Electronic Supplementary Material (ESI) for New Journal of Chemistry.

ESI for

Understanding the efficiency of ionic liquids-DMSO as solvents for carbohydrates: Use of solvatochromic- and related physicochemical properties

Thaís A. Bioni, Mayara L. de Oliveira, Marcella T. Dignani, and Omar A. El Seoud,*

Institute of Chemistry, the University of São Paulo, 748 Prof. Lineu Prestes Av., 05508-000 São Paulo, SP, Brazil. Email (elseoud.usp@gmail.com)

Table ESI-1. ^{1}H NMR spectral data for the synthesized ionic liquids.[a]

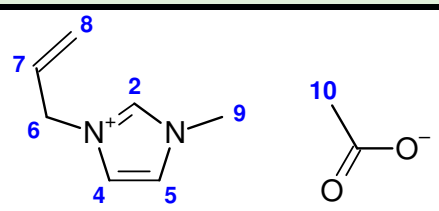
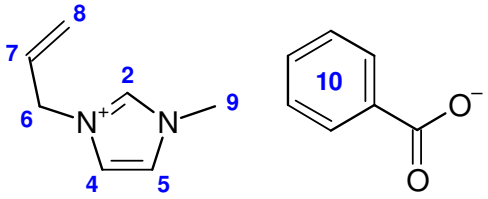
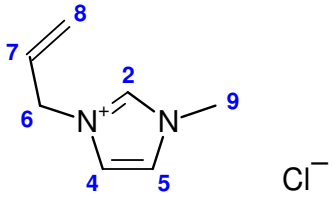
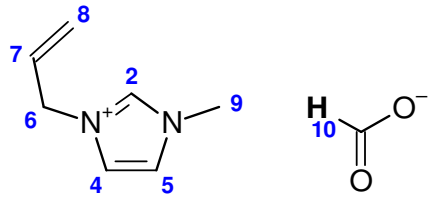
Cation	Cation hydrogen number (number of hydrogens; δ ppm; peak multiplicity)[b]
 **AlMeImAc**	H2 (1H; 10,7; s), H4/5 (2H; 7,6-7,9; dd), H6 (2H; 4,94; d), H7 (1H; 5,94; m), H8 (2H; 5,25-5,39; dd), H9 (3H; 3,99; s), H10 (3H, 1,92; s).
 **AlMeImBz**	H2 (1H; 10,8; s), H4/5 (2H; 7,93; dd), H6 (2H; 4,64; d), H7 (1H; 5,76; m), H8 (2H; 5,12-5,26; dd), H9 (3H; 3,73; s), H10 (5H, 7,3-7,9; m).
 **AlMeImCl**	H2 (1H; 10,4; s), H4/5 (2H; 7,7-7,9; dd), H6 (2H; 5,02; d), H7 (1H; 5,98; m), H8 (2H; 5,31-5,40; dd), H9 (3H; 4,06; s).
 **AlMeImFor**	H2 (1H; 10,7; s), H4/5 (2H; 7,6-7,8; dd), H6 (2H; 4,89; d), H7 (1H; 5,96; m), H8 (2H; 5,29-5,39; dd), H9 (3H; 3,95; s), H10 (1H, 8,95; s).

