Supporting Information

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Clusters of the Ionic Liquid 1-Hydroxyethyl-3-methylimidazolium Picrate: From Theoretical Prediction in the Gas Phase to Experimental Evidence in the Solid State

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Synthesis and characterization of Hydroxyethyl)-3-methylimidazolium picrate (EtOHmimPic):

Synthetic procedure of EtOHmimCl IL is described in our previous work.¹EtOHmimCl (1.86 g, 10.77 mmol) was dissolved in 5 ml of water and then aqueous solution of NaPic (2.16g, 12.92 mmol) was added slowly with stirring. White precipitate appeared and stirred solution for 3 hrs at room temperature. DCM was added in to the solution to dissolve the white precipitate and washed the reaction mixture 2-3 times with DCM and DCM solution was washed with cold water and checked the Chloride ion with AgNO₃ and dried DCM with anhydrous MgSO₄. The DCM solution was further treated with activated charcoal to remove coloured impurities and then passed through column containing alumina and celite.

In order to remove volatile components and water, the IL was dried under constant stirring at a temperature of 298 K for about 24 h at a reduced pressure of 2 Pa; there was no detectable mass loss of a 2 g sample during this period of time. Finally, the water content was below 100 ppm as proved by Karl Fischer titration. After drying, the samples were handled under argon atmosphere.

EtOHmimPic IL: State: Yellow solid; Melting Point: 90.0 °C; ¹H-NMR (600 MHz, DMSO-d₆): δ (ppm) 9.11 (s, 1H, C₂-H), 8.60 (s, 2H), 7.72 (t, J = 1.8 Hz, 1H), 7.71 (t, J = 1.8 Hz, 1H), 4.24 (t, J = 4.8 Hz, 2H), 3.89 (s, 3H), 3.74 (t, J = 4.8 Hz, 2H); ¹³C-NMR (151 MHz, D₂O): δ (ppm) 162.0, 140.6, 136.2, 127.1, 126.5, 123.6, 122.5, 59.7, 51.4, 35.7; FTIR (KBr, cm⁻¹): 3417, 3155, 3086, 2959, 2894, 2824, 1630, 1611, 1563, 1496, 1483, 1438, 1369, 1334, 1277, 1163, 1081, 937, 907, 795, 746, 704, 651, 621.