Electronic Supplementary Information

Title: Selective hydrogenation of biomass derived substrates using ionic liquid-stabilized Ruthenium nanoparticles

Authors: J. Julis, M. Hölscher and W. Leitner

Characterization of IL-stabilized ruthenium nanoparticles

XRD

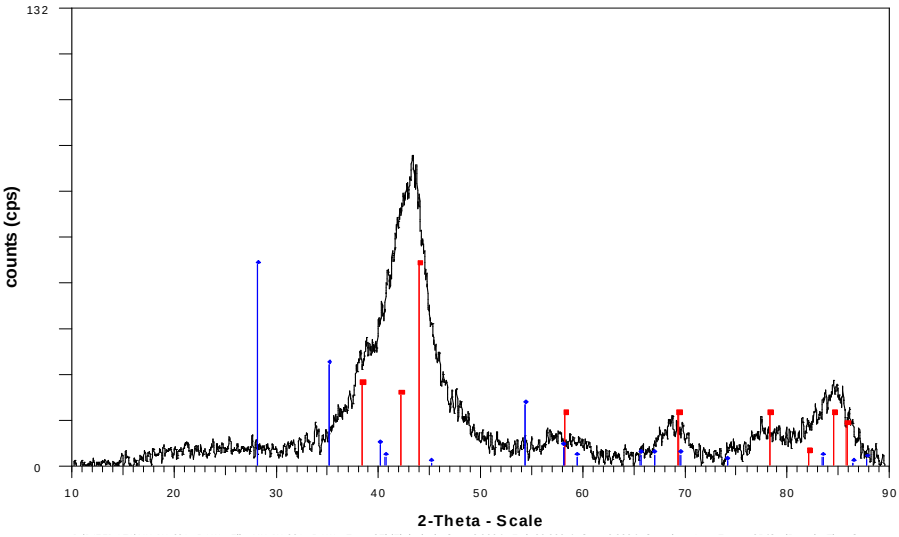


Figure 1. X-ray diffractogram of Ru@[C_{12}MIM][BTA] (washed with acetone).
blue: reflexes of RuO; **red**: reflexes of Ru

TEM

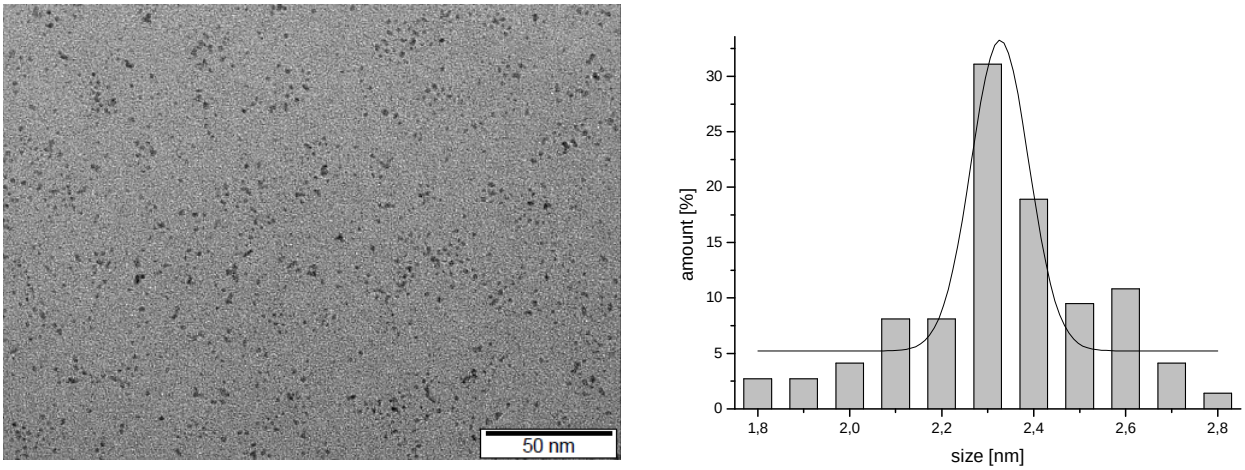


Figure 2. TEM image of Ru@[EMIM][Acetate] (left) and size distribution for 100 particles (right).