Table ESI-1, continue

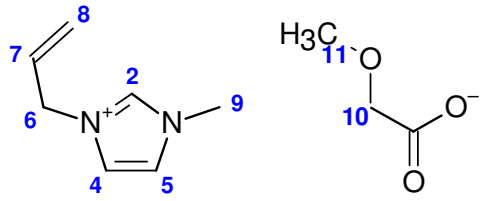
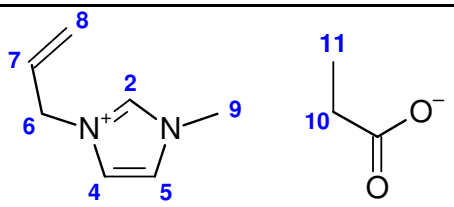
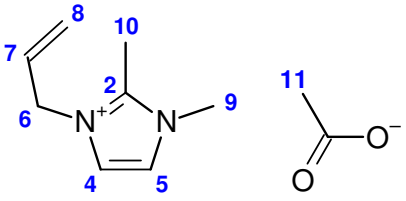
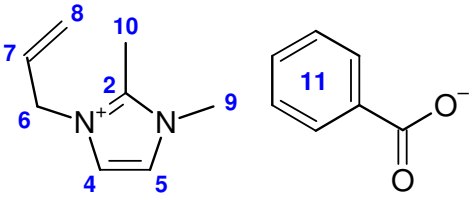
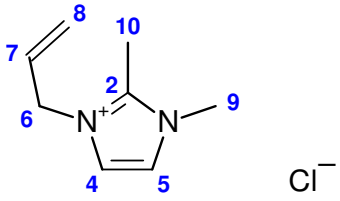
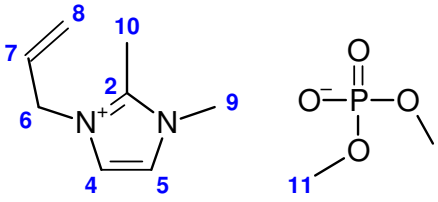
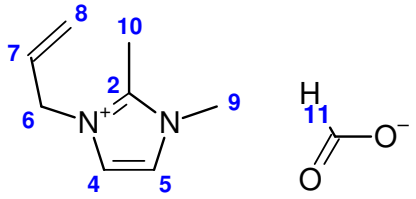
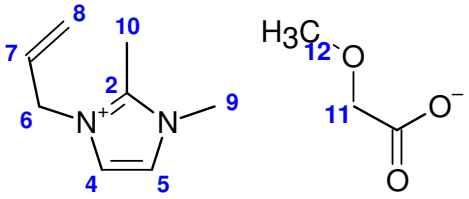
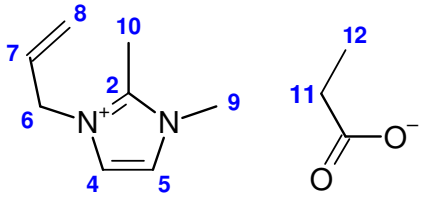
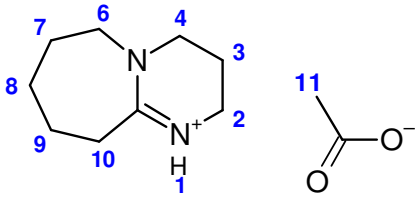
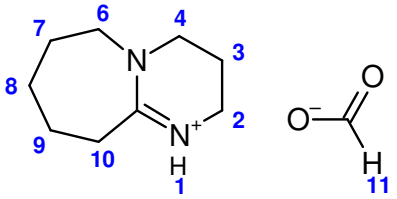
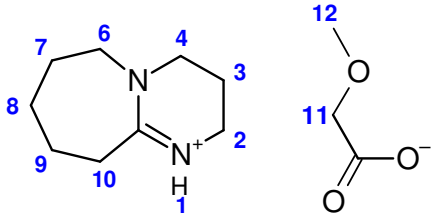
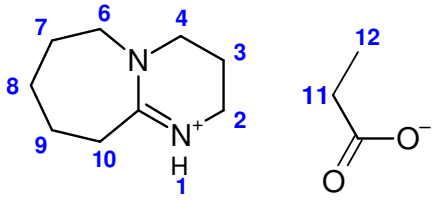
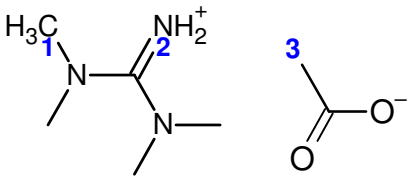
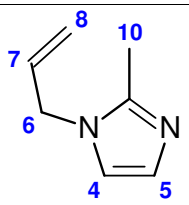
Cation	Hidrogen Number (Number of hydrogens; δ ppm; peak multiplicity)[b]
 **AlMeImMeOAc**	H2 (1H; 10,35; s), H4/5 (2H; 7,7-7,9; dd), H6 (2H; 4,89; d), H7 (1H; 5,96; m), H8 (2H; 5,29-5,39; dd), H9 (3H; 3,95; s), H10 (3H, 2,65; s).
 **AlMeImPr**	H2 (1H; 11,15; s), H4/5 (2H; 7,7-7,9; dd), H6 (2H; 4,89; d), H7 (1H; 5,96; m), H8 (2H; 5,29-5,39; dd), H9 (3H; 3,95; s), H10 (2H; 4,05; s), H11(3H, 2,45; s).
 **AlMe$_2$ImAc**	H4/5 (2H; 7,87; d), H6 (2H; 4,94; d), H7 (1H; 5,94; m), H8 (2H; 5,25-5,39; dd), H9 (3H; 3,99; s), H10 (3H; 2,74; s), H11 (3H, 1,96; s).
 **AlMe$_2$ImBz**	H4/5 (2H; 7,6-7,9; dd), H6 (2H; 4,64; d), H7 (1H; 5,76; m), H8 (2H; 5,12-5,26; dd), H9 (3H; 3,73; s), H10 (3H; 2,48; s), H11 (5H, 7,3-7,9; m).
 **AlMe$_2$ImCl**	H4/5 (2H; 7,6-7,9; dd), H6 (2H; 5,02; d), H7 (1H; 5,98; m), H8 (2H; 5,31-5,40; dd), H9 (3H; 4,06; s), H10 (3H; 2,83; s).
 **AlMe$_2$ImMe$_2$P**	H4/5 (2H; 7,6-7,9; dd), H6 (2H; 4,93; d), H7 (1H; 5,95; m), H8 (2H; 5,25-5,38; dd), H9 (3H; 3,98; s), H10 (3H; 2,73; s), H11 (6H, 3,53; s).

