Synthesis and Applications of Polymeric *N*-Heterocyclic Carbene Palladium Complex-Grafted Silica as a Novel Recyclable Nano-Catalyst for Heck and Sonogashira Coupling Reactions

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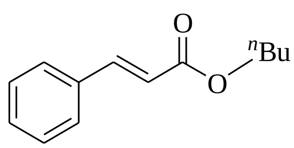
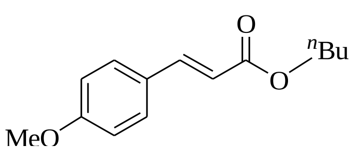
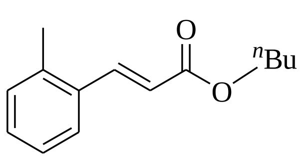
Characterization data of arylated-alkene compounds (Table 2) 1-5



(1): ^{1}H-NMR (250 MHz, $CDCl_3$): 0.83-0.9 (t, 3H, J = 7.3 Hz) ppm, 1.17-1.42 (m, 2H), 1.54-1.69 (m, 2H), 4.12 (t, 2H, J = 6.8 Hz), 6.32 (d, 1H, J = 16 Hz), 7.17-7.29 (m, 3H), 7.41-7.62 (m, 2H), δ 7.80 (d, 1H, J = 16 Hz). ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 167.1, 144.5, 134.4, 130.2, 129.8, 128.1, 118.2, 64.3, 30.7, 19.1 13.7 ppm.



(2): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 0.93-0.99 (t, J= 7.5 Hz, 3H), 1.38-1.47 (m, 2H), 1.62-1.71 (m, 2H), 3.82 (s, 3H), 4.21 (t, J= 6.7 Hz, 2H), 6.32 (d, J=16.0,1H), 6.68-6.92 (m, 2H), 7.45-7.49 (m, 2H), 7.76 (d, J= 16.0, 1H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 167.3, 162.4, 144.1, 129.6, 127.0, 115.6, 114.2, 64.2, 55.2, 30.7, 19.1, 13.6 ppm.



(3): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 0.81-0.87 (m, J= 7.5 Hz, 3H,), 1.40-1.46 (m, 2H), 1.67-1.73 (m, 2H), 2.3 (s, 3H), 4.22 (m, 2H, J= 7.5 Hz), 6.27 (d, J=16.0, 1H), 7.47-7.54 (m, 3H), 7.62 (d, 1H), 8.30 (d, 1H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 142.2, 130.7, 129.9, 129.1, 128.9, 127.7, 127.3, 124.1, 119.2, 64.4, 30.7, 19.7, 19.2, 13.7 ppm.

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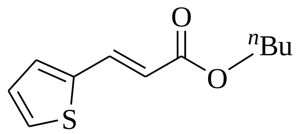
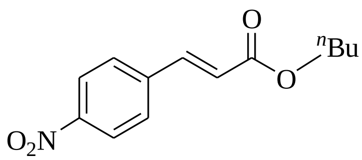
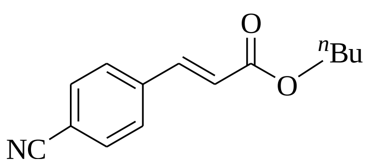


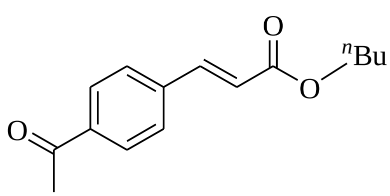
(4): ^{1}H-NMR (250 MHz, $CDCl_3$) δ (ppm): 0.87 (t, 3 H, *J* = 7.5), 1.31-1.42 (m, 2H) , 1.54-1.62 (m, 2H), 4.11 (t, 2H, *J* = 7.5 Hz), 6.17 (d, 1H, *J* = 17.5), 7.18-7.27 (m, 2H), 7.41 (d, 1H, *J*=8.2), 7.57 (d, 1H, *J* = 17.5), ^{13}C-NMR (62.9 MHz,$CDCl_3$) δ (ppm): 166.2, 136.9, 136.5, 127.7, 126.9, 125.8, 116.9, 63.3, 29.7, 18.1, 12.7.



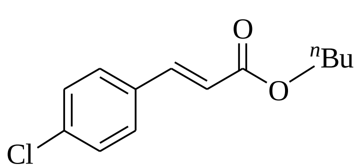
(6): ^{1}H-NMR (250 MHz, $CDCl_3$): 0.93 (t, 3H, J = 7.5) ppm, 1.36-1.45 (m, 2H), 1.63-1.69 (m, 2H), 4.17 (t, 2H, J= 7.5 Hz), 6.53 (d, 1H, J = 15.5 Hz), 7.63-7.70 (m, 3H), δ 8.20 (d, 2H, J = 8.7 Hz); ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 184.0, 166.5, 155.5, 138.7, 133.5, 129.5, 123.3, 87.7, 54.4, 28.8, 15.5 ppm.