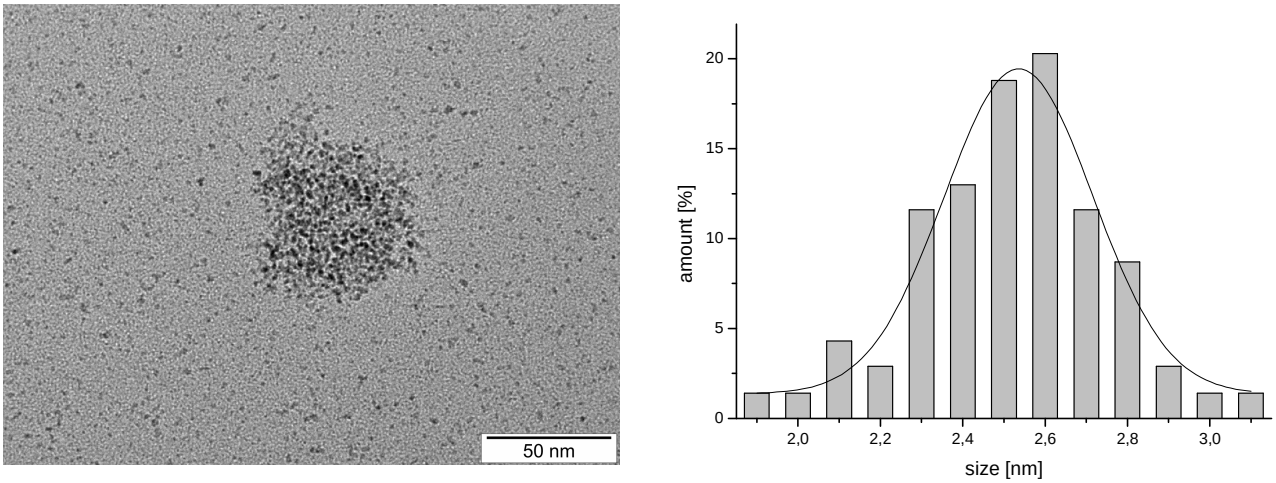
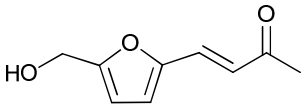


Figure 3. TEM image of Ru@[EMIM][Acetate] left and size distribution for 100 particles (right) after catalysis.

All other Ru@IL systems were characterized by the same methods. TEM images and particles size distributions look similar.

NMR data of isolated products

4-(5-hydroxymethyl-2-furyl)-3-butene-2-one (**1**)

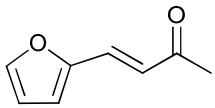


(**1**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 2.27 (s, 3 H), 4.58 (s, 2 H), 6.44 (d, 1 H, J_3= 3.5 Hz), 6.50 (d, 1 H, J_3= 16.0 Hz), 6.79 (d, 1 H, J_3= 3.5 Hz), 7.34 (d, 1 H, J_3= 16.0 Hz) ppm.

^{13}C-NMR (100 MHz, d_6-acetone): δ 27.5 (s, 1 C), 57.4 (s, 1 C), 110.5 (s, 1 C), 117.6 (s, 1 C), 124.6 (s, 1 C), 130.1 (s, 1 C), 151.2 (s, 1 C), 159.6 (s, 1 C), 206.2 (s, 1 C) ppm.

4-(2-Furyl)-3-buten-2-on (**2**)

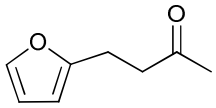


(**2**)

^{1}H-NMR (300 MHz, $CDCl_3$): δ 2.30 (s, 3 H), 6.46 (dd, 1 H, J = 1.8 Hz / 3.5 Hz), 6.64 (d, 1 H, J = 3.5 Hz), 6.90 (q, 2 H, J = 15.8/1.8 Hz), 7.48 (d, 1 H, J = 1.8 Hz) ppm.

^{13}C-NMR (75 MHz, $CDCl_3$): δ 27.9 (s, 1 C), 112.6 (s, 1 C), 115.7 (s, 1 C), 124.3 (s, 1 C), 129.4 (s, 1 C), 145.0 (s, 1 C), 150.9 (s, 1 C), 197.9 (s, 1 C) ppm.

4-(2-Furyl)-butan-2-on (**3**)

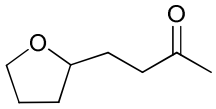


(**3**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 2.09 (s, 3 H), 2.78 (dt, 4 H, *J*= 7.3 / 50.1 Hz), 5.92 (m, 1 H), 6.19 (m, 1 H), 7.22 (m, 1 H) ppm.

^{13}C-NMR (150 MHz, DMSO): δ 22.2 (s, 1 H), 29.9 (s, 1 H), 41.7 (s, 1 H), 105.2 (s, 1 H), 110.2 (s, 1 H), 141.1 (s, 1 H), 154.5 (s, 1 H), 207.3 (s, 1 H) ppm.

