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Study on Guanidine-based task-specific ionic liquids as catalysts for direct aldol reactions without solvent

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^{1}H NMR spectra were recorded as solutions in $CDCl_3$ at room temperature on a Bruker spectrometer using Me_4Si as standard at 300 MHz.

Compound 1 (Table 1, Entry 1). 2-(hydroxyl (4-nitrophenyl) methyl) cyclopentanone, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 1.55-2.76(m, 7H), 3.01(bs, 1H), 5.42(s, 1H), 7.73-8.32(m, 4H), ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 1.55-2.76(m, 7H), 4.78(bs, 1H), 4.83(d, J=9.1 Hz, 1H), 7.73-8.32(m, 4H).

Compound 2 (Table 1, Entry 7). 4-hydroxy-3-methyl-4- (4-nitrophenyl) butan-2-one, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 1.08(d, J=6 Hz, 3H), 2.26(s, 3H), 2.84(bs, 1H), 5.29(d, J=2.4 Hz, 1H), 7.52-8.25(m, 4H); ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 1.03(d, J=6 Hz, 3H), 2.23(s, 3H), 2.91(bs, 1H), 4.87(d, J=7.9 Hz, 1H), 7.52-8.25(m, 4H).

Compound 3 (Table 2, Entry 1). 4-hydroxy-4- (4- nitrophenyl) butan-2-one, ^{1}H-NMR (300 MHz, $CDCl_3$) (ppm): 2.21 (s, 3H), 2.84 (m, 2H), 3.5 (bs 1H), 5.25 (m, 1H), 7.52 (d, J=6 Hz, 2H), 8.19 (d, J = 6.9 Hz, 2H).

Compound 4 (Table 2, Entry 2). 2-(hydroxyl (4-nitrophenyl) methyl) cyclohexanone, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 1.30-2.61(m, 9H), 3.23(bs, 1H), 5.49(s, 1H), 7.51-8.23(m, 4H), ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 1.30-2.61(m, 9H), 4.12(bs, 1H), 4.89(d, J=8.4 Hz, 1H), 7.51-8.23(m, 4H).

Compound 5 (Table 2, Entry 3). 3-hydroxy-3- (4-nitrophenyl)-1-phenylpropan-1-one,

^{1}H-NMR (300 MHz, $CDCl_3$) (ppm): 3.38(m, 1H), 3.8(bs, 1H), 5.45(m, 1H), 7.47-8.42 (m, 9H).

Compound 6 (Table 2, Entry 4). 3-(hydroxyl (4-nitrophenyl) methyl) pentan-2-one, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 0.82(t, J=6 Hz, 3H), 1.68-1.75(m, 2H), 2.18(s, 1H), 2.79(m, 1H), 3.24(bs, 1H), 5.10(d, J=3 Hz, 1H), 7.51-8.22(m, 4H), ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 0.90(t, J=6 Hz, 3H), 1.48-1.55(m, 2H), 2.14(s, 3H), 2.84(m, 1H), 3.27(bs, 1H), 4.92(d, J=6 Hz, 1H), 7.51-8.24(m, 4H).

Compound 7 (Table 2, Entry 5). 4-hydroxy-3-methyl-4- (3-nitrophenyl) butan-2-one, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 1.07(d, J=6.9 Hz, 3H), 2.25(s, 3H), 2.88(m, 1H), 5.29(S, 1H), 7.52-8.23(m, 4H); ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 1.02(d, J=7.3 Hz, 3H), 2.25(s, H), 2.97(m, 1H), 4.88(d, J=7.1 Hz, 1H), 7.52-8.23(m, 4H).

Compound 8 (Table 2, Entry 6). 4-hydroxy-3-methyl-4- (4-aldehydephenyl) butan-2-one, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 1.02 (d, J=7.2 Hz, 3H), 2.17(s, 3H), 2.80(m, 1H), 5.18(m, 1H), 7.45-7.82(m, 4H), 9.94(s, 1H); ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 0.92(d, J=7.2 Hz, 3H), 2.17(s, 3H), 2.86(m, 1H), 4.79(m, 1H), 7.45-7.82(m, 4H), 9.94(s, 1H).

Compound 9 (Table 2, Entry 7). 2-((benzol [*d*] [1,3] dioxol-6-yl)(hydroxy) methyl)-cyclopentanone, ^{1}H-NMR (300 MHz, $CDCl_3$; syn) (ppm): 1.52-2.44(m, 7H), 4.62(d, J=2.0 Hz, 1H), 5.97(s, 2H), 6.78-6.89(m, 3H); ^{1}H-NMR (300 MHz, $CDCl_3$; anti) (ppm): 1.52-2.44(m, 7H), 4.62(d, J=9.2 Hz, 1H), 5.97(s, 2H), 6.78-6.89(m, 3H).