Supporting Information:

Estimation of Properties of Ionic Liquids 1-Alkyl-3-methylimidazolium Lactate Using Semiempirical Method

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Table S1. Values of molar volume, V , and the molecular volume, V_m, of ILs at 298.15 K

ionic liquid	V/ $cm^3 \cdot mol^{-1}$	V_m(Ex)/ nm^3	V_m(Cal)/ nm^3	ionic liquid	V/ $cm^3 \cdot mol^{-1}$	V_m(Ex)/ nm^3	V_m(Cal)/ nm^3
$[C_2mim][Lact]^{[a]}$	168.9	0.2804	0.2804	$[C_2mim][Gly]$	157.2	0.2612	0.2612
$[C_3mim][Lact]$	185.6(Cal)		0.3082	$[C_3mim][Gly]$	174.0	0.2890	0.2890
$[C_4mim][Lact]^{[b]}$	202.3	0.3359	0.3360	$[C_4mim][Gly]$	190.7	0.3168	0.3168
$[C_5mim][Lact]^{[a]}$	219.1	0.3639	0.3638	$[C_5mim][Gly]$	207.4	0.3446	0.3446
$[C_6mim][Lact]$	235.8(Cal)		0.3916	$[C_6mim][Gly]$	224.2	0.3724	0.3724
$[C_2mim][Ala]$	177.5	0.2948	0.2948	$[C_2mim][BF_4]$	154.7	0.2569	0.2569
$[C_3mim][Ala]$	194.0	0.3222	0.3226	$[C_3mim][BF_4]$	171.4	0.2848	0.2847
$[C_4mim][Ala]$	210.2	0.3492	0.3504	$[C_4mim][BF_4]$	188.1	0.3124	0.3125
$[C_5mim][Ala]$	227.1	0.3772	0.3782	$[C_5mim][BF_4]$	204.8	0.3402	0.3403
$[C_6mim][Ala]$	244.5	0.4062	0.4060	$[C_6mim][BF_4]$	221.6	0.3681	0.3681
$[C_2mim][Pro]$	154.8	0.2572	0.2572	$[C_2mim][OAc]$	148.8	0.2471	0.2471
$[C_3mim][Pro]$	171.6	0.2851	0.2850	$[C_3mim][OAc]$	164.6	0.2734	0.2749
$[C_4mim][Pro]$	188.2	0.3126	0.3128	$[C_4mim][OAc]$	180.7	0.3002	0.3027
$[C_5mim][Pro]$	205.0	0.3406	0.3406	$[C_5mim][OAc]$	197.0	0.3272	0.3305
$[C_6mim][Pro]$	221.8	0.3685	0.3684	$[C_6mim][OAc]$	213.3	0.3543	0.3583

[*a*]: in this work; [*b*]: ref. 6; (Ex) means the experimental value; (Cal) means the calculated value.

Table S2. The values of ionic volume, V_i(IL), ionic parachor, P_i, and ionic molar refraction, R_{mi} at 298.15 K

ion	V_i(IL)/nm^3	P_i	R_{mi}
$[C_2mim]^+$	0.1745	277.7	30.87
$[C_3mim]^+$	0.2023	315.3	35.50
$[C_4mim]^+$	0.2301	352.9	40.13
$[C_5mim]^+$	0.2579	390.5	44.76
$[C_6mim]^+$	0.2857	428.1	49.39

$[Lact]^-$	0.1059	168.5	18.74
$[Ala]^-$	0.1203	200.6	22.35
$[Pro]^-$	0.0827	110.7	13.87
$[Gly]^-$	0.0867	143.2	17.06
$[BF_4]^-$	0.0824	133.9	12.35
$[OAc]^-$	0.0726	91.4	12.43
$[PF_3(CF_2CF_3)_3]^-$	0.3660	512.6	

Table S3. The parameters of fitting lines for the estimated values vs the corresponding experimental values

	V_m(Cal) *vs* V_m(Ex)/nm^3	P(Cal) *vs* P(Ex)	R_m(Cal) *vs* R_m(Ex)
intercept	-3.267×10^{-4}	1.593	-0.3549
slope	1.003	1.004	1.008
standard deviation	0.0011	9.4	0.34
correlation coefficient	0.9997	0.9982	0.9990