4-(2-Tetrahydrofuryl)-butan-2-on (**4**)

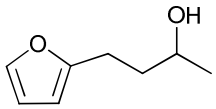


(**4**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 1.42 (m, 1 H), 1.68 (m, 1 H), 1.81 (m, 2 H), 1.95 (m, 1 H), 2.12 (s, 3 H), 2.52 (m, 2 H), 3.66 (m, 1H), 3.78 (m, 2 H) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ 25.8 (s, 1 C), 29.6 (s, 1 C), 30.0 (s, 1 C), 31.4 (s, 1 C), 40.5 (s, 1 C), 67.7 (s, 1 C), 78.4 (s, 1 C), 208.8 (s, 1 C) ppm.

4-(2-Furyl)-butan-2-ol (**5**)

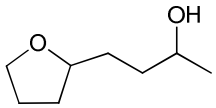


(**5**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 1.21 (d, 3 H, J_3= 6.4 Hz), 1.78 (m, 2 H), 2.73 (m, 2 H), 3.82 (m, 1 H), 5.99 (m, 1 H), 6.29 (m, 1 H), 7.29 (s, 1 H) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ 23.5 (s, 1 C), 24.4 (s, 1 C), 37.4 (s, 1 C), 67.3 (s, 1 C), 105.6 (s, 1 C), 110.2 (s, 1 C), 141.0 (s, 1 C), 155.9 (s, 1 C) ppm.

4-(2-Tetrahydrofuryl)-butan-2-ol (**6**)



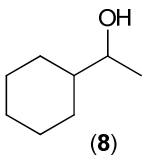
(**6**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 1.08 (dd, 3 H, J = 6.2 Hz / 1.9 Hz), 1.45 (m, 5 H), 1.82 (m, 3 H), 3.63 (m, 1 H, C*H*OH), 3.72 (m, 3 H) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ 23.3 (d, 1 C), 25.6 (d, 1 C), 31.4 (d, 1 C), 31.9 (d, 1 C), 36.0 (d, 1 C), 67.5 (d, 1 C), 67.6 (s, 1 C), 79.5 (d, 1 C) ppm.

MS (EI): *m/z* 145([M^++H], 44), 143 (11), 127 (81), 109 (46), 71 (100), 67 (10).

1-Cyclohexylethanol (**8**)

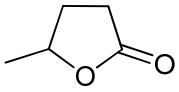


(**8**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 0.94 (m, 2 H), 1.10 (d, 3 H, J_3= 6.5 Hz), 1.16 (m, 4 H), 1.72 (m, 5 H), 1.86 (s, 1 H), 3.50 (qn, 1 H, J_3= 6.2 Hz) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ 20.3 (s, 1 C), 26.1 (s, 1 C), 26.2 (s, 1 C), 26.5 (s, 1 C), 28.4 (s, 1 C), 28.7 (s, 1 C), 45.1 (s, 1 C), 72.1 (s, 1 C) ppm.

5-methylfuran-2-one (**11**)

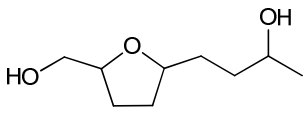


(**11**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 1.34 (d, 3 H, J_3= 6.3 Hz), 1.77 (m, 1 H), 2.31 (dt, 1 H, J_3= 6.3), 2.48 (sx, 2 H, J_3= 6.8 Hz), 4.58 (sx, 1 H, J_3= 6.3 Hz) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ 21.0 (s, 1 C), 29.1 (s, 1 C), 29.6 (s, 1 C), 77.4 (s, 1 C), 177.5 (s, 1 C) ppm.

4-(5-hydroxymethyl-2-tetrahydrofuryl)-2-butanol (**9**)



(**9**)

^{1}H-NMR (400 MHz, $CDCl_3$): δ 1.15 (d, 1 H, J_3= 6.1 Hz), 1.31 (m, 2 H), 1.56 (m, 6 H), 1.91 (m, 2 H), 3.45 (m, 1 H), 3.68 (m, 1 H), 3.86 (m, 3 H) ppm.

^{13}C-NMR (100 MHz, $CDCl_3$): δ 23.5 (d, 1 C), 26.9 (d, 1 C), 31.3 (d, 1 C), 31.9 (d, 1 C), 35.7 (d, 1 C), 65.0 (d, 1 C), 67.8 (d, 1 C), 79.8 (d, 1 C), 80.4 (d, 1 C) ppm.