m, 4H), 1.51-1.63 (m, 4H), 1.02-1.40 (m, 10H), 0.99 (t, 3H, $J = 7.7$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 143.9, 138.7, 128.3, 127.5, 127.4, 108.7, 94.5, 77.2, 72.8, 70.5, 29.7, 29.4, 29.3, 29.0, 28.9, 28.8, 26.1, 23.4, 19.5, 13.4; HRMS (EI) calcd for $\text{C}_{22}\text{H}_{32}\text{O}$ [M^+] 312.2453, found 312.2446.

[(Z)-6-Trimethylsilyl-4-hexen-2-ynyl] benzyl ether (4): ^1H NMR (300 MHz, CDCl_3) δ 7.19-7.30 (m, 5H), 5.95 (dt, 1H, $J = 10.5, 8.9$ Hz), 5.42 (d, 1H, $J = 10.9$ Hz), 4.57 (s, 2H), 4.28 (d, 2H, $J = 1.7$ Hz), 1.81 (d, 2H, $J = 8.8$ Hz), 0.01 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.8, 137.6, 128.4, 128.1, 127.8, 105.6, 88.8, 84.1, 71.2, 58.0, 22.9, -1.6; HRMS (EI) calcd for $\text{C}_{16}\text{H}_{22}\text{OSi}$ [M^+] 258.1440, found 258.1435.

[(Z)-8-Trimethylsilyl-6-octen-4-ynyl] benzyl ether (5): ^1H NMR (300 MHz, CDCl_3) δ 7.20-7.32 (m, 5H), 5.82 (dt, 1H, $J = 10.4, 8.8$ Hz), 5.27 (d, 1H, $J = 10.5$ Hz), 4.47 (s, 2H), 3.55 (t, 2H, $J = 6.3$ Hz), 2.43 (qd, 2H, $J = 7.0, 1.9$ Hz), 1.76-1.83 (m, 4H), 0.00 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 139.5, 138.5, 128.3, 127.7, 127.6, 106.5, 93.2, 78.2, 73.0, 69.0, 29.2, 22.4, 16.4, -1.6; HRMS (EI) calcd for $\text{C}_{18}\text{H}_{26}\text{OSi}$ [M^+] 286.1753, found 286.1751.

[(Z)-4-Hepten-2-ynyl] benzoate (6): ^1H NMR (400 MHz, CDCl_3) δ 8.07 (d, 2H, $J = 7.7$ Hz), 7.55 (t, 1H, $J = 7.5$ Hz), 7.43 (t, 2H, $J = 7.5$ Hz), 5.95 (dt, 1H, $J = 10.8, 7.4$ Hz), 5.45 (dt, 1H, $J = 10.8, 1.8$ Hz), 5.06 (d, 2H, $J = 2.1$ Hz), 2.31 (qd, 2H, $J = 6.9, 1.3$ Hz), 1.00 (t, 3H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 165.9, 147.1, 133.1, 129.7, 129.6, 128.3, 107.5, 86.9, 83.4, 53.4, 23.7, 13.2; HRMS (EI) calcd for $\text{C}_{14}\text{H}_{14}\text{O}_2$ [M^+] 214.0994, found 214.0995.

[(Z)-6-Nonen-4-ynyl] benzoate (7): ^1H NMR (300 MHz, CDCl_3) δ 8.05 (d, 2H, $J = 7.8$ Hz), 7.55 (t, 1H, $J = 7.4$ Hz), 7.43 (t, 2H, $J = 7.5$ Hz), 5.83 (dt, 1H, $J = 10.6, 7.3$ Hz), 5.40 (d, 1H, $J = 10.6$ Hz), 4.44 (t, 2H, $J = 6.3$ Hz), 2.39 (td, 2H, $J = 7.00, 1.8$ Hz), 2.24-2.34 (qd, 2H, $J = 7.5, 0.9$ Hz), 1.97-2.06 (m, 2H), 1.00 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 166.3, 144.3, 132.7, 130.4, 129.5, 128.2, 108.5, 92.5, 78.0, 63.6, 28.1, 23.3, 16.4, 13.2; HRMS (EI) calcd for $\text{C}_{16}\text{H}_{18}\text{O}_2$ [M^+] 242.1307, found 242.1334.