Table S4. The estimated values and the corresponding experimental values of parachor and surface tension for the ILs

IL	ρ /g·cm^{-3}	γ(Ex) /mJ·m^{-2}	P(Ex)	P(Cal)	γ(Cal)/mJ·m^{-2}	$\Delta\gamma$/mJ·m^{-2}
$[C_2mim][Lact]$	1.1861	48.8	446.2	446.2	48.8	0
$[C_3mim][Lact]$				483.8	46.2	
$[C_4mim][Lact]$	1.1282	44.0	521.2	521.4	44.1	-0.1
$[C_5mim][Lact]$	1.1060	42.4	559.1	559.0	42.4	0
$[C_6mim][Lact]$				596.6	41.0	
$[C_2mim][Ala]$	1.1209	52.7	478.3	478.3	52.4	0.3
$[C_3mim][Ala]$	1.0978	50.1	516.2	515.9	49.7	0.4
$[C_4mim][Ala]$	1.0794	47.7	552.9	553.5	47.7	0
$[C_5mim][Ala]$	1.0610	46.0	591.6	591.1	45.6	0.4
$[C_6mim][Ala]$	1.0426	43.4	627.9	628.7	43.4	0
$[C_2mim][Pro]$	1.1900	39.6	388.4	388.4	39.6	0
$[C_3mim][Pro]$	1.1554	38.4	427.2	426.0	38.0	0.4
$[C_4mim][Pro]$	1.1279	37.0	464.2	463.6	36.8	0.2
$[C_5mim][Pro]$	1.1038	35.7	501.1	501.2	35.7	0
$[C_6mim][Pro]$	1.0835	34.8	538.6	538.8	34.8	0
$[C_2mim][OAc]$	1.1437	38.1	369.1	369.1	37.8	0.3
$[C_3mim][OAc]$	1.1190	36.8	405.0	406.7	37.2	-0.4
$[C_4mim][OAc]$	1.0968	35.2	441.1	444.3	36.5	-1.3
$[C_5mim][OAc]$	1.0773	34.1	476.9	481.9	35.8	-1.7
$[C_6mim][OAc]$	1.0606	33.0	512.1	519.5	35.1	-2.1
$[C_2mim][PF_3(CF_2CF_3)_3]$	1.70926	34.8	790.3	790.3	34.8	0
$[C_3mim][PF_3(CF_2CF_3)_3]$	1.66756	34.1	826.3	827.9	34.4	-0.3
$[C_4mim][PF_3(CF_2CF_3)_3]$	1.62962	33.2	860.6	865.5	34.0	-0.8
$[C_5mim][PF_3(CF_2CF_3)_3]$	1.59516	32.4	894.8	903.1	33.6	-1.2
$[C_6mim][PF_3(CF_2CF_3)_3]$	1.56356	31.7	929.2	940.7	33.3	-1.6

[C_2mim][Gly]	1.1589	48.1	420.9	418.3	46.9	1.2
[C_3mim][Gly]	1.1358	45.6	455.9	455.9	45.6	0.0
[C_4mim][Gly]	1.1109	43.5	493.1	493.5	43.7	-0.2
[C_5mim][Gly]	1.0947	41.9	526.9	531.1	42.8	-0.9
[C_6mim][Gly]	1.0755	40.6	567.3	568.7	41.3	-0.7
[C_2mim][BF_4]	1.2798	50.1	411.6	411.6	50.1	0
[C_3mim][BF_4]	1.2361	47.0	449.1	499.2	47.1	-0.1
[C_4mim][BF_4]	1.2015	44.7	486.4	486.8	44.8	-0.1
[C_5mim][BF_4]	1.1719	42.9	524.2	524.4	42.9	0
[C_6mim][BF_4]	1.1463	41.0	560.9	562.0	41.3	-0.3

P(Cal) = P_- + P_+; γ(Cal) was calculated by Eq. (7); $\Delta\gamma = \gamma$(Ex) – γ(Cal).