Table ESI-1, continue

Cation	Hidrogen Number (Number of hydrogens; δ ppm; peak multiplicity)[b]
 **$AlMe_2ImFor$**	H4/5 (2H; 7,5-7,8; dd), H6 (2H; 4,89; d), H7 (1H; 5,96; m), H8 (2H; 5,29-5,39; dd), H9 (3H; 3,95; s), H10 (3H; 2,72; s), H11 (1H; 8,7; s).
 **$AlMe_2ImMeOAc$**	H4/5 (2H; 7,6-7,9; dd), H6 (2H; 4,89; d), H7 (1H; 5,96; m), H8 (2H; 5,29-5,39; dd), H9 (3H; 3,95; s), H10 (3H; 2,72; s), H11 (2H; 4,05; s), H12 (3H; 2,35; s).
 **$AlMe_2ImPr$**	H4/5 (2H; 7,6-7,8; dd), H6 (2H; 4,89; d), H7 (1H; 5,96; m), H8 (2H; 5,29-5,39; dd), H9 (3H; 3,95; s), H10 (3H; 2,72; s), H11 (2H, 2,05; qua). H12 (3H; 0,95; tri).
 **DBUHAc**	H1 (1H; 11,97; s), H2/4/6 (6H; 3,49; m), H3 (2H; 2,81; m), H7/8/9 (6H; 1,75; m), H10/11 (5H; 2,02; s).
 **DBUHFor**	H1/11 (2H; 11,97; s), H2/4/6 (6H; 3,49; m), H3 (2H; 2,81; m), H7/8/9 (6H; 1,75; m), H10 (2H; 2,01; tri).
	H1 (1H; 11,97; s), H2/4/6/12 (9H; 3,49; m), H3 (2H; 2,92; m), H7/8/9 (6H; 1,75; m), H10 (2H; 2,02; tri), H11 (2H, 3,90, s).

DBUHMeOAc	

Table ESI-1, continue

Cation	Hidrogen Number (Number of hydrogens; δ ppm; peak multiplicity)[b]
 **DBUHPr**	H1 (1H; 11,97; s), H2/4/6 (6H; 3,49; m), H3 (2H; 2,81; m), H7/8/9 (6H; 1,75; m), H10 (2H; 2,02; qui), H11 (2H; 2,25; qua), H12 (3H; 1,13; tri).
 **TGMHAc**	H1 (12H; 2,99; s), H2 (2H; 7,82; s), H3 (3H; 1,97; s).
	H4/5 (2H; 7,6-7,9; dd), H6 (2H; 4,94; d), H7 (1H; 5,94; m), H8 (2H; 5,2-5,4; dd), H10 (3H, 2,84, s).

a-At 300 MHz. Values of δ are in ppm from internal TMS.

b-The abbreviations for peak splitting are: s: singlet; d: doublet; dd: doublet of doublets; tri: triplet; qua: quartet; qui: quintet; m: multiplet.