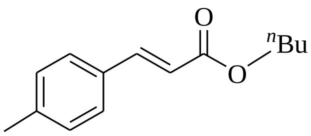
(7): ^{1}H-NMR (250 MHz, $CDCl_3$): 0.84-0.90 (t, 3H, J = 7.3 Hz) ppm, 1.30-1.39 (m, 2H, J = 7.3 Hz),δ 7.51–7.72 (m, 5H), 1.58-1.66 (m, 2H, J = 7.3 Hz), 4.11 (t, 2H, J = 6.6 Hz), 6.47 (d, 1H, J = 16 Hz), δ 7.51–7.60 (m, 5H) ; 13C-NMR (62.9 MHz, $CDCl_3$): δ 166.14, 142.0, 138.6, 132.5, 128.7, 121.8, 118.3, 113.2, 64.7, 30.6, 19.1, 13.6 ppm.



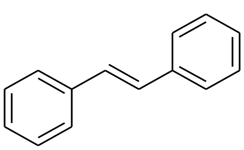
(8): ^{1}H-NMR (250 MHz, $CDCl_3$): 0.86-0.92 (m, 3H, J = 7.3 Hz) ppm, 1.32-1.48 (m, 2H), 1.59-1.65 (m, 2H), 2.53 (S, 3H), 4.15 (m, 2H, J= 7.5 Hz), 6.47 (d, 1H, J = 16 Hz), 7.22-7.58 (m, 5H); ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 195.5, 172.5, 155.0, 146.5, 141.5, 132.6, 130.8, 125.5, 88.3, 45.0, 33.4, 23.4, 16.0 ppm.



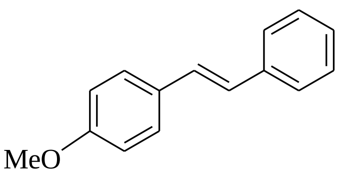
(9): ^{1}H-NMR (250 MHz, CDCl3): δ 0.95 (t, J= 7.4 Hz, 3H), 1.37-1.46 (m, 2H), 1.62-1.70 (m, 2H), 4.17 (t, J= 6.7 Hz, 2H), 6.42 (d, J= 16.0, 1H), 7.26-7.33 (m, 2H), 7.42-7.45 (m, 2H), 7.60 (d, J= 16.0, 1H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 166.7, 143.0, 136.0, 132.9, 129.1, 118.8, 64.4, 30.6, 19.1, 13.7 ppm.



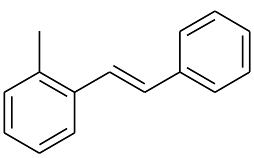
(10): ^{1}H-NMR (250 MHz, $CDCl_3$): 0.88 (t, 3H, J = 7.5 Hz) ppm, 1.20 (m, 2H, J =7.3 Hz), 1.99 (m, 2H, J = 6 Hz), 2.80 (s, 3H), 4.90 (t, 2H, J = 6.5 Hz), 6.60 (d, 1H, J = 16 Hz), 7.25 (d, 2H, J = 8.5 Hz), 7.55 (d, 2H, J = 8.5 Hz), δ 7.87 (d, 1H, J = 16 Hz); ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 175.5, 150.6, 144.5, 130.0, 129.0, 128.5, 119.0, 70.5, 41.3, 25.7, 17.5, 13.0 ppm.



(14): 1H-NMR (250 MHz, $CDCl_3$): δ 7.26 (s, 2H) ppm, 7.30 (t, 2H, J = 7.5 Hz), 7.36 (t, 4H, J = 7.5 Hz), δ 7.55 (d, 4H, J = 7.5 Hz); ^{13}C-NMR (62.9 MHz, $CDCl_3$): 137.3, 128.7, 127.6, 126.5 ppm.

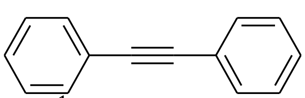


(15): ^{1}H-NMR (250 MHz, $CDCl_3$): 3.77 (s, 3H) ppm, 6.80 (d, 2H, J = 8.5 Hz), 6.89 (d, 1H, J = 16.5 Hz), 6.99 (d, 1H, J = 16.0 Hz), 7.18 (t, 1H, J = 6.5 Hz), 7.28 (t, 2H, J = 7.5 Hz), 7.37 (d, 2H, J =8.5 Hz),δ 7.42 (d, 2H, J = 7.5 Hz); ^{13}CNMR (62.9 MHz, $CDCl_3$): δ 160.5, 138.8, 130.9, 129.5, 128.0, 127.5, 127.0, 126.5, 126.0, 116.5, 57.5 ppm.



