Supporting Information

Palladium(II) Acetate in Pyridine as an Effective Catalyst for Highly Regioselective Hydroselenation of Alkynes

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General Comments. ^1H and ^{13}C NMR spectra (300, 400 and 75 MHz, respectively) were determined by using CDCl_3 as the solvent with Me_4Si as the internal standard. Chemical shifts in ^1H and ^{13}C NMR were measured relative to CDCl_3 and converted to δ (Me_4Si) value by using δ (CDCl_3) = 7.26 and 77.0 ppm, respectively. IR spectra were recorded on FT-IR instrument. Mass spectra were run by EI ionization (70 eV).

FIGURE 1. ^1H NMR Spectra of Crude Products from the $\text{Pd}(\text{OAc})_2$ -Catalyzed Hydroselenation of 1-Octyne in THF (a) and in Pyridine (b)

The following products are known compounds and CAS registry numbers are listed below.

2-Phenylseleno-1-octene (Table 2, entry 1) [63831-77-6].

2-Phenylseleno-3-phenyl-1-propene (Table 2, entry 4) [63831-80-1].

2-Phenylseleno-2-propen-1-ol (Table 2, entry 6) [104828-93-5].

4-Phenylseleno-4-hexenenitrile (Table 2, entry 2).

TLC: R_f = 0.38 (hexane/ethyl acetate = 84/16).

Yellow oil; ^1H NMR (300 MHz, CDCl_3) δ 1.89 (quint, J = 7.2 Hz, 2H), 2.33 (t, J = 7.1 Hz, 2H), 2.43 (t, J = 7.2 Hz, 2H), 5.25 (s, 1H), 5.58 (s, 1H), 7.31-7.56 (m, 5H); ^{13}C NMR (75 MHz, CDCl_3) δ 15.8, 23.9, 36.5, 118.8, 119.4, 128.2, 129.5, 134.8, 134.9, 140.6; IR (NaCl) 3061, 2936, 2245, 1611, 1475, 1437, 1213, 1022, 912, 877, 741, 692 cm^{-1} . Anal. Calcd for $\text{C}_{12}\text{H}_{13}\text{NSe}$: C, 57.61; H, 5.24; N, 5.60. Found: C, 57.74; H, 5.21; N, 5.67.

2-Phenylseleno-1-hexene-1-ol (Table 2, entry 3).

TLC: R_f = 0.41 (hexane/ethyl acetate = 64/36).

Yellow oil; ^1H NMR (300 MHz, CDCl_3) δ 1.44-1.64 (m, 4H), 2.29 (t, J = 7.1 Hz, 2H), 3.31 (s, 1H), 3.52 (t, J = 6.3 Hz, 2H), 5.10 (s, 1H), 5.51 (s, 1H), 7.27-7.57 (m, 5H); ^{13}C NMR (75 MHz, CDCl_3) δ 26.0, 32.7, 39.0, 62.7, 117.1, 129.1, 130.1, 130.5, 136.0, 144.8; IR (NaCl) 3308, 3074, 2936, 2862, 2370, 1610, 1578, 1475, 1437, 1067, 1022, 870, 739, 691 cm^{-1} . Anal. Calcd for $\text{C}_{12}\text{H}_{16}\text{OSe}$: C, 56.47; H, 6.32. Found: C, 56.18; H, 6.22.

2-Phenylseleno-5-methyl-1-hexene (Table 2, entry 5).

TLC: Rf = 0.28 (hexane).

Yellow oil; ^1H NMR (300 MHz, CDCl_3) δ 0.77 (d, J = 6.3 Hz, 6H), 1.34 (dt, J = 6.6, 6.6 Hz, 2H), 1.47 (quint, J = 6.6 Hz, 1H), 2.21 (t, J = 8.0 Hz, 2H), 5.03 (s, 1H), 5.42 (s, 1H), 7.19-7.50 (m, 5H); ^{13}C NMR (75 MHz, CDCl_3) δ 22.3, 27.3, 36.2, 37.9, 116.0, 127.8, 129.1, 129.3, 134.9, 144.0; IR (NaCl) 3067, 2955, 2928, 2868, 2852, 1609, 1580, 1475, 1468, 1366, 1022, 739, 691 cm^{-1} . Anal. Calcd for $\text{C}_{13}\text{H}_{18}\text{Se}$: C, 61.66; H, 7.16. Found: C, 61.93; H, 7.28.

1-Phenylseleno-1-(*p*-methoxyphenyl)-ethene (Table 2, entry 7).

This hydroselenation product is unstable and makes it difficult to isolate. Therefore, only ^1H NMR spectra data is shown, as a reference.

TLC: Rf = 0.42 (hexane/ethyl acetate = 80/20).

Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 3.83 (s, 3H), 5.32 (s, 1H), 5.84 (s, 1H), 7.16-7.53 (m, 9H).