Table ESI-2: Molar volume data calculated from the molar mass and density of LIs, and molar volume calculated by the Molinspiration software.

Ionic liquid	Molar mass / g.mol^{-1}	Density[1,2] / g.cm^{-3}	Molar volume[a] cm^3.mol^{-1}	Molar volume[3,b] cm^3.mol^{-1}
BuMeImAc	198.26	1.0532	188.25	205.46
BuMeImCl	174.67	1.086	160.84	176.25
EtMeImCl	146.62	1.1362	129.04	142.65
PrMeImCl	160.64	1.1014	145.85	159.45
C_5O_2MeImCl	192.64	1.14	168.98	177.42
OcMeImCl	230.78	1.0104	228.40	243.46
Me_2ImDMP	222.18	1.277	173.99	198.96
EtMeImAc	170.21	1.027	165.74	171.86
EtMeImDEP	264.26	1.1572	228.36	249.36
EtMeImDMP	236.21	1.1572	204.12	215.76
HxMeImCl	202.72	1.03	196.82	209.86
EtMeImMS	206.26	1.247	165.41	184.31
EtMeImDBP	320.36	1.075	298.01	316.57
AlMeImCl	158.63	1.1408	154.01	153.82
BuEtImTAc	266.26	1.183	225.07	234.71
Bu_2ImCl	216.75	1.0082	214.99	226.66

a - Molar volume calculated through the molar mass divided by the density of the IL. Density data from:

b - Acronyms for the ionic liquids.

BuMeImAc: 1-Butyl-3-methylimidazolium acetate; BuMeImCl: 1-Butyl-3-methylimidazolium chloride; EtMeImCl: 1-ethyl-3-methylimidazolium chloride; PrMeImCl: 1-propyl-3-methylimidazolium chloride; C_5O_2MeImCl: 1- (3,6-dioxa) - (1-heptyl) - 3-methylimidazolium chloride; OcMeImCl: 1-Octyl-3-methylimidazolium chloride; Me_2ImDMP: 1,3-dimethylimidazolium dimethylphosphate; EtMeImAc: 1-

ethyl-3-methylimidazolium acetate; EtMeImDEP: 1-ethyl-3-methylimidazolium diethylphosphate; EtMeImDMP: 1-ethyl-3-methylimidazolium dimethyl phosphate; HxMeImCl: 1-hexyl-3-methylimidazolium chloride; EtMeImMS: 1-ethyl-3-methylimidazolium methyl sulfonate; EtMeImDBP: 1-ethyl-3-methylimidazolium dibutylphosphate; AlMeImCl: 1-allyl-3-methylimidazolium chloride; BuEtImTAc: 1-Butyl-3-ethylimidazolium trifluoroacetate; Bu_2ImCl: 1,3-dibutylimidazolium chloride.

Table ESI-3. Values of the empirical polarity (E_T(MePMBr$_2$), E_T(WB), E_T(RB)), Lewis acidity (*SA*), Lewis basicity (*SB*), dipolarity (*SD*), polarizability (*SP*), molar volume (V_M), refractive index (n) and Lorentz-Lorenz refractive index function *f(n)* employed in the correlations of part **II** of **Table 3,** molecular solvents, see text.[a]