Table S5. Experimental values of R_m, n_D, $10^{24}\alpha_p$ and predicted values of R_m(Cal) for ILs at 298.15 K

Ionic liquid	R_m(Ex)	R_m(Cal)	n_D	$10^{24}\alpha_p$
[C_2mim][Lact]	49.61	49.61	1.4995	19.68
[C_3mim][Lact]		54.24		21.52
[C_4mim][Lact]	58.90	58.87	1.4939	23.36
[C_5mim][Lact]	63.51	63.50	1.4915	25.20
[C_6mim][Lact]		68.13		27.03
[C_2mim][Ala]	53.22	53.22	1.5106	21.12
[C_3mim][Ala]	57.57	57.85	1.5044	22.84
[C_4mim][Ala]	62.14	62.48	1.5019	24.66
[C_5mim][Ala]	66.72	67.11	1.4984	26.47
[C_6mim][Ala]	71.67	71.14	1.4970	28.44
[C_2mim][Gly]	47.93	47.93	1.5214	19.02
[C_3mim][Gly]	52.53	52.56	1.5155	20.84
[C_4mim][Gly]	57.13	57.19	1.5107	22.67
[C_5mim][Gly]	61.73	61.82	1.5066	24.49
[C_6mim][Gly]	65.35	66.45	1.4944	25.93
[C_2mim][Pro]	44.74	44.74	1.4897	17.75
[C_3mim][Pro]	49.50	49.37	1.4886	19.64
[C_4mim][Pro]	54.05	54.00	1.4862	21.45
[C_5mim][Pro]	58.68	58.63	1.4841	23.28
[C_6mim][Pro]	63.33	63.26	1.4828	25.13

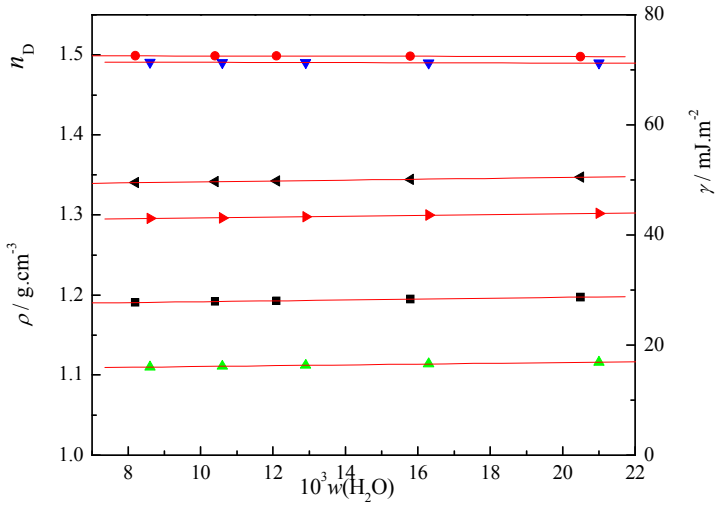

Figure S1. Plot of the density, surface tension, and refractive index *vs* the amount of water in [C_2mim][Lact] and [C_5mim][Lact] at 298.15 K

■ [C_2mim][Lact] $\rho = 1.1861 + 0.54654\ w_2$, $s = 3.5 \times 10^{-5}$, $r = 0.999$;

▲ [C_5mim][Lact] $\rho = 1.1058 + 0.49126\ w_2$, $s = 9.6 \times 10^{-5}$, $r = 0.999$;

◀ [C_2mim][Lact] $\gamma = 48.8 + 80.4\ w_2$, $s = 0.018$, $r = 0.99$;

▶ [C_5mim][Lact] $\gamma = 42.3 + 75.3\ w_2$, $s = 0.032$, $r = 0.99$;

● [C_2mim][Lact] $n_D = 1.4995 - 0.0804\ w_2$, $s = 1.8 \times 10^{-5}$, $r = 0.99$;

▼ [C_5mim][Lact] $n_D = 1.4914 - 0.0783\ w_2$, $s = 3.3 \times 10^{-5}$, $r = 0.99$.