Supporting Information

Cyano-bridged copper(II)-copper(I) mixed-valence coordination polymer as source for copper oxide nanoparticles with good catalytic activity in C-N, C-O and C-S cross-coupling reactions

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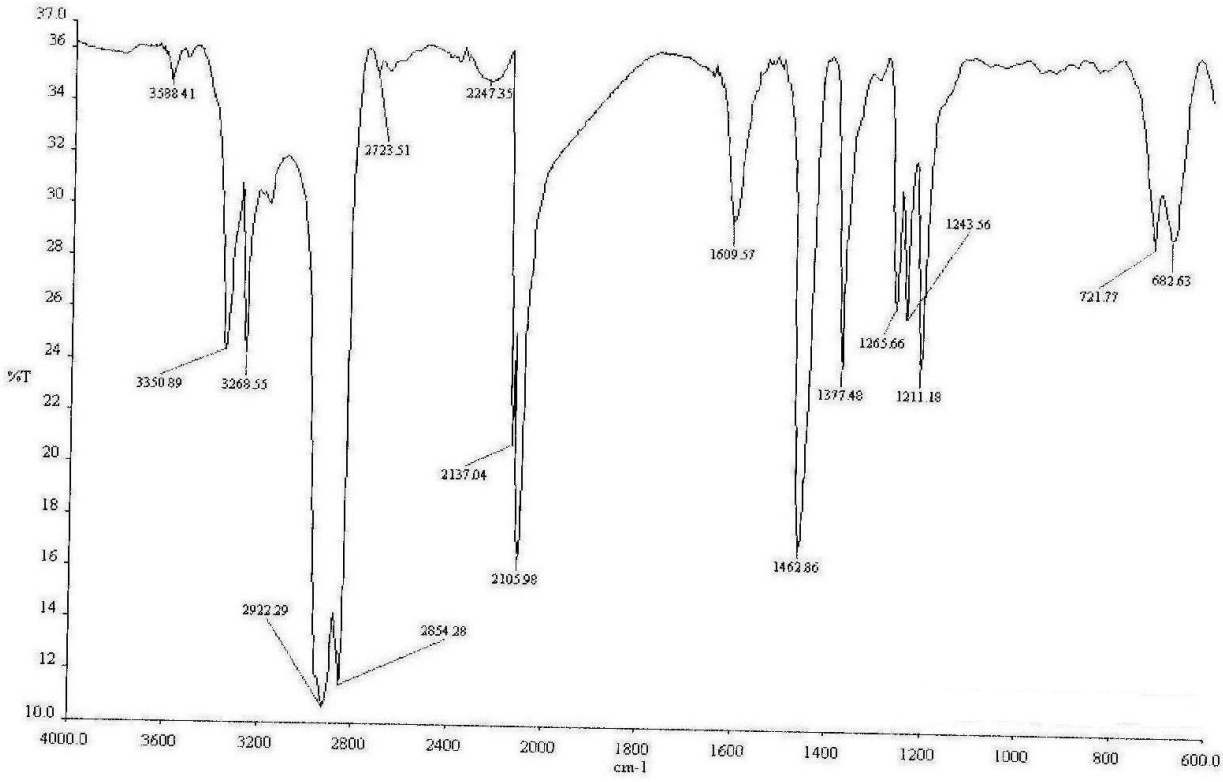
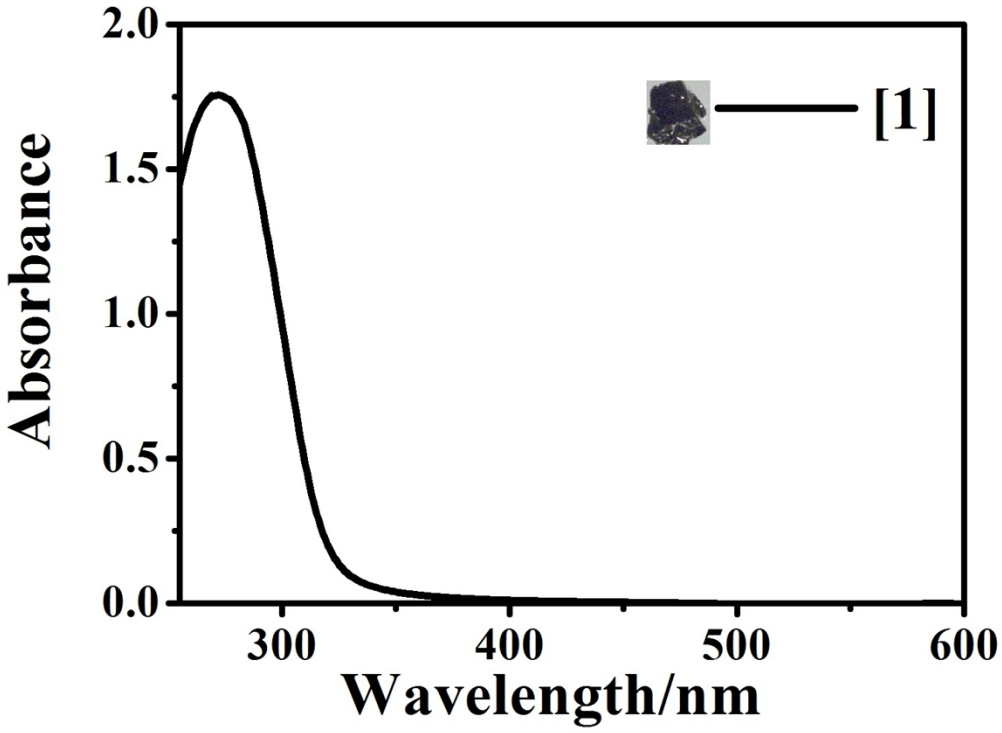
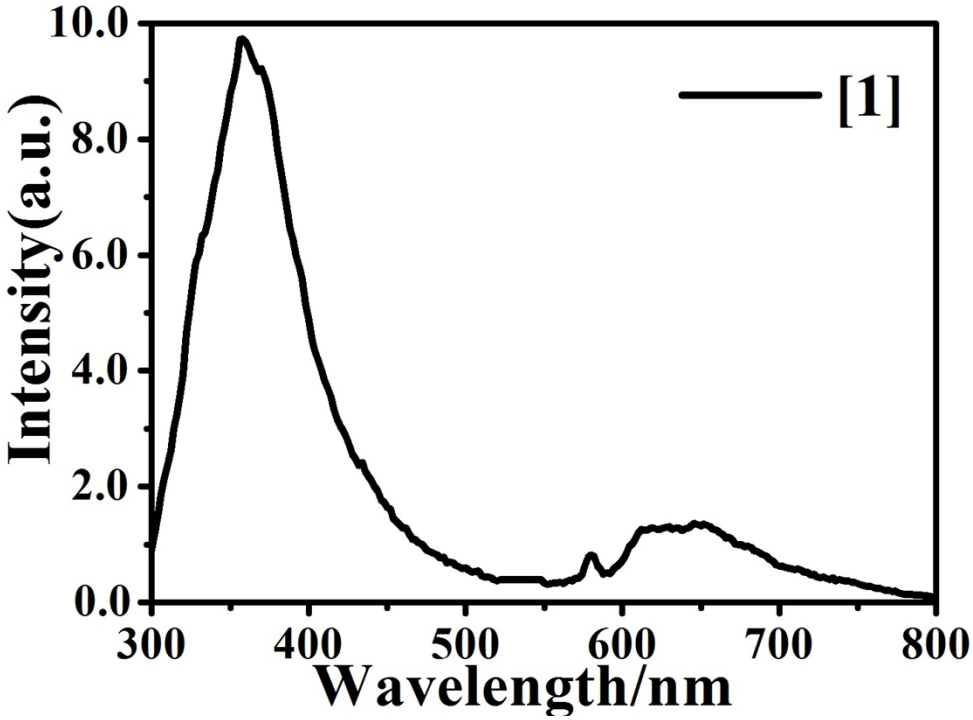