Solvent	E_T(MePMBr$_2$)[b,4] / kcal.mol^{-1}	E_T(RB)b,[b,5] / kcal.mol^{-1}	E_T(WB)[b,6] / kcal.mol^{-1}	*Sb,*[b,7]	*SB*[b,8]	*SD*[b,9]	*SP*[b,10]	V_M / cm^3.mol^{-1}	n	*f* (n)
Methanol	58.56	55.4	64.6	0.61	0.55	0.964	0.590	40.45	1.3314	0.20480
Ethanol	56.03	51.9	60.7	0.40	0.66	0.810	0.624	58.38	1.3611	0.22130
1-Pronanol	54.8	50.7	58.7	0.37	0.78	0.777	0.647	74.84	1.3870	0.23543
1-Butanol	54.15	49.7	57.7	0.34	0.81	0.682	0.662	91.51	1.3993	0.24205
1-Hexanol	53.07	48.8	57.06	0.32	0.88	0.567	0.688	124.61	1.4178	0.25190
1-Octanol	52.26	48.1	56.1	0.30	0.92	0.473	0.699	156.90	1.429	0.25780
2-Propanol	53.54	48.4	57.06	0.28	0.83	0.853	0.619	76.46	1.3776	0.23033
Butan-2-ol	52.29	47.1	55.73	0.22	0.89	0.728	0.647	91.74	1.3978	0.24124
2-Methyl-2-propanol	50.59	43.3	51.85	0.15	0.93	0.732	0.632	95.64	1.3870	0.23543
Benzyl alcohol	54.56	50.4	58.8	0.41	0.46	0.808	0.855	103.58	1.5396	0.31356
Chloroform	46.12	39.1	48.6	0.05	0.07	0.640	0.773	80.17	1.4590	0.27338
Dichloromethane	48.13	40.7	49.7	0.04	0.18	0.791	0.754	64.02	1.4244	0.25538
1.2-Dichloroethane	48.55	41.3	51.1	0.03	0.13	0.738	0.771	78.97	1.4448	0.26605
Chlorobenzene	46.36	36.8	44.3	0	0.18	0.564	0.819	104.41	1.5241	0.30602
Acetone	51.06	42.2	52.0	0	0.48	0.907	0.652	74.03	1.3588	0.22004
Acetonitrile	53.19	45.6	55.4	0.04	0.29	1.023	0.632	52.23	1.3440	0.21184
DMAc	51.98	42.9	51.5	0.03	0.65	0.994	0.765	92.98	1.4375	0.26225
DMF	52.39	43.2	53.3	0.03	0.61	0.978	0.762	77.10	1.4305	0.25859
DMSO	53.38	45.1	55.1	0.07	0.65	1.000	0.834	71.03	1.4790	0.28357
1,4-Dioxane	45.69	36.0	44.0	0	0.44	0.303	0.730	85.29	1.4203	0.25322

Table ESI-3, continue.

Solvent	E_T(MePMBr$_2$)[a] / kcal.mol^{-1}	E_T(RB) / kcal.mol^{-1}	E_T(WB) / kcal.mol^{-1}	*SA*	*SB*	*SD*	*SP*	V_M / cm^3.mol^{-1}	n	*f* (n)
Ethyl acetate	47.22	38.1	47.6	0	0.54	0.617	0.647	97.68	1.3720	0.22728
Pyridine	49.66	40.5	48.99	0.03	0.58	0.761	0.842	80.56	1.5093	0.29874
THF	47.69	37.4	44.7	0	0.59	0.645	0.707	81.24	1.4073	0.24632

a- All data are for 25 ^{o}C. We calculated all solvent descriptorsusing the equations listed in **Table 2** of text.

b- We use (b plus a number) to denote the reference number in ESI where these data were taken from.

Table ESI-4: λ_{max} values of the probes used to determine the solvatochromic parameters.

LI	E_T(WB)	SA	SB		SD and SP	
	λ_{max} WB	λ_{max} Fe	λ_{max} MNI	λ_{max} NI	λ_{max} DMANF	λ_{max} antraceno
AlMeImAc	495.4	594.5	452.9	452.1	446.7	380.7
AlMeImBz	501.9	594.3	428.4	432.1	452.0	382.0
AlMeImCl	489.7	592.7	426.6	432.6	444.6	380.2
AlMeImFor	495.5	594.2	445.4	451.2	447.8	381.0
AlMeImMeOAc	498.1	594.0	427.6	433.5	446.5	380.7
AlMeImPr	501.3	594.6	427.7	426.8	447.3	380.9
$AlMe_2ImAc$	509.8	597.2	451.2	449.3	447.5	380.9
$AlMe_2ImBz$	517.6	597.0	448.6	452.3	453.8	382.4
$AlMe_2ImCl$	506.9	595.1	442.7	449.3	445.1	380.3
$AlMe_2ImMe_2P$	513.31	595.6	442.1	446.9	443.4	379.9
$AlMe_2ImFor$	503.6	595.4	437.7	433.9	446.2	380.6
$AlMe_2ImMAc$	508.3	595.2	436.0	441.4	446.6	380.7
$AlMe_2ImPr$	513.0	597.3	436.4	434.4	448.4	381.1
DBUAc	485.34	608.3	427.8	428.3	442.7	379.8
DBUFor	490.67	608.1	426.7	429.2	442.7	379.8
DBUMAc	492.36	607.9	429.0	430,0	443.7	380.0
DBUPr	490.17	608.7	435.9	435.9	449.8	381.5
TMGAc	493.3	593.4	423.5	426.3	440.7	379.3

