Electronic Supplementary Information for Dalton Transactions

Electronic Supporting Information: NMR & IR Data

Dioxo-molybdenum(VI) complexes as catalysts for the hydrosilylation of aldehydes and ketones

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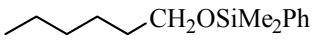
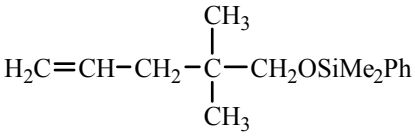
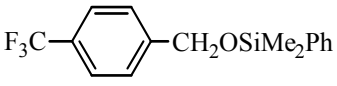


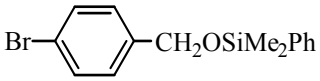
(Hexyloxy)-dimethyl-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.57-7.50 (m, 2H), 7.23-7.17 (m, 3H), 3.52 (t, 2H, J_{H-H} = 6.3 Hz), 1.53-1.44 (m, 2H), 1.32-1.16 (m, 6H), 0.83 (t, 3H, J_{H-H} = 6.3 Hz), 0.32 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 134.2, 133.7, 133.3, 130.0, 63.1, 33.0, 31.3, 25.8, 23.01, 14.1, -1.6; IR (neat) cm^{-1}: 3070, 2955, 2858, 1467, 1428, 1377, 1255, 1119, 1054, 998, 880, 831, 791, 742, 700, 649, 471.



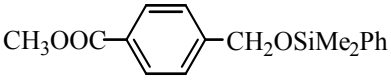
[(2,2-dimethyl-4-pentenyl)oxy]-dimethyl-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.56-7.50 (m, 2H), 7.22-7.15 (m, 3H), 5.82-5.67 (m, 1H), 4.91 (d, 2H, J_{H-H} = 8 Hz), 3.21 (s, 2H), 2.02 (d, 2H, J_{H-H} = 7.5 Hz), 0.83 (s, 6H), 0.31 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 138.4, 137.3, 134.2, 133.3, 129.7, 117.1, 71.5, 43.9, 24.1, 1.0, -1.4; IR (neat) cm^{-1}: 3070, 2975, 2700, 1469, 1260, 1100, 920, 870, 700, 470.



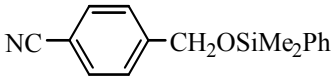
Dimethyl-phenyl-(4-trifluoromethyl-benzyloxy)-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.55-7.52 (m, 2H), 7.36-7.32 (m, 2H), 7.25-7.22 (m, 3H), 7.12-7.09 (m, 2H), 4.45 (s, 2H), 0.30 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 145.4, 139.9, 137.5, 133.8, 133.3, 130.1, 128.3, 126.6, 125.3, 64.2, -1.8; IR (neat) cm^{-1}: 3051, 2959, 2864, 1620, 1428, 1326, 1255, 1164, 1119, 1066, 1018, 830, 790, 700, 650, 620, 592, 472.



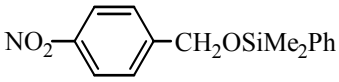
(4-Bromo-benzyloxy)-dimethyl-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.52-7.45 (m, 4H), 7.25-7.17 (m, 3H), 6.90-6.88 (m, 2H), 4.07 (s, 2H), 0.31 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 139.8, 137.2, 133.6, 131.4, 130.1, 128.5, 128.0, 120.9, 64.5, -1.7; IR (neat) cm^{-1}: 2959, 1594, 1487, 1251, 1069, 830, 700, 470.



Methyl-[4-(dimethyl-phenyl-silyloxy)-methyl]-benzoate. ^{1}H NMR (300 MHz, C_6D_6) δ 8.09-8.07 (m, 2H), 7.54-7.42 (m, 4H), 7.23-7.14 (m, 3H), 4.50 (s, 2H), 3.47 (s, 3H), 0.30 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 165.1, 139.5, 137.6, 135.3, 134.2, 131.2, 130.8, 129.0, 127.6, 64.2, 53.6, -1.6; IR (neat) cm^{-1}: 3069, 2959, 1721, 1428, 1255, 1119, 1064, 831, 790, 699, 650, 470.