(16): ^{1}H-NMR (250 MHz, $CDCl_3$) δ (ppm): 2.33 (s, 3H), 6.90 (d, 1H, *J*=16.0),7.53-7.07 (m, 10H). ^{13}C-NMR (62.9 MHz, $CDCl_3$) δ (ppm): 137.7, 136.4, 135.8, 130.4, 130.0, 128.7, 128.4, 127.6, 126.6, 126.5, 126.2, 125.4, 19.9.

Characterization data of arylated-alkyne compounds (Table 3) 6-9



(1): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.16-7.23 (m, 6H), 7.39-7.44 (m, 4H), ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 131.2, 128.5, 128.2, 123.3, 89.5 ppm.

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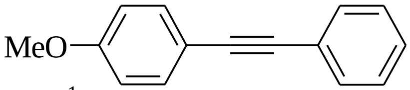
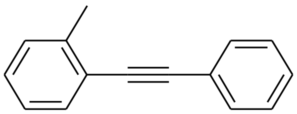
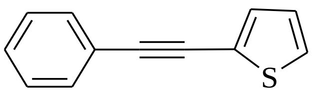


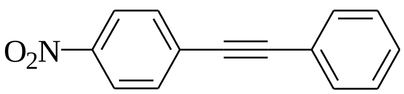
(2): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.37-7.43 (m, 4H), 7.22-7.25 (m, 3 H), 6.79 (d, 2 H, J=8.2), 3.75 (s, 3H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 159.6, 133.0, 131.4, 128.3, 127.9, 123.6, 115.3, 114.0, 89.3, 88.0, 55.2 ppm .



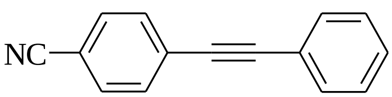
(3): 1H-NMR ($CDCl_3$, 250 MHz): δ (ppm): 2.44 (s, 3 H), 7.14-7.46 (m, 9 H); ^{13}C-NMR ($CDCl_3$, 62.9 MHz): δ (ppm): 20.75, 86.01, 94.25, 123.01, 125.58, 128.17, 128.30, 128.35, 129.46, 131.51, 131.83, 140.19;



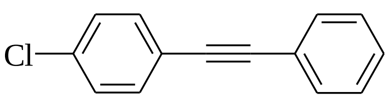
(4): ^{1}H-NMR (DMSO-d_6, 250 MHz): δ (ppm): 7.01-7.68 (m, 8 H); ^{13}C-NMR (DMSO-d_6, 62.9 MHz): δ (ppm): 87.30, 94.51, 128.33, 128.43, 129.20, 131.51, 132.50



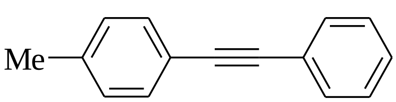
(6): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 8.22 (d, 2H), 7.64-7.69 (d, 2H), 7.54-7.57 (m, 2H), 7.37-7.41 (m, 3H) ppm; 13C-NMR (62.9 MHz, $CDCl_3$): δ 146.9, 132.2, 131.8, 130.2, 129.2, 123.6, 122.0, 94.7, 87.5 ppm.



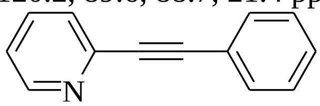
(7): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.28-7.31 (m, 6H), 7.44-7.53 (m, 3H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 132.0, 131.7, 129.1, 128.5, 128.2, 122.2, 118.5, 111.4, 93.7, 87.7 ppm.



(8): ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.13-7.25 (m, 3H), 7.33-7.43 (m, 6H) ppm; ^{13}C-NMR (62.9 MHz, $CDCl_3$): δ 134.2, 132.8, 131.6, 128.7, 128.5, 128.4 122.9, 121.8, 90.3, 88.2 ppm.



(9): [1]H-NMR ($CDCl_3$, 250 MHz): δ 7.52-7.48 (m, 2H), 7.41 (d, 2H), 7.29–7.26 (m, 3H), 7.10 (d, 2H), 2.30 (s, 3H) ppm; [13]C-NMR (62.9 MHz, $CDCl_3$): δ 138.3, 131.5, 129.0, 128.2, 128.0, 123.4, 120.2, 89.6, 88.7, 21.4 ppm.



(12): [1]H-NMR (250 MHz, $CDCl_3$): δ 8.69 (s, 1H), 8.46-8.47 (m, 1H), 7.71-7.74 (m, 1H), 7.45-7.51 (m, 2H), 7.28-7.31 (m, 4H) ppm; [13]C-NMR (62.9 MHz, $CDCl_3$): δ (ppm): 152.2, 148.5, 138.4, 131.6, 128.8, 128.4, 126.4, 123.0 ppm.