[(Z)-12-Pentadecen-10-ynyl] benzoate (8): ^1H NMR (300 MHz, CDCl_3) δ 8.02 (d, 2H, $J = 7.9$ Hz), 7.50 (t, 1H, $J = 7.7$ Hz), 7.42 (t, 2H, $J = 7.2$ Hz), 5.77 (dt, 1H, $J = 10.7, 7.2$ Hz), 5.39 (d, 1H, $J = 10.8$ Hz), 4.29 (t, 2H, $J = 6.6$ Hz), 2.25-2.31 (m, 4H), 1.76-1.72 (m, 2H), 1.30-1.51 (m, 12H), 0.97 (t, 3H, $J = 7.8$ Hz); ^{13}C NMR (75 MHz, CDCl_3) δ 166.6, 144.0, 132.7, 130.5, 129.5, 128.2, 108.7, 94.4, 77.2, 65.0, 29.3, 29.2, 29.0, 28.8, 28.8, 28.7, 26.0, 23.4, 19.5, 13.4; HRMS (EI) calcd for $\text{C}_{22}\text{H}_{30}\text{O}_2$ [M^+] 326.2246, found 326.2248.

[(Z)-6-Trimethylsilyl-4-hexen-2-ynyl] benzoate (9): ^1H NMR (300 MHz, CDCl_3) δ 8.04 (d, 2H, $J = 7.2$ Hz), 7.53 (t, 1H, $J = 7.4$ Hz), 7.40 (t, 2H, $J = 7.8$ Hz), 6.01 (dt, 1H, $J = 10.5, 8.8$ Hz), 5.34 (d, 1H, $J = 10.6$ Hz), 5.04 (d, 2H, $J = 1.8$ Hz), 1.82 (d, 2H, $J = 8.8$ Hz), 0.00 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 165.9, 143.1, 133.1, 129.8, 129.7, 128.3, 105.1, 86.7, 84.4, 53.6, 23.0, -1.7; HRMS (EI) calcd for $\text{C}_{16}\text{H}_{20}\text{O}_2\text{Si}$ [M^+] 272.1233, found 272.1222.

[(Z)-8-Trimethylsilyl-6-octen-4-ynyl] benzoate (10): ^1H NMR (300 MHz, CDCl_3) δ 8.00 (d, 2H, $J = 7.1$ Hz), 7.51 (t, 1H, $J = 7.5$ Hz), 7.39 (t, 2H, $J = 7.6$ Hz), 5.85 (dt, 1H, $J = 10.4, 8.7$ Hz), 5.28 (d, 1H, $J = 10.6$ Hz), 4.41 (t, 2H, $J = 6.3$ Hz), 2.51 (qd, 2H, $J = 7.0, 1.8$ Hz), 1.92-2.02 (m, 2H), 1.77 (d, 2H, $J = 8.7$ Hz), 0.00 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 166.4, 139.9, 132.8, 130.2, 129.5, 128.3, 106.2, 92.2, 78.8, 63.7, 28.2, 22.5, 16.4, -1.7; HRMS (EI) calcd for $\text{C}_{18}\text{H}_{24}\text{O}_2\text{Si}$ [M^+] 300.1546, found 300.1550.

***N*-Ethyl-*N*-[(*Z*)-4-hepten-2-ynyl] benzamide (11):** ^1H NMR (300 MHz, CDCl_3) δ 7.36-7.48 (m, 5H), 5.95 (dt, 1H, $J = 10.2, 7.4$ Hz), 5.44 (d, 1H, 10.7 Hz), 4.33 (b, 2H), 3.57 (b, 2H), 2.32 (qd, 2H, $J = 7.5, 1.1$ Hz), 1.24 (b, 3H), 1.03 (t, 3H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 170.8, 146.4, 136.1, 129.6, 128.3, 107.7, 88.2, 77.2, 42.9, 40.2, 33.9, 23.6, 13.3, 12.4; HRMS (EI) calcd for $\text{C}_{16}\text{H}_{19}\text{NO}$ [M^+] 241.1467, found 241.1460.

***N*-Ethyl-*N*-[(*Z*)-4-hepten-2-ynyl] *p*-toluenesulfonamide (12):** ^1H NMR (300 MHz, CDCl_3) δ 7.73 (d, 2H, $J = 8.3$ Hz), 7.27 (d, 2H, $J = 8.0$ Hz), 5.81 (dt, 1H, $J = 10.7, 7.4$ Hz), 5.18 (d, 1H, $J = 10.7$ Hz), 4.30 (d, 2H, $J = 1.7$ Hz), 3.28 (q, 2H, $J = 7.2$ Hz), 2.40 (s, 3H), 2.03 (qd, 2H, $J = 7.5, 1.1$ Hz), 1.20 (t, 3H, $J = 7.2$ Hz), 0.92 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 145.8, 143.1, 135.9, 129.3, 127.5, 107.3, 85.9, 82.0, 41.1, 36.5, 23.4, 21.4, 13.2, 13.1; HRMS (EI) calcd for $\text{C}_{16}\text{H}_{21}\text{NO}_2\text{S}$ [M^+] 291.1293, found 291.1312.

