

Supporting information

DABCO-functionalized silica-copper (I) complex: a novel and recyclable heterogeneous nanocatalyst for palladium-free Sonogashira cross-coupling reaction

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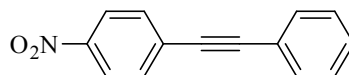
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Data for the prepared organic compounds¹⁻⁴

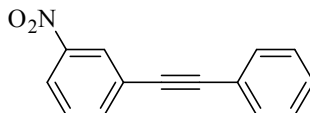
1-Nitro-4-phenylethynyl-benzene



Yellow solid, melting point: 117-119 °C

¹H-NMR (400 MHz, CDCl₃, ppm, TMS): δ = 8.1 (d, J = 9.0 Hz, 2H), 7.8 (d, J = 8.8 Hz, 2H), 7.5 (m, 2H), 7.3 (m, 3H), ¹³C-NMR (100 MHz, CDCl₃): δ = 145.0, 130.2, 128.7, 127.1, 126.3, 124.6, 122.8, 120.2, 93.7, 86.3. FT-IR (KBr, cm⁻¹): ν = 3106, 2215, 1580, 1340, 1115.

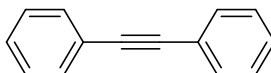
1-Nitro-3-phenylethynyl-benzene



Pale yellow solid, melting point: 68-70 °C

¹H-NMR (400 MHz, CDCl₃, ppm, TMS): δ = 8.29 (m, 1H), 7.8 (ddd, J = 8.0, 2.1, 1.2 Hz, 1H), 7.65 (ddd, J = 14.3, 7.6, 3.0 Hz, 3H), 7.48-7.52 (m, 1H), 7.33-7.34 (m, 3H). ¹³C-NMR (100 MHz, CDCl₃): δ = 149.3, 136.3, 132.9, 127.5, 126.1, 125.5, 124.3, 123.1, 121.6, 120.2, 89.8, 87.8. FT-IR (KBr, cm⁻¹): ν = 2920, 2209, 1589, 1503, 1337, 840.

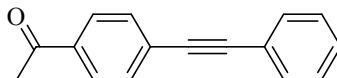
1,2-diphenylethyne



White solid, melting point: 58-60 °C

$^1\text{H-NMR}$ (400 MHz, CDCl_3 , ppm, TMS): $\delta = 7.55\text{-}7.60$ (m, 4H), $7.27\text{-}7.39$ (m, 6H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): $\delta = 132.6, 129.4, 127.3, 122.3, 88.5$.

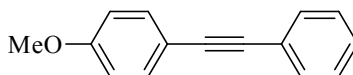
1-(4-Phenylethynyl-phenyl)-ethanone



Pale yellow solid, melting point: 98-100 °C

$^1\text{H-NMR}$ (300 MHz, DMSO, ppm, TMS): $\delta = 7.9$ (d, $J = 8.5$ Hz, 2H), 7.6 (d, $J = 8.5$ Hz, 2H), 7.5 (m, 2H), 7.3 (m, 3H), 2.7 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): $\delta = 198, 138.2, 133.6, 130.6, 127.5, 125.2, 124.1, 120.6, 94.7, 86.6, 25.6$. FT-IR (KBr, cm^{-1}): $\nu = 3075, 2926, 2219, 1680, 1612, 1450, 1423, 1273, 1169$.

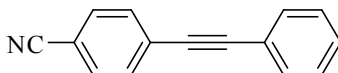
1-Methoxy-4-phenylethynyl-benzene



White solid, melting point: 60-62 °C

$^1\text{H-NMR}$ (400 MHz, CDCl_3 , ppm, TMS): $\delta = 7.56$ (m, 2H), 7.46 (d, $J = 9.5$ Hz, 2H), 7.30 (m, 3H), 6.89 (d, $J = 8.7$ Hz, 2H), 3.87 (s, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): $\delta = 156.5, 135.7, 130.5, 128.3, 126.6, 125.2, 114.9, 112.5, 88.6, 86.2, 50.7$.

4-(Phenylethynyl)benzonitrile



Pale yellow solid, melting point: 108–110 °C.

$^1\text{H-NMR}$: δ 7.35–7.38 (m, 3H), 7.48–7.53 (m, 2H), 7.55–7.57 (m, 4H); $^{13}\text{C-NMR}$: δ = 133, 134.7, 131.7, 127.8, 126, 124.9, 122.9, 119.3, 113.6, 95.2, 85.7.

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2. F. Yang, X. Cui, Y. Li, J. Zang, G. Ren and Y. Wu, *Tetrahedron*. 2007, **63**, 1963-1969.
3. A. Elangovan, Y.-H. Wang and T.-I. Ho, *Org. Lett.* 2003, **5**, 1841-1844.
4. F. Monnier, F. Turtaut, L. Duroure and M. Taillefer, *Org. Lett.* 2008, **10**, 3203-3206.