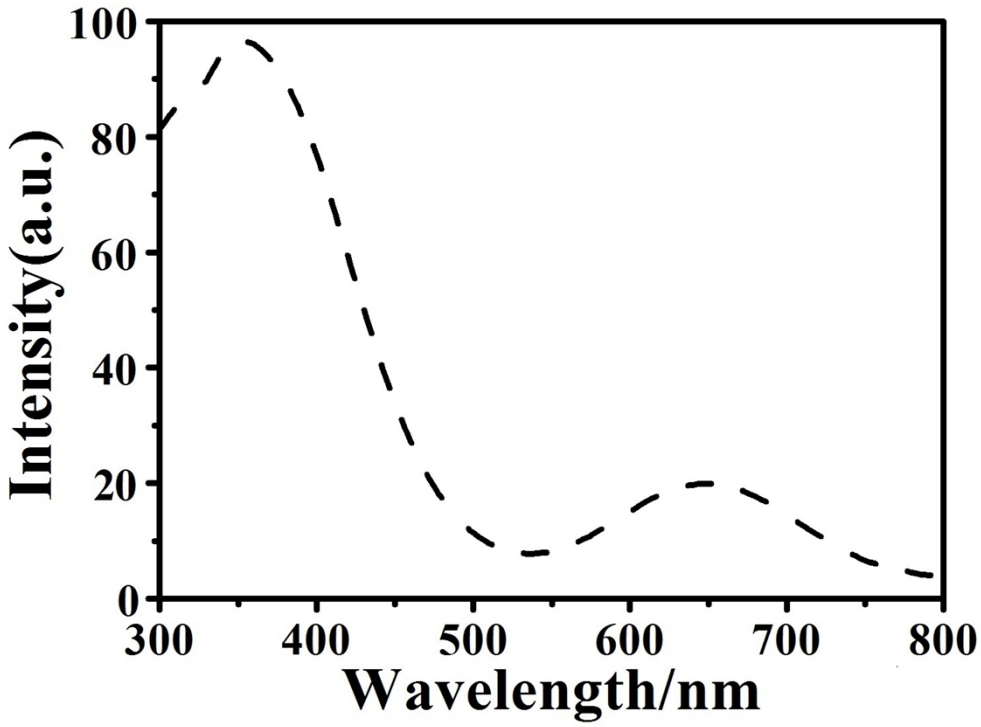
S1. Infrared spectrum of **1.**



S2. Electronic spectrum for **1** in DMSO.

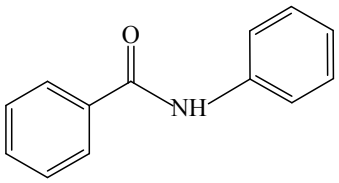


S3. Normalised emission spectrum for **1** in DMSO.



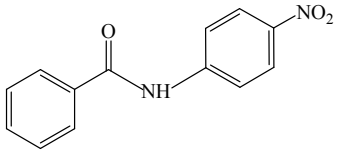
S4. Emission spectrum for **1** in the solid state (λ_{ex} 270 nm).

***N*-Phenylbenzamide:**[1]



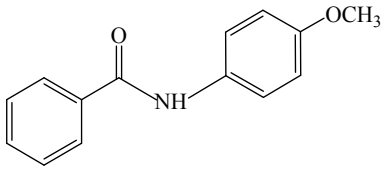
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85(d, J=7.4Hz, 2H), 7.76 (s, 1H), 7.61(d, J=6.0Hz, 2H), 7.52 (d, J=6.4Hz, 1H), 7.45 (t, J=8.4Hz, 2H), 7.36 (t, J=7.2Hz, 2H), 7.12 (t, J=6.4Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 166.2, 138.5, 135.1, 132.0, 129.4, 129.0, 127.2, 124.8, 120.4.