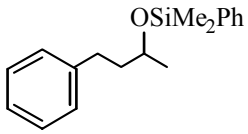


4-[(Dimethyl-phenyl-silyloxy)-methyl]-benzonitrile. ^{1}H NMR (300 MHz, C_6D_6) δ 7.53-7.43 (m, 2H), 7.25-7.18 (m, 5H), 7.11-6.95 (m, 2H), 4.38 (s, 2H), 0.31 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ146.1, 137.3, 134.3, 133.8, 133.4, 132.4, 132.0, 126.7, 118.9, 64.1, -1.8; IR (neat) cm^{-1}: 3069, 2958, 1610, 1427, 1253, 1118, 1088, 820, 790, 700, 647, 547, 471.



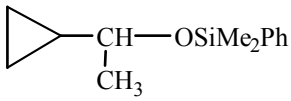
Dimethyl-(4-nitro-benzyloxy)-phenyl-silane. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18-8.16 (m, 2H), 7.60-7.55 (m, 2H), 7.47-7.38 (m, 3H), 7.10-7.09 (m, 2H), 4.76 (s, 2H), 0.45 (s,

6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.7, 147.5, 137.1, 133.8, 130.2, 128.4, 127.2, 123.9, 64.2, -1.5 ; IR (neat) cm^{-1}: 2958, 1520, 1344, 1064, 824, 710, 560, 470.

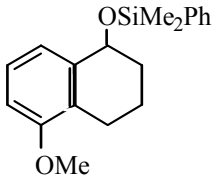


Dimethyl-(1-methyl-3-phenyl-propoxy)-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.59-7.56 (m, 3H), 7.22-7.02 (m, 7H), 3.76-3.68 (m, 1H), 2.68-2.49 (m, 2H), 1.76-1.71 (m, 2H), 1.05 (d, *J* = 6 Hz, 3H), 0.30 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 142.3, 139.7, 137.5, 137.1, 134.3, 130.0, 127.6, 71.9, 69.0, 35.7, 34.8, 23.2, -1.8; IR (neat) cm^{-1}: 2959, 2865, 1452, 1385, 761, 700, 570, 470.

(4-*tert*-Butyl-cyclohexyloxy)-dimethyl-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.72-7.69 (m, 2H), 7.33-7.25 (m, 3H), 3.66-3.56 (m, 1H), 2.04-2.0 (m, 2H), 1.70-1.63 (m, 2H), 1.50-1.40 (m, 5H), 0.83 (s, 9H), 0.38 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 138.7, 133.8, 129.4, 127.7, 72.3, 47.2, 34.8, 34.2, 27.6, 26.1, -1.3; IR (neat) cm^{-1}: 2953, 2862, 1428, 1365, 1255, 1119, 1089, 831, 795, 696, 649, 470.



(1-Cyclopropylethoxy)-dimethyl-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.59-7.51 (m, 2H), 7.24-7.15 (m, 3H), 3.20-3.16 (m, 1H), 1.18 (d, J_{H-H} = 6 Hz, 3H), 0.81-0.78 (m, 1H), 0.24-0.15 (m, 4H), 0.32 (s, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 139.0, 135.1, 133.3, 129.6, 24.05, 19.36, 4.75, 2.25, -0.59; IR (neat) cm^{-1}: 3070, 3004, 2871, 1428, 1371, 1252, 1117, 969, 881, 828, 786, 699, 643, 471.



[(5-Methoxy-1,2,3,4-tetrahydro-1-naphthalenyl)oxy]-dimethyl-phenyl-silane. ^{1}H NMR (300 MHz, C_6D_6) δ 7.63-7.62 (m, 2H), 7.24-7.17 (m, 3H), 7.55 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H), 7.10 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H), 6.46 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H), 4.83-4.80 (m, 1H), 3.42 (s, 3H), 2.64-2.61 (m, 2H), 1.95-1.84 (m, 1H), 1.73 (m, 3H), 0.39 (d, $J_{H\text{-}H}$ = 3 Hz, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 156.8, 142.1, 140.9, 133.8, 129.1, 128.1, 127.6, 124.8, 122.7, 108.5, 82.0, 55.8, 35.7, 22.5, 19.6, 1.2, 0.05; IR (neat) cm^{-1}: 1582, 1460, 1247, 1112, 826.