Table ESI-5. Dipolarity (*SD*), dielectric constant (ε) and molar volume (V_M) for molecular solvents.

Solvent	ε^{11}	SD^{9}	V_M*
Acetone	0.907	21.01	74.08
Bromobenzene	0.497	5.45	104.67
Butyl acetate	0.535	5.07	131.7
Butylamine	0.296	4.71	98.84
Chlorobenzene	0.537	5.69	101.41
Dibutylether	0.175	3.083	169.13
Dibenzyl ether	0.509	3.821	190.09
Trichloromethane	0.614	4.807	80.12
Pentane	0	1.837	115.26
1-Methylnaphthalene	0.51	2.915	142.2
Acetonitrile	0.974	36.64	52.23
Allyl alcohol	0,839	20.7	68.01
Methanol	0.904	33.0	40.45
1,2-Dichloroethane	0.742	10.42	79.17
Ethylbenzene	0.237	2.446	122.6
Ethylacetate	0.603	6.081	97.68
3-Methylpentane	0	1.886	129.79
Methylcyclohexane	0	2.024	127.51
1,1,1-Trichloroethane	0.5	7.243	101.06
Propylbenzene	0.209	2.37	139.44
Acetonitrile	0.974	36.64	52.23
Fluorobenzene	0.511	5.465	93.94
Nitromethane	0.954	37.27	53.54
Benzene	0.27	2.283	89.16

* Molar volume calculated through the molar mass divided by the density of solvents.

Table ESI-6. Dielectric constant (ε) and molar volume (V_M) data[12] for ionic liquids.

Ionic Liquid	V_M / nm^3	ε
$EtMeImPF_6$	0.265	14.7
$BuMeImPF_6$	0.305	14
$HxMeImPF_6$	0.351	11.1
$OcMeImPF_6$	0.397	9.7
$EtMeImTfN_2$	0.388	11.5
$PrMeImTfN_2$	0.41	10.6
$BuMeImTfN_2$	0.428	9.4
$PeMeImTfN_2$	0.451	7.9
$HxMeImTfN_2$	0.474	7
$OcMeImTfN_2$	0.52	6.5
EtMeImTfO	0.287	15.8
BuMeImTfO	0.327	13.5
BuMeImCl	0.243	15
$Me_2ImMeOSO_3$	0.27	17.2
$EtMeImMeOSO_3$	0.326	-
$Bu3MePyBF_4$	0.293	15.3
$PrMePyrTfN_2$	0.431	9.1
$BuMePyrTfN_2$	0.453	7

$EtMeImPF_6$: 1-ethyl-3-methylimidazolium hexafluorophosphate; $BuMeImPF_6$: 1-butyl-3-methylimidazolium hexafluorophosphate; $HxMeImPF_6$: 1-hexyl-3-methylimidazolium hexafluorophosphate; $OcMeImPF_6$: 1-methyl-3-octylimidazolium hexafluorophosphate; $EtMeImTfN_2$: 1-ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide; $PrMeImTfN_2$: 1-propyl-3-methylimidazole bis (trifluoromethylsulfonyl) imide; $BuMeImTfN_2$: 1-butyl-3-methylimidazole bis (trifluoromethylsulfonyl) imide; $PeMeImTfN_2$: 1-methyl-3-pentylimidazole bis (trifluoromethylsulfonyl) imide; $HxMeImTfN_2$: 1-hexyl-3-methylimidazole bis (trifluoromethylsulfonyl) imide; $OcMeImTfN_2$: 1-ethyl-3-methylimidazole bis (trifluoromethylsulfonyl) imide; EtMeImTfO: 1-ethyl-3-methylimidazolium