***N*-(4-Nitrophenyl)-benzamide:**[2]



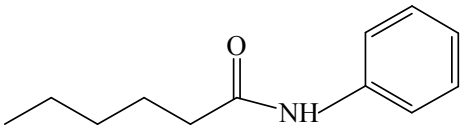
Yellow solid; ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.14 (s, 1H), 8.01(d, J = 8.6Hz, 2H), 7.84 (d, J=7.2Hz, 2H), 7.76 (d, J=6.4Hz, 2H), 7.36 (t, J=8.1Hz, 1H), 7.31 (t, J=7.6Hz 2H); ^{13}C NMR (400 MHz, DMSO-d_6): δ 166.6, 145.1, 142.6, 134.2, 131.6, 128.1, 127.8, 124.2, 119.6.

***N*-(4-Methoxyphenyl)-benzamide:**[2]



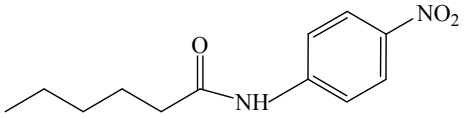
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J=8.4Hz, 2H), 7.74 (s, 1H), 7.53-7.41 (m, 5H), 6.85 (d, J=7.8Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 165.8, 156.9, 135.2, 131.6, 131.3, 128.9, 127.4, 122.4, 114.5, 55.6.

N-Phenylhexanamide:[3]



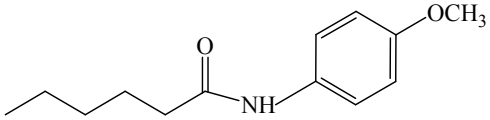
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, J=7.6Hz, 2H), 7.30 (t, J=7.8Hz, 2H), 7.12 (s, 1H), 7.06 (t, J= 6.4Hz, 1H), 2.33 (t, J=7.8Hz, 2H), 1.74 (m, 2H), 1.35-1.32 (m, 4H), 0.90-0.86 (m, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 171.9, 138.2, 129.2, 124.4, 120.1, 38.1, 31.6, 25.5, 22.6, 14.1.

***N*-(4-Nitrophenyl)-hexanamide:**[3]



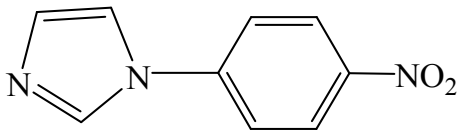
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, J=8.4Hz, 2H), 7.40 (d, J=4.8 Hz, 2H), 7.14 (s, 1H), 2.34 (t, J=6.8Hz, 2H), 1.78 (m, 2H), 1.40-1.34 (m, 4H), 0.96-0.89(m, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 172.6, 145.2, 142.5, 137.6, 128.2, 124.2, 119.8, 38.2, 31.4, 25.2, 22.6, 14.2.

***p*-Hexananisidide:**[4]



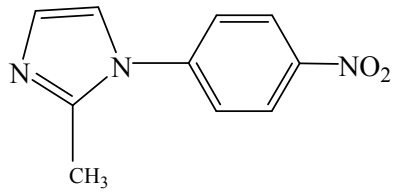
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, J = 4.8Hz, 2H), 7.25 (s, 1H), 6.70 (d, J = 7.8Hz, 2H), 3.60 (s, 3H), 2.26 (t, J = 8.6Hz, 2H), 1.60-1.68 (m, 2H), 1.36-1.28 (m, 4H), 0.88-0.84 (m, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 171.2, 155.6, 130.9, 121.8, 114.3, 55.6, 37.4, 31.2, 25.3, 22.6, 14.1.

1-(4-Nitrophenyl)-1*H*-imidazole:[5]



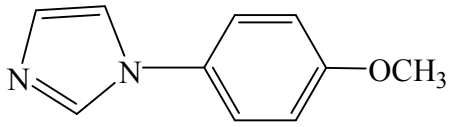
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (d, J=6.4Hz, 2H), 7.95 (s, 1H), 7.52 (d, J=9.2Hz, 2H), 7.35 (s, 1H), 7.20 (d, J=4.8Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 146.6, 142.2, 135.4, 131.6, 125.8, 121.2, 117.6.

