

Supporting Information

for

Syntheses with Organoboranes. XI. Allylboration of Vinylic Epoxides with Allylic Dialkylboranes

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Characterization of new compounds

trans-2-Allyl-3-cyclopenten-1-ol (5a): ^1H NMR, ^1H - ^1H COSY NMR (CDCl_3 , δ , ppm) 2.12 (t, $J=6.9$ Hz, 2H, $\text{C}_{(6)}\text{H}_2$), 2.25 (dd, $J=17.0$, 3.5 Hz, 1H, $\text{C}_{(5)}\text{H}$), 2.62 (m, 1H, $\text{C}_{(2)}\text{H}$), 2.69 (dd, $J=17.1$, 6.4 Hz, 1H, $\text{C}_{(5)}\text{H}$), 4.13 (dt, $J=6.4$, 3.5 Hz, 1H, HC-OH), 4.98-5.12 (m, 2H, $=\text{CH}_2$), 5.67 (s, 2H, $\text{HC}_{(3)}=\text{C}_{(4)}\text{H}$), 5.82 (ddt, $J=17.2$, 10.2, 6.9 Hz, 1H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 37.39, 41.50, 54.37, 76.96, 116.08, 128.13, 132.62, 136.66.

1-Allyl-3-cyclopenten-1-ol (6a): ^1H NMR (CDCl_3 , δ , ppm) 1.88 (s, 1H, OH), 2.30-2.60 (m, 6H, 3 x CH_2), 5.10-5.28 (m, 2H, $=\text{CH}_2$), 5.69 (s, 2H, $\text{HC}=\text{CH}$), 5.91 (ddt, $J=17.7$, 9.5, 7.2 Hz, 1H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 45.64, 46.66, 80.30, 118.60, 128.56, 134.25.

trans-4-Allyl-2-cyclopenten-1-ol: ^1H NMR (CDCl_3 , δ , ppm) 1.57 (s, 1H, OH), 1.80-1.92 (m, 2H, CH_2), 2.04-2.16 (m, 2H, CH_2), 2.97 (m, 1H, $\text{C}_{(4)}\text{H}$), 4.85 (m, 1H, HC-OH), 4.96-5.16 (m, 2H, $=\text{CH}_2$), 5.65–5.85 (m, 2H, 2 x $=\text{CH}$), 5.94 (dd, $J=5.9$, 2.0 Hz, 1H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 39.76, 39.93, 43.63, 71.14, 115.94, 133.02, 136.69, 139.41.

5,5-Dimethyl-3,4-epoxy-1-cyclopentene (3b): ^1H NMR (CDCl_3 , δ , ppm) 1.08 (s, 3H, CH_3), 1.15 (s, 3H, CH_3), 3.44 (t, $J=2.5$ Hz, $\text{CH}_{(\text{ep})}$), 3.75 (m, 1H, $\text{CH}_{(\text{ep})}$), 5.75 (dt, $J=5.7$ Hz, $J=2.2$ Hz, 1H, $\text{HC}_{(2)}=$), 5.97 (d, $J=5.8$ Hz, 1H, $\text{HC}_{(1)}=$); ^{13}C NMR (CDCl_3 , δ , ppm) 21.24, 25.50, 45.15, 58.58, 63.19, 128.30, 148.58.

(5Z)-8-Methyl-1,5,7-nonatrien-4-ol (4b): ^1H NMR, ^1H - ^1H COSY NMR (CDCl_3 , δ , ppm) 1.68 (s, 1H, OH), 1.76 (s, 3H, CH_3), 1.81 (s, 3H, CH_3), 2.31 (t, $J=6.8$ Hz, 2H, CH_2), 4.64 (q, $J=7.4$ Hz, 1H, HC-OH), 5.06-5.22 (m, 2H, $=\text{CH}_2$), 5.32 (t, $J=9.6$ Hz, 1H, $=\text{C}_{(5)}\text{H}$), 5.82 (m, 1H, $=\text{C}_{(2)}\text{H}$), 6.08 (d, $J=11.6$ Hz, 1H, $=\text{C}_{(7)}\text{H}$), 6.27 (t, $J=11.2$ Hz, 1H, $=\text{C}_{(6)}\text{H}$); ^{13}C NMR (CDCl_3 , δ , ppm) 17.92, 26.24, 41.95, 66.87, 117.76, 119.86, 126.35, 130.13, 134.31, 137.70.