trifluoromethylsulfonate; BuMeImTfO: 1-butyl-3-methylimidazolium trifluoromethylsulfonate; BuMeImCl: 1-butyl-3-methylimidazolium chloride; $Me_2ImMeOSO_3$: 1,3-dimethylimidazolium methyl sulfonate; $EtMeImMeOSO_3$: 1-ethyl-3-methylimidazolium methyl sulfonate; $Bu3MePyBF_4$: 1-butyl-3-methylpyridinium tetrafluoroborate; $PrMePyrTfN_2$: 1-propyl-1-methylpyrrolidinium bis (trifluoromethylsulfonyl) imide; $BuMePyrTfN_2$: 1-butyl-1-methylpyrrolidinium bis (trifluoromethylsulfonyl) imide.

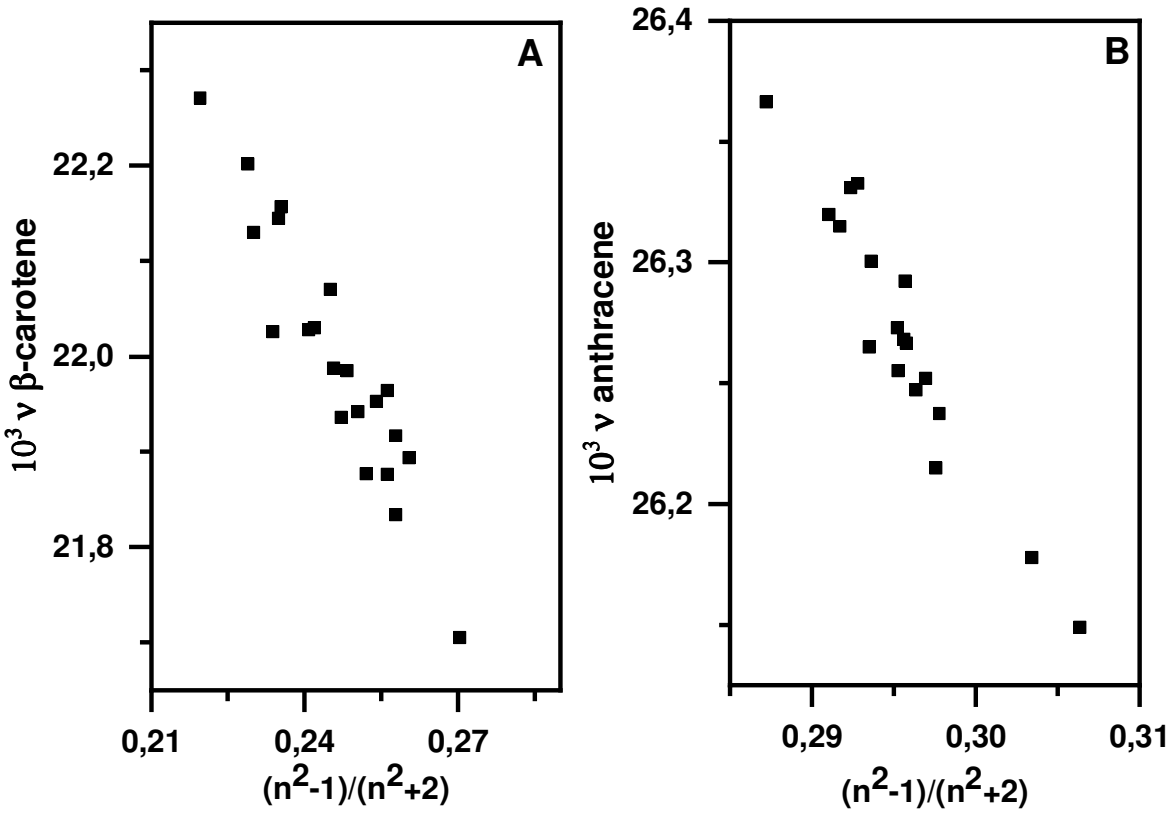


Figure ESI-1: Part (A) Relationship between ν of β-carotene and the Lorenz-Lorentz refractive index function f(n) for 21 molecular solvents.[13] Part (B) Relationship between ν of anthracene and the Lorenz-Lorentz refractive index function f(n) for 18 BMs of the present work.