***N*-Ethyl-*N*-[6-trimethylsilyl-(*Z*)-4-hexen-2-ynyl] *p*-toluenesulfonamide (13):** ^1H NMR (300 MHz, CDCl_3) δ 7.74 (d, 2H, $J = 8.2$ Hz), 7.28 (d, 2H, $J = 7.8$ Hz), 5.89 (dt, 1H, $J = 10.4,$

9.2 Hz), 5.10 (d, 1H, $J = 10.7$ Hz), 4.32 (d, 2H, $J = 1.3$ Hz), 3.29 (q, 2H, $J = 7.1$ Hz), 2.41 (s, 3H), 1.62 (d, 2H, $J = 8.7$ Hz), 1.20 (t, 3H, $J = 7.1$ Hz), 0.02 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.1, 141.5, 136.0, 129.4, 127.7, 105.1, 85.5, 82.9, 41.1, 36.6, 22.7, 21.4, 13.1, -1.8; HRMS (EI) calcd for $\text{C}_{18}\text{H}_{27}\text{NO}_2\text{SSi}$ [M^+] 349.1532, found 349.1531.

[(Z)-5-octen-3-ynyl] tosylate (15) ^1H NMR (300 MHz, CDCl_3) 7.79 (d, 2H, $J = 8.2$ Hz), 7.33 (d, 2H, $J = 8.2$ Hz), 5.84 (dt, 1H, $J = 10.7, 7.4$ Hz), 5.31 (d, 1H, $J = 10.7$ Hz), 4.10 (t, 2H, $J = 7.2$ Hz), 2.69 (td, 2H, $J = 7.1, 1.9$ Hz), 2.43 (s, 3H), 2.22 (t, 2H, $J = 7.4$ Hz), 0.97 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (100 MHz, CDCl_3) 145.4, 144.8, 132.8, 129.8, 127.8, 107.8, 87.8, 79.9, 67.7, 23.4, 21.4, 20.3, 13.2; HRMS (EI) calcd for $\text{C}_{15}\text{H}_{18}\text{O}_3\text{S}$ [M^+] 278.0977, found 278.0970.

Table S-1. Calculated energies (in hartree) of chelation and non-chelation metallacyclobutane intermediates of the reaction derived from Scheme 3 in the text.^a

method	(n=1) substrate			(n=3) substrate		
	chelation (A)	non-chelation (B)	(A)–(B)	chelation (A)	non-chelation (B)	(A)–(B)
HF	–7522.3206	–7522.3004	–0.0202	–7600.0707	–7599.9436	–0.1271
SVWN5 ³	–7513.8146	–7513.8055	–0.0092	–7591.2684	–7591.2475	–0.0210
B3LYP ⁴	–7538.6523	–7538.6467	–0.0056	–7616.8543	–7616.8458	–0.0085
B3P86 ⁴	–7546.4100	–7546.4232	0.0132	–7624.9339	–7624.9132	–0.0207
HF*	–7577.3298	–7577.3180	–0.0118	–7635.4842	–7635.3638	–0.1204

^a All energies were calculated at the HF optimized geometry with 3-21G** basis set.² All except HF* are calculated with the 3-21G** basis set and HF* refers to calculation with the DGDZVP basis set.

[(Z)-4-Hepten-2-ynyl] benzyl ether (1)

[(Z)-6-Nonen-4-ynyl] benzyl ether (2)

[(Z)-12-pentadecen-10-ynyl] benzyl ether (3)

[(Z)-6-Trimethylsilyl-4-hexen-2-ynyl] benzyl ether (4)

[(Z)-8-Trimethylsilyl-6-octen-4-ynyl] benzyl ether (5)

[(Z)-4-Hepten-2-ynyl] benzoate (6)

[(Z)-6-Nonen-4-ynyl] benzoate (7)

[(Z)-12-Pentadecen-10-ynyl] benzoate (8)

[(Z)-6-Trimethylsilyl-4-hexen-2-ynyl] benzoate (9)

[(Z)-8-Trimethylsilyl-6-octen-4-ynyl] benzoate (10)

***N*-Ethyl-*N*-[(*Z*)-4-hepten-2-ynyl] benzamide (11)**

***N*-Ethyl-*N*-[(*Z*)-4-hepten-2-ynyl] *p*-toluenesulfonamide (12)**

***N*-Ethyl-*N*-[6-trimethylsilyl-(*Z*)-4-hexen-2-ynyl] *p*-toluenesulfonamide (13)**

[(Z)-7-decen-5-ynyl] tosylate (14)

[(Z)-5-octen-3-ynyl] tosylate (15)

Notes and References

(1) Love, J. A.; Morgan, J. P.; Trnka, T. M.; Grubbs, R. H. *Angew. Chem., Int. Ed.* **2002**, *41*, 4035.

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

(3) Vosco, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200.

(4) Beck, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.