2-Allyl-5,5-dimethyl-3-cyclopenten-1-ol (5b): ^1H NMR (CDCl_3 , δ , ppm) 0.88 (s, 3H, CH_3), 0.91 (s, 3H, CH_3), 2.10-2.24 (m, 3H), 3.58 (d, 6.8 Hz, 1H, HC-OH), 4.95-5.15 (m, 2H, $=\text{CH}_2$), 5.45 (d, $J=6.2$ Hz, 1H, $=\text{CH}$), 5.52 (dd, $J=6.4$, 2.1 Hz, 1H, $=\text{CH}$), 5.78-5.96 (m, 1H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 23.80, 26.51, 39.22, 49.72, 50.27, 85.22, 115.42, 124.82, 136.69, 141.11.

1-Allyl-2,2-dimethyl-3-cyclopenten-1-ol (6b): ^1H NMR (CDCl_3 , δ , ppm) 1.02 (s, 6H, 2 x CH_3), 2.28 (d, $J=6.8$ Hz, 2H, CH_2), 2.42-2.58 (m, 2H, CH_2), 5.08-5.22 (m, 2H, $=\text{CH}_2$), 5.56-5.64 (m, 2H, 2 x $=\text{CH}$), 5.92-6.08 (m, 1H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 20.07, 20.35, 36.92, 44.41, 46.14, 82.09, 117.63, 128.62, 134.37, 139.58.

(2Z)-1-(2-Cyclohexenyl)-2,4-pentadien-1-ol (7): mp 41-42 °C: ^1H NMR (CDCl_3 , δ , ppm) 1.35-1.60 (m, 1H), 1.66-1.88 (m, 4H), 1.90-2.06 (m, 2H), 2.30 (m, 1H), 4.44 (dd, $J=9.0, 6.3$ Hz, 1H, HC-OH), 5.10-5.32 (m, 2H, $=\text{CH}_2$), 5.46 (t, $J=10.4$ Hz, 1H, $=\text{C}_{(2)}\text{H}$), 5.56 (dd, $J=10.5, 2.1$ Hz, 1H, $=\text{C}_{(7)}\text{H}$), 5.80 (m, 1H, $=\text{C}_{(8)}\text{H}$), 6.12 (t, $J=11.1$ Hz, 1H, $=\text{C}_{(3)}\text{H}$), 6.62 (dt, $J=16.6, 10.8$ Hz, 1H, $=\text{C}_{(2)}\text{H}$); ^{13}C NMR (CDCl_3 , δ , ppm) 21.18, 24.39, 25.17, 41.75, 70.79, 119.24, 127.21, 129.99, 131.45, 131.91, 132.25.

1-Allyl-3-cyclohexen-1-ol (11a): ^1H NMR (CDCl_3 , δ , ppm) 1.63 (t, $J=7.8$ Hz, 2H, CH_2), 1.80 (s, 1H, OH), 1.95-2.20 (m, 4H, 2 x CH_2), 2.25 (d, $J=6.8$ Hz, 2H, CH_2), 5.05-5.19 (m, 2H, $=\text{CH}_2$), 5.65 (m, 2H, HC=CH), 5.92 (ddt, $J=16.5, 10.7, 7.4$ Hz, 1H, HC=CH_2); ^{13}C NMR (CDCl_3 , δ , ppm) 22.76, 33.04, 37.81, 45.42, 69.81, 118.67, 124.37, 126.50, 133.62.

cis-2-Allyl-3-cyclohepten-1-ol (cis-9b): ^1H NMR, ^1H - ^1H COSY NMR (CDCl_3 , δ , ppm) 1.53 (m, 2H, $\text{C}_{(6)}\text{H}_2$), 1.61 (s, 1H, OH), 1.74 (m, 1H, $\text{C}_{(7)}\text{H}$), 1.98-2.22 (m, 3H, $\text{C}_{(5)}\text{H}_2$, $\text{C}_{(7)}\text{H}$), 2.25-2.38 (m, 2H, $\text{C}_{(8)}\text{H}_2$), 2.55 (m, 1H, $\text{C}_{(2)}\text{H}$), 3.83 (s, 1H, CH-OH), 4.98-5.15 (m, 2H, $=\text{CH}_2$), 5.31 (dddd, $J=10.8, 4.4, 2.1, 1.0$ Hz, 1H, $=\text{C}_{(3)}\text{H}$), 5.81 (ddt, $J=17.1, 10.2, 6.9$ Hz, 1H, $=\text{C}_{(9)}\text{H}$), 6.02 (m, 1H, $=\text{C}_{(4)}\text{H}$); ^{13}C NMR (CDCl_3 , δ , ppm) 20.12, 28.53, 37.89, 37.96, 43.89, 69.71, 116.21, 131.48, 134.07, 137.18.

