

Supplementary Information

The dipolarity/polarisability of 1-alkyl-3-methylimidazolium ionic liquids as function of anion structure and the alkyl chain length

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Content

Catalán solvent parameter data and the UV/Vis absorption maxima of dissolved dye **1**

UV/Vis absorption maxima of **2** and **3** in [Rmim] Ionic Liquids with R = *n*-hexyl, *n*-octyl, and *n*-decyl for various anions

Results of the correlation of the determined π^* values with the product of α with β for [Rmim] Ionic Liquids with 6 various anions

Catalán solvent parameter data and the UV/Vis absorption maxima of dissolved dye 1

solvent	$\tilde{\nu}_{\max(1)} / 10^{-3} \text{cm}^{-1}$ a)	$SP^{b)}$	$SdP^{b)}$	$SA^{b)}$	$SB^{b)}$
<i>n</i> -hexane	17.67	0.616	0	0	0.056
cyclohexane	17.51	0.683	0	0	0.073
triethylamine	17.33	0.660	0.108	0	0.885
CCl ₄	17.21	0.768	0	0	0.104
diethyl ether	17.12	0.617	0.385	0	0.562
<i>p</i> -xylene	17.01	0.778	0.175	0	0.160
toluene	16.95	0.782	0.284	0	0.128
benzene	16.92	0.793	0.270	0	0.124
THF	16.42	0.714	0.634	0	0.591
acetic acid	16.45	0.651	0.676	0.689	0.390
chloroform	16.39	0.783	0.614	0.047	0.071
anisole	16.31	0.820	0.543	0.084	0.299
dichloromethane	16.29	0.761	0.769	0.040	0.178
acetone	16.21	0.651	0.907	0	0.475
1,2-dichloroethane	16.23	0.771	0.742	0.030	0.126
ethanol	16.18	0.633	0.783	0.400	0.658
methanol	16.15	0.608	0.904	0.605	0.545
1-butanol	16.16	0.674	0.655	0.341	0.809
trifluoroethanol	16.08	0.543	0.922	0.893	0.107
1,1,2,2-tetrachloroethane	16.08	0.845	0.792	0	0.017
nitromethane	16.05	0.710	0.954	0.078	0.236
dimethylformamide	15.82	0.759	0.977	0.031	0.613
benzyl alcohol	15.75	0.861	0.788	0.409	0.461
1,2-ethandiol	15.75	0.777	0.910	0.717	0.534
formamide	15.72	0.814	1.006	0.549	0.414
dimethylsulfoxide	15.65	0.830	1.000	0.072	0.647

a) S. Spange, R. Sens, Y. Zimmermann, A. Seifert, I. Roth, S. Anders and K. Hofmann, *New J. Chem.*, 2003, **27**, 520.

b) J. Catalán, *J. Phys. Chem. B*, 2009, **113**, 5951.

UV/Vis absorption maxima of 2 and 3 in [Rmim] Ionic Liquids with R = *n*-hexyl, *n*-octyl, and *n*-decyl for various anions

Ionic Liquid	$\tilde{\nu}_{\max(2)} / 10^{-3}\text{cm}^{-1}$	$\tilde{\nu}_{\max(3)} / 10^{-3}\text{cm}^{-1}$
[C ₆ mim]Cl	14.35	16.84
[C ₈ mim]Cl	14.31	16.83
[C ₁₀ mim]Cl	14.29	16.84
[C ₆ mim]NO ₃	15.41	17.04
[C ₈ mim]NO ₃	15.20	16.95
[C ₁₀ mim]NO ₃	15.15	16.95
[C ₆ mim]N(CN) ₂	15.77	17.12
[C ₈ mim]N(CN) ₂	15.68	17.09
[C ₁₀ mim]N(CN) ₂	15.65	17.12
[C ₆ mim]BF ₄	16.18	17.12
[C ₈ mim]BF ₄	16.05	17.15
[C ₁₀ mim]BF ₄	15.95	17.18
[C ₆ mim]PF ₆	16.72	17.27
[C ₈ mim]PF ₆	16.56	17.30
[C ₁₀ mim]PF ₆	16.47	17.21
[C ₆ mim]CF ₃ SO ₃	16.16	17.18
[C ₈ mim]CF ₃ SO ₃	16.00	17.21
[C ₁₀ mim]CF ₃ SO ₃	15.97	17.21
[C ₆ mim]Ntf ₂	16.98	17.27
[C ₈ mim]Ntf ₂	16.84	17.21
[C ₁₀ mim]Ntf ₂	16.75	17.21

Results of the correlation of the determined π^* values with the product of α with β for [Rmim] Ionic Liquids with 6 various anions

Anions: Cl⁻, NO₃⁻, N(CN)₂⁻, BF₄⁻, PF₆⁻, Ntf₂⁻

General formula: $\pi^* = A + B(\alpha \times \beta)$

Cation	A	B	r^2	sd	n	F
[Bmim]	0.12	3.14	0.85	0.05	6	0.0093
[C ₆ mim]	0.42	2.00	0.88	0.03	6	0.0050
[C ₈ mim]	0.44	1.80	0.79	0.03	6	0.0167
[C ₁₀ mim]	0.57	1.22	0.64	0.03	6	0.0560

r^2 = correlation coefficient; sd = standard deviation; n = number of solvents; F = significance.