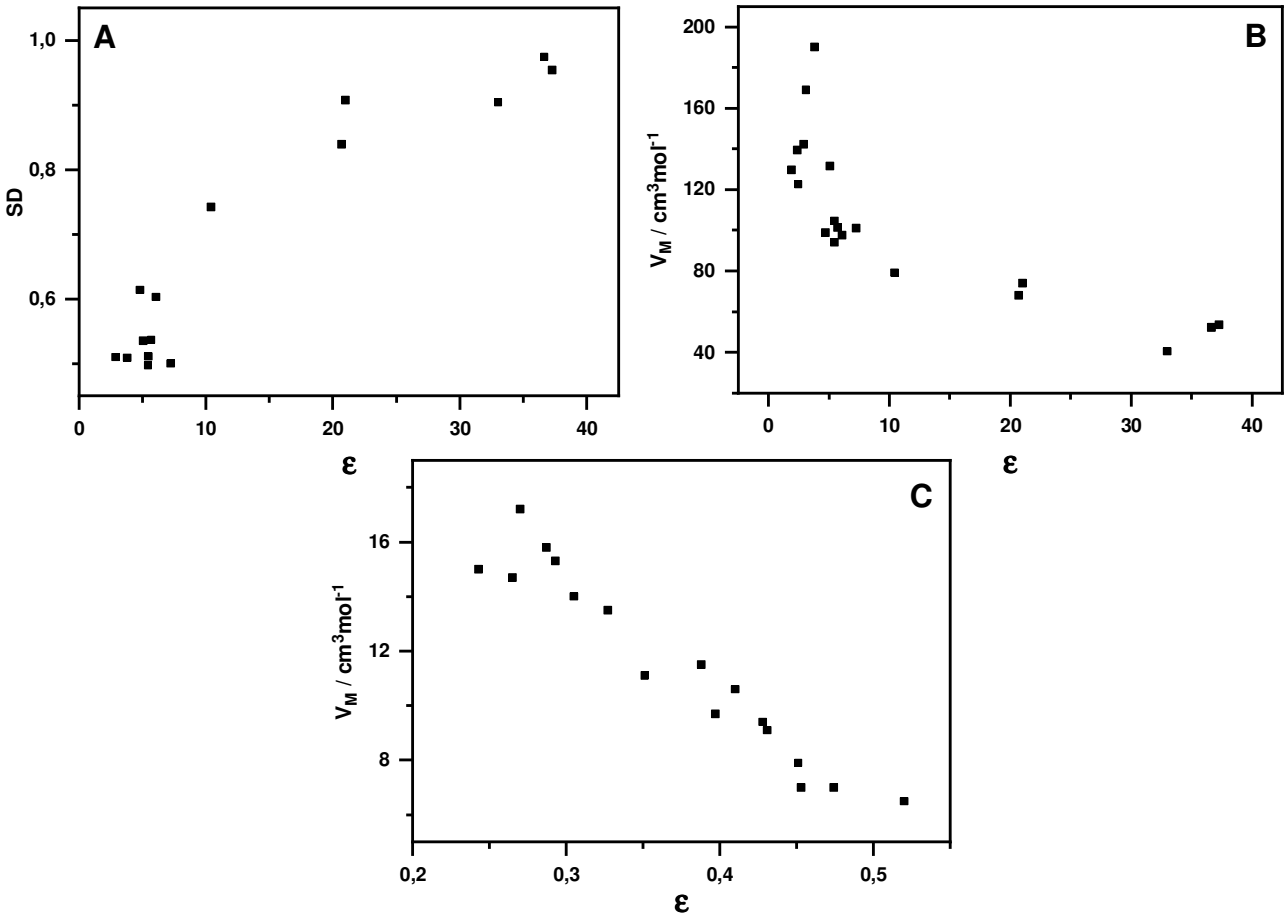


Figure ESI-2: Correlation between the values of (ε)[11] and SD[9] Catalán (part A) and (ε) and V_M (part B) for molecular solvents (**Table ESI-5**). Part (C) Correlation between the values of (ε) and V_M of 18 Lis[13] (**Table ESI-6**).

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