2-Methyl-1-(4-nitrophenyl)-1H-imidazole:[6]



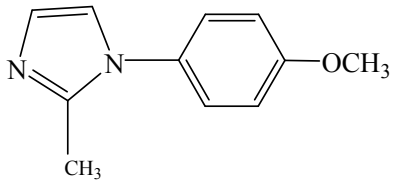
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, J = 6.0Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.01 (d, J = 6.4Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 147.3, 144.5, 143.2, 128.6, 126.1, 125.3, 120.4, 29.8.

1-(4-Methoxyphenyl)-1*H*-imidazole:[7]



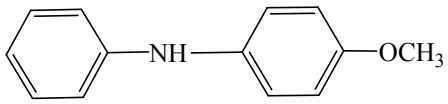
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.30-7.22 (m, 2H), 7.12 (d, J=6.4 Hz, 2H), 6.92-6.96 (m, 2H), 3.82 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 159.4, 136.3, 131.1, 130.4, 123.5, 118.1, 115.5, 55.8.

1-(4-Methoxyphenyl)-2-methyl-1*H*-imidazole:[8]



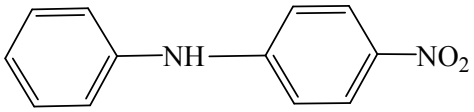
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (d, J=7.4Hz, 2H), 6.94-6.91 (m, 4H), 3.82 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 159.2, 131.1, 130.6, 128.3, 126.7, 121.1, 114.6, 55.4, 29.8.

4-methoxy-N-phenylbenzenamine:[9]



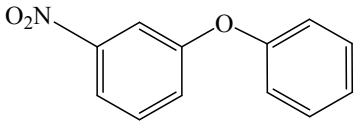
Colorless solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (d, J = 6.4Hz, 2H), 7.24-7.10 (m, 5H) 6.88 (d, J = 7.4Hz, 2H), 5.51 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 153.4, 145.7, 135.5, 129.2, 123.4, 120.1, 115.1, 55.2.

4-nitro-N-phenylbenzenamine:[9]



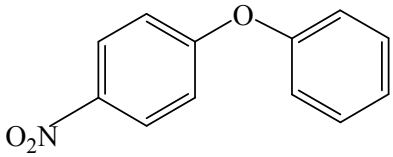
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, J = 7.2Hz, 2H), 7.40 (t, J = 8.4 Hz, 2H) 7.20-7.10 (m, 3H), 6.91 (d, J = 8.6Hz, 2H), 6.31 (s, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 151.3, 138.2, 137.5, 129.6, 127.6, 125.6, 123.4, 114.1.

1-Nitro-3-phenoxybenzene:[4]



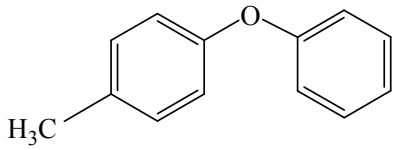
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, J = 7.4Hz, 1H), 7.61 (t, J = 8.4Hz, 1H), 7.34–7.23 (m, 3H), 7.04 (t, J =6.6Hz, 1H), 6.94-6.91 (m, 2H), 6.80 (d, J = 8.4Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 158.5, 155.6, 149.4, 130.6, 129.8, 124.5, 122.1, 120.9, 116.6, 115.5.

1-Nitro-4-phenoxybenzene:[4]



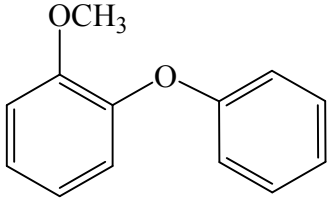
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (d, J = 9.2Hz, 2H), 7.46–7.42 (m, 2H), 7.28-7.24 (m, 1H), 7.09 (m, 2H), 7.01 (d, J = 9.2Hz, 2H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 163.4, 154.9, 142.3, 130.1, 126.4, 125.2, 120.1, 117.3.