trans-2-Allyl-3-cyclohepten-1-ol (trans-9b): ^1H NMR, ^1H - ^1H COSY NMR (CDCl_3 , δ , ppm) 1.30-1.52 (m, 1H, $\text{C}_{(6)}\text{H}$), 1.60-1.82 (m, 2H, $\text{C}_{(7)}\text{H}$, $\text{C}_{(6)}\text{H}$), 1.79 (s, 1H, OH), 2.02-2.14 (m, 3H, $\text{C}_{(5)}\text{H}_2$, $\text{C}_{(7)}\text{H}$), 2.18-2.40 (m, 2H, $\text{C}_{(8)}\text{H}_2$), 2.42-5.50 (m, 1H, $\text{C}_{(2)}\text{H}$), 3.49 (td, $J=8.3, 3.2$ Hz, 1H, HC-OH), 4.98-5.20 (m, 2H, $=\text{CH}_2$), 5.45 (dd, $J=11.3, 4.5$ Hz, 1H, $=\text{C}_{(3)}\text{H}$), 5.70-5.95 (m, 2H, 2 x $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 23.59, 28.05, 36.46, 39.01, 45.23, 71.59, 116.35, 131.62, 132.96, 136.77.

1-Allyl-3-cyclohepten-1-ol (11b): ^1H NMR, ^1H - ^1H COSY NMR (CDCl_3 , δ , ppm) 1.46-1.64 (m, 2H, $\text{C}_{(6)}\text{H}_2$), 1.77 (dd, $J=6.7, 4.6$ Hz, 2H, $\text{C}_{(7)}\text{H}_2$), 1.83 (s, 1H, OH), 2.06-2.22 (m, 2H, $\text{C}_{(5)}\text{H}_2$), 2.24-2.44 (m, 4H, $\text{C}_{(2)}\text{H}_2$, $\text{C}_{(8)}\text{H}_2$), 5.04-5.20 (m, 2H, $=\text{CH}_2$), 5.59 (dt, $J=10.7, 6.6$ Hz, 1H, $=\text{C}_{(3)}\text{H}$), 5.78-6.08 (m, 2H, 2 x $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 22.12, 28.53, 39.64, 43.72, 45.69, 71.38, 118.41, 126.27, 134.02, 134.86.

trans-4-Allyl-2-cycloocten-1-ol (10c): ^1H NMR (CDCl_3 , δ , ppm) 1.30-1.70 (m, 7H, OH, 3 x CH_2), 1.74-1.88 (m, 2H, CH_2), 2.08 (t, $J=6.8$ Hz, 2H, CH_2), 2.75 (m, 1H, $\text{C}_{(4)}\text{H}$), 4.68 (dt, $J=8.0, 5.5$ Hz, 1H, HC-OH), 4.94-5.10 (m, 2H, $=\text{CH}_2$), 5.35 (dd, $J=12.5, 6.6$ Hz, 1H, $=\text{CH}$), 5.57 (ddd, $J=12.1, 5.4, 1.4$ Hz, 1H, $=\text{CH}$), 5.79 (ddt, $J=17.0, 10.1, 6.9$ Hz, 1H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 22.64, 25.61, 32.98, 36.26, 37.73, 41.46, 69.49, 115.84, 132.22, 134.43, 137.12.

2-(2-Cyclohexenyl)-3-buten-1-ol (16a): ^1H NMR, ^1H - ^1H COSY NMR (CDCl_3 , δ , ppm) 0.80-1.54 (m, 3H), 1.59-1.78 (m, 2H, OH), 1.88-2.01 (m, 2H), 2.15-2.24 (m, 1H), 3.49 (m, 1H, $\text{CH}_2\text{-OH}$), 3.69 (m, 1H, $\text{CH}_2\text{-OH}$), 5.00-5.25 (m, 2H, $=\text{CH}_2$), 5.50-5.76 (m, 3H, $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 21.97, 25.88, 27.10, 36.38, 51.95, 63.38, 118.33, 128.41, 129.01, 138.37.

2-(2-Cyclohexenyl)-2-methyl-3-buten-1-ol (16b): ^1H NMR (CDCl_3 , δ , ppm) 0.92 (s, 3H, CH_3), 1.08-1.38 (m, 2H), 1.48-1.82 (m, 3H, OH), 1.85-2.02 (m, 2H), 3.50 (s, 2H, $\text{CH}_2\text{-OH}$), 4.95-5.27 (m, 2H, CH_2), 5.48-5.85 (m, 2H, 2 x $=\text{CH}$); ^{13}C NMR (CDCl_3 , δ , ppm) 17.14, 23.73, 24.31, 25.13, 40.59, 44.78, 68.30, 115.50, 127.77, 128.83, 143.72.