

Electronic supporting information

Surface-active ionic liquids for Palladium-catalysed cross coupling in water: Effect of ionic liquid concentration on the catalytically active species

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1. Table S1: Critical micelle concentrations for all involved ionic liquids

Ionic Liquid	CMC [mM] ^a	
	Conductivity ^b	Surface tension ^c
1	14.53 [1]	13.25 [1]
2	13.75 [2]	10.33 [2]
3	2.69 [3]	2.31 [3]
4	4.32	3.24
5	5.52	4.33
6	5.69	5.07
7	5.04	4.91
8	4.17	5.61

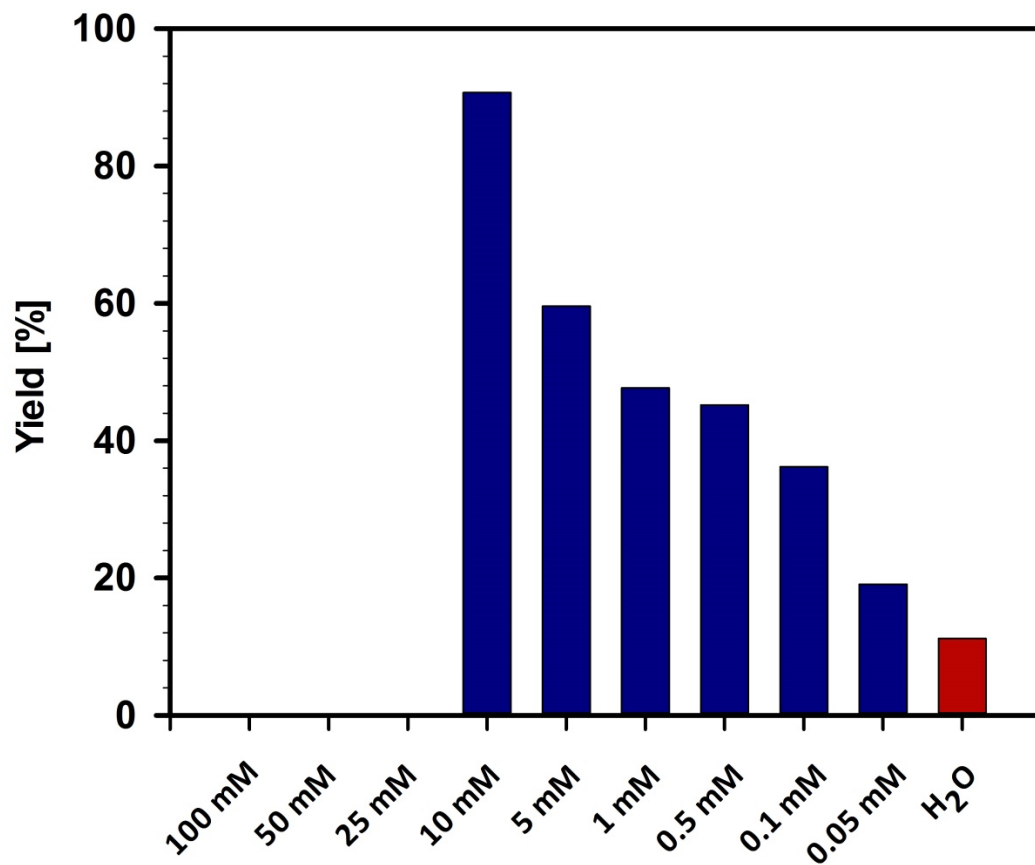
^a Solutions were prepared with doubly-distilled Millipore Milli-Q water. Samples were equilibrated at 25 °C with a HAAKE K15 thermostat before measurements. ^b Conductivity measurement were performed on a Mettler Toledo SevenExcellence system. InLAB® 741-ISM electrode (cell constant k = 0.105). The conductimeter was calibrated with a standard KCl solution and measurements were performed in duplicate; ^c Surface tension was determined with the Du Noüy ring method on a Krüss tensiometer at RT. Each measurement was repeated 5 times.

¹ A. Cognigni, P. Gaertner, R. Zirbs, H. Peterlik, K. Prochazka, C. Schröder and K. Bica, *Phys. Chem. Chem. Phys.*, 2016, **18**, 13375–13384.