1-methyl-4-phenoxybenzene:[4]



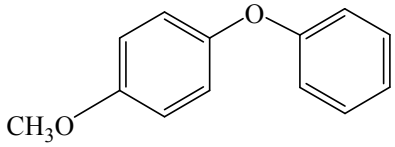
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.31 (m, J = 4.2Hz, 2H), 7.17-7.15 (m, J = 6.4Hz, 2H), 7.10-7.07 (m, J = 7.8Hz, 1H), 7.01-6.99 (m, J = 8.4Hz 2H), 6.95-6.93 (m, J = 6.8Hz 2H), 2.35 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 158.4, 154.8, 133.2, 130.1, 129.8, 123.1, 119.4, 118.5, 22.9.

1-methoxy-2-phenoxybenzene:[4]



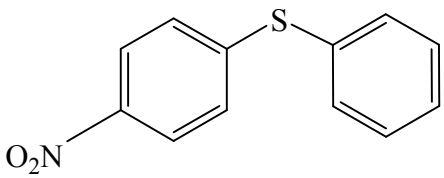
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.32-7.25 (m, J = 6.4Hz, 2H), 7.15 (t, *J* = 9.2 Hz, 1H), 7.05-6.80 (m, J = 7.8Hz, 6H), 3.81 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 157.8, 151.2, 145.1, 129.8, 124.9, 122.4, 121.0, 117.1, 112.6, 56.1.

1-methoxy-4-phenoxybenzene:[4]



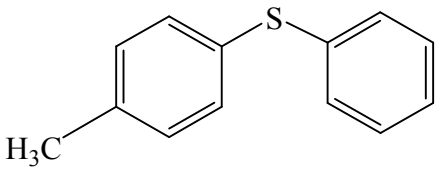
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 7.34-7.30 (m, J = 8.4Hz, 2H), 7.09-7.05 (m, J = 6.0Hz 1H), 7.03-6.97 (m, J = 4.2Hz, 4H), 6.93–6.90 (m, J = 6.4Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): δ 158.7, 156.3, 150.1, 129.9, 122.4, 121.1, 117.8, 115.4, 55.8.

4-Nitrophenyl phenyl sulfide:[10]



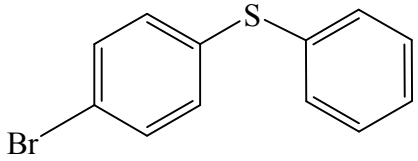
Yellow solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.02 (d, J = 6.4Hz, 2H), 7.30-7.22 (m, 3H), 7.05 (d, J = 4.8Hz, 2H), 6.71 (d, J = 7.4Hz, 1H); ^{13}C NMR ($CDCl_3$, 400 MHz): δ 158.9, 142.9, 136.1, 131.2, 125.8, 124.6, 115.1.

4-Tolylphenyl sulfide:[10]



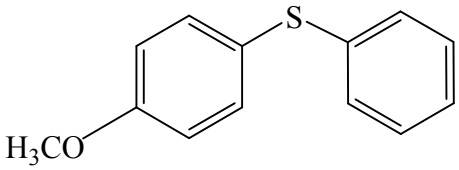
Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32-7.25 (m, 6H), 7.22-7.15 (m, 3H), 2.36 (s, 3H); ^{13}C NMR ($CDCl_3$, 400 MHz): δ 137.7, 137.3, 132.5, 131.4, 130.2, 129.8, 129.3, 126.5, 21.4.

4-Bromophenyl phenyl sulfide:[10]



Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.42-7.38 (m, J = 6.4Hz, 2H), 7.35-7.24 (m, 5H). 7.18-7.16 (m, J = 7.4Hz, 2H); ^{13}C NMR ($CDCl_3$, 400 MHz): δ 135.9, 132.8, 132.5, 132.1, 129.2, 128.1.

***p*-Anisyl phenyl sulfide:**[10]



Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.38-7.36 (m, J = 8.4Hz, 2H), 7.21-7.10 (m, 5H), 6.89-6.84 (m, J = 4.8Hz, 2H), 3.62 (s, 3H); ^{13}C NMR ($CDCl_3$, 400 MHz): δ 159.9, 138.8, 135.6, 129.1, 128.3, 125.9, 124.4, 115.1, 55.5.

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