Supplementary Material for PCCP

PCCP issue on ionic liquids: B921391K- Revised Electronic Supplementary Information

Thermo-solvatochromism in binary mixtures of water and ionic liquids: On the relative importance of solvophobic interactions

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Figures

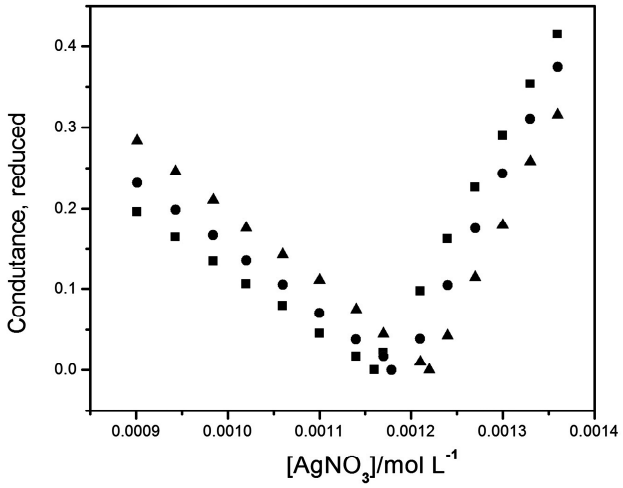


Figure *ESI*-1: Determination of log P of the IL by condutometric titration of the chloride ion in the aqueous phase by standardized $AgNO_3$ solution; the symbols employed are ▲; ●; ■, for the AlMeImCl, AlBuImCl, AlHxImCl, respectively

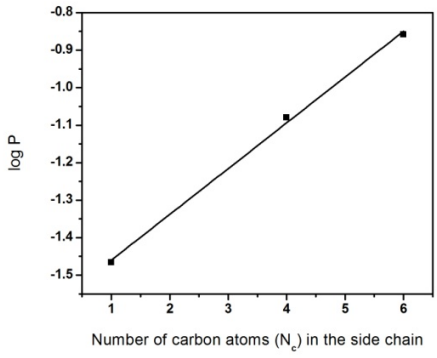


Figure *ESI*-2: Dependence of log P of the ILs on Nc, the number of carbon atoms in the R group of AlRImCl. The correspond equation is: Log P = -1.582 + 0.122 N_C ; r = 0.9968

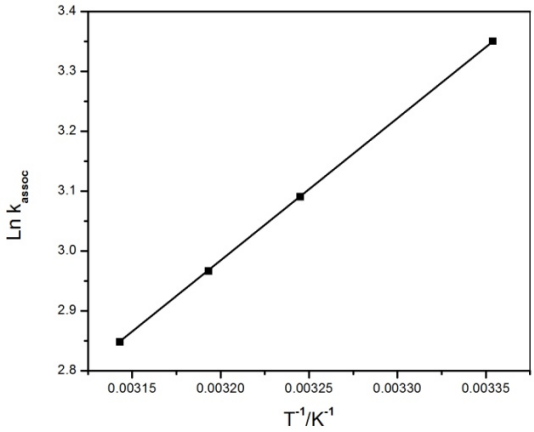


Figure *ESI*-3: Representative van´t Hoff plot of the dependence of K_{assoc} of IL-W (AlBuImCl) on T. The corresponding equation is: $\ln K_{assoc} = -4.66 + 2387.94.T^{-1}$; r = 0.9968

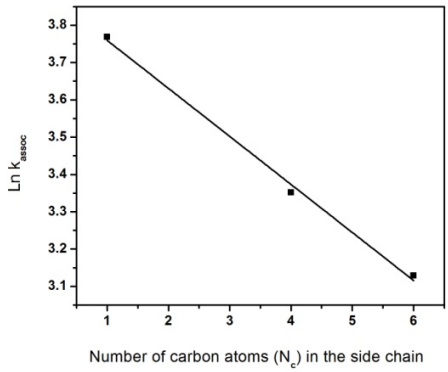
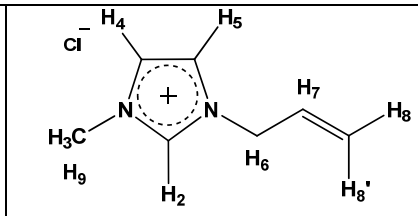
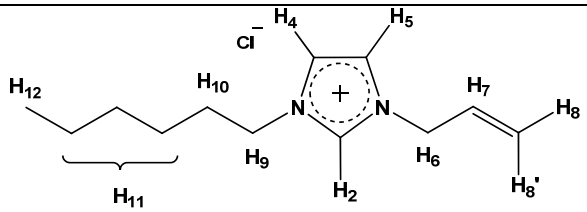


Figure *ESI*-4: Dependence of ln Kassoc on N_C, the number of carbon atoms in the alkyl group of the IL; at 25°C The corresponding equation is: ln K_{assoc} = 3.8882 – 0.1287.N_C; r = 0.9930.

Tables

Table *ESI*-1, Molecular structures and ^{1}H NMR spectral results of AlMeImCl[a] and AlHxImCl.[b]

				
	δ/ppm	**J/Hz**	δ/ppm	J/Hz
H2	9.400 (s)	-	10.829 (s)	-
H4	7.787 (t)	J_{4-9} = 3.4	7.468 (t)	J_{4-9} = 3.2
H5	7.807 (t)	J_{4-5} = 1.5	7.511 (t)	J_{4-5} = 1.4
H6	4.902 (d)	J_{6-7} = 6.0	5.076 (d)	J_{6-7} = 6.4
H7	6.124 to 5.993 (m)	J_{7-8} = 10.2	6.142 to 5.942 (m)	J_{7-8} = 7.6
H8	5.359 (dq)	$J_{8-8'}$ = 1.2	5.552 (dq)	$J_{8-8'}$ = 0.6
H8’	5.320 (dq)	J_{7-8} = 15.0	5.513 (dq)	J_{7-8} = 13.2
H9	3.901 (s)	-	4.348 (t)	J_{9-10} = 7.4-
H10	-	-	1.933 (qt)	J_{10-11} = 7.3
H11	-	-	1.318 (ls)	J_{11-12} = 6.8
H12	-	-	0.874 (t)	-

a- At 300 MHz and 25 ºC, solvent DMSO reference TMS. The following abbreviations were employed for peak multiplicity: d, doublet; dq, double quartet, ls, large singlet, m, multiplet, q, quintet, s, singlet; and t, triplet, respectively

b- At 200 MHz and 25 ºC, solvent $CDCl_3$ reference TMS

Table *ESI*-2

Dependence of the association constant of the IL-W complex solvent on T

Binary mixture	Temperature, °C	K_{assoc}, L mol^{-1}
AlMeImCl/W	25	43.30
	35	37.73
	40	35.32
	45	33.15
	60[a]	27.69
AlBuImCl/W	10[a]	43.63
	25	28.55
	35	22.00
	40	19.44
	45	17.26
	60[a]	12.30
AlHxImCl/W	10[a]	36.54
	25	22.83
	35	17.16
	40	14.93
	45	13.09
	60[a]	9.01

a- Values calculate by using the van't Hoff equation plot.