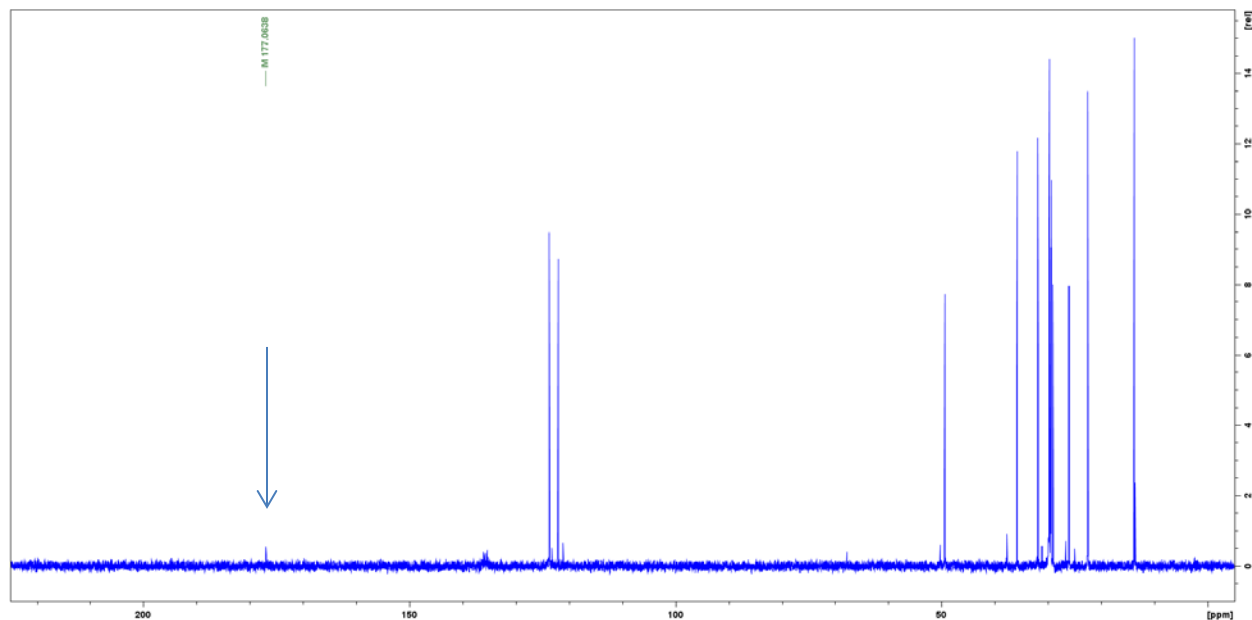
² A. Cognigni, S. Kampichler and K. Bica, *J. Colloid Interface Sci.*, 2017, **492**, 136–145.

³ X.-f. Liu, L.-l. Dong and Y. Fang, *J. Surfactants Deterg.*, 2011, **14**, 203–210.

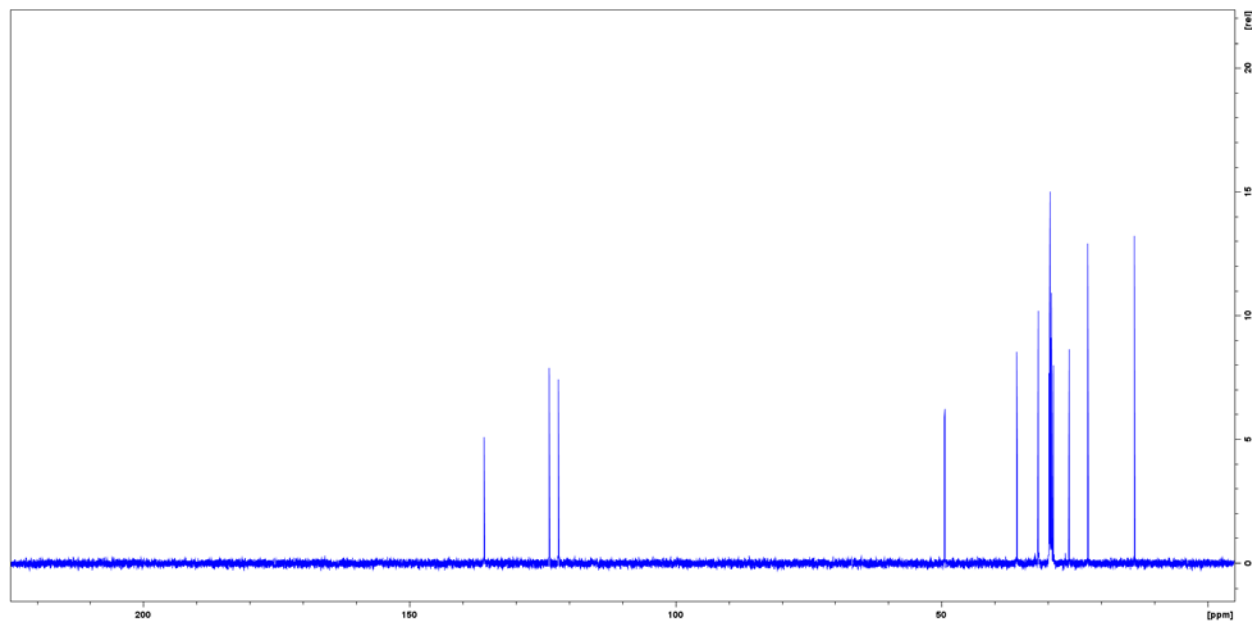
2. Figure S1: Concentration dependence of the Heck reaction of ethyl acrylate 9 and iodobenzene 10 in aqueous solution of ionic liquids [C₁₂mim]Cl 1 using DBU as base.



3. Figure S2: Copy of ^{13}C NMR spectroscopy showing the formation of a Pd-carbene at 177 ppm.



Conditions: 2 mL $[\text{C}_{12}\text{mimCl}] \mathbf{2}$ solution (50 mM) in D_2O , 0.02 mmol $\text{Pd}_2\text{allyl}_2\text{Cl}_2$ and 0.02 mmol K_2CO_3 ; 30 min at 80 °C under air.



Conditions: $[\text{C}_{12}\text{mimCl}] \mathbf{2}$ solution (50 mM) in D_2O