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Electronic Supplementary Information

Assessment of certain ionic liquids for separation of binary mixtures based on gamma infinity data measurements[†]

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Table 1S The sources and mass fraction purities of materials

Chemical name ^a	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
Pentane	Aldrich	≥ 0.99	—	—	—
Hexane	Fluka	≥ 0.99	—	—	—
3-Methylpentane	Aldrich	≥ 0.99	—	—	—
2,2,-Dimethylbutane	Aldrich	≥ 0.99	—	—	—
Heptane	Aldrich	≥ 0.995	—	—	—
Octane	Aldrich	≥ 0.99	—	—	—
2,2,4-Trimethylpentane	Aldrich	≥ 0.99	—	—	—
Nonane	Aldrich	≥ 0.99	—	—	—
Decane	Aldrich	≥ 0.99	—	—	—
Cyclopentane	Aldrich	≥ 0.99	—	—	—
Cyclohexane	Aldrich	≥ 0.99	—	—	—
Methylcyclohexane	Aldrich	≥ 0.99	—	—	—
Cycloheptane	Aldrich	≥ 0.98	—	—	—
Cyclooctane	Fluka	≥ 0.99	—	—	—
Pent-1-ene	Aldrich	≥ 0.985	—	—	—
Hex-1-ene	Aldrich	≥ 0.99	—	—	—
Cyclohexene	Aldrich	≥ 0.99	—	—	—
Hept-1-ene	Aldrich	≥ 0.99	—	—	—
Oct-1-ene	Aldrich	≥ 0.98	—	—	—
Dec-1-ene	Aldrich	≥ 0.97	—	—	—
Pent-1-yne	Aldrich	≥ 0.99	—	—	—
Hex-1-yne	Aldrich	≥ 0.97	—	—	—
Hept-1yne	Aldrich	≥ 0.98	—	—	—
Oct-1-yne	Aldrich	≥ 0.97	—	—	—
Benzene	Aldrich	≥ 0.998	—	—	—

Chemical name ^a	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
Toluene	Aldrich	≥ 0.998	–	–	–
Ethylbenzene	Aldrich	≥ 0.998	–	–	–
<i>o</i> -Xylene	Aldrich	≥ 0.99	–	–	–
<i>m</i> -Xylene	Aldrich	≥ 0.99	–	–	–
<i>p</i> -Xylene	Aldrich	≥ 0.99	–	–	–
<i>n</i> -Propylbenzene	Aldrich	≥ 0.98	–	–	–
Cumene	Aldrich	≥ 0.99	–	–	–
(<i>iso</i> -Propylbenzene)					
Styrene	Aldrich	≥ 0.999	–	–	–
Prop-1-en-2-ylbenzene	Aldrich	≥ 0.99	–	–	–
α-Methylstyrene)					
Thiophene	Aldrich	≥ 0.99	–	–	–
Pyridine	Aldrich	≥ 0.998	–	–	–
Methanol	Aldrich	≥ 0.999	–	–	–
Ethanol	Aldrich	≥ 0.998	–	–	–
Propan-1-ol	Aldrich	≥ 0.999	–	–	–
Propan-2-ol	Fluka	≥ 0.999	–	–	–
Butan-1-ol	Aldrich	≥ 0.998	–	–	–
Butan-2-ol	Aldrich	≥ 0.995	–	–	–
2-Methyl-propan-1-ol	Aldrich	≥ 0.998			
2-Methyl-propan-2-ol	Aldrich	≥ 0.997	–	–	–
(<i>tert</i> -Butanol)					
1-Pentanol	Aldrich	≥ 0.998	–	–	–
Water	own source	–	distillation, filtration	≥ 0.999	density
Methyl acetate	Aldrich	≥ 0.998	–	–	–

Chemical name ^a	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
Methyl propanoate	Aldrich	≥ 0.99	—	—	—
Methyl butanoate	Aldrich	≥ 0.99	—	—	—
Ethyl acetate	Aldrich	≥ 0.998	—	—	—
Oxolane (Tetrahydrofuran, THF)	Aldrich	≥ 0.999	—	—	—
1,4-Dioxane	Aldrich	≥ 0.998	—	—	—
2-Methoxy-2-methylpropane (<i>tert</i> -Butyl methyl ether, MTBE)	Aldrich	≥ 0.998	—	—	—
2-Ethoxy-2-methylpropane (<i>tert</i> -Butyl ethyl ether, ETBE)	Aldrich	≥ 0.99	—	—	—
2-Methoxy-2-methylbutane (<i>tert</i> -Amyl methyl ether, TAME)	Aldrich	≥ 0.97	—	—	—
Ethoxyethane (Diethyl ether)	Aldrich	≥ 0.999	—	—	—
1-Propoxypropane (Di- <i>n</i> -propyl ether)	Aldrich	≥ 0.99	—	—	—
2-Propan-2-yloxypropane (Di- <i>iso</i> -propyl ether)	Fluka	≥ 0.99	—	—	—
1-Butoxybutane (Di- <i>n</i> -butyl ether)	Aldrich	≥ 0.993	—	—	—
Propan-2-one (Acetone)	Aldrich	≥ 0.999	—	—	—

Chemical name^a	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
Pentan-2-one	Aldrich	≥ 0.99	—	—	—
Pentan-3-one	Aldrich	≥ 0.99	—	—	—
Butanal	Fluka	≥ 0.99	—	—	—
Acetonitrile	Fluka	≥ 0.999	—	—	—
1-Nitropropane	Aldrich	≥ 0.985	—	—	—
Dicyanoazanide; 1-benzyl-3-methylimidazol-3-ium	Io-Li-Tec	≥ 0.980	vacuum heating	—	—
(1-Benzyl-3-methylimidazolium dicyanamide)					
bis(trifluoromethylsulfonyl)azanide; 1-benzyl-3-methylimidazol-3-ium	Io-Li-Tec	≥ 0.990	vacuum heating	—	—
(1-Benzyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide)					

^a Names in parentheses are common names used in text.

Acetone	\bar{p} /kPa	130.8	131.9	130.9	130.5	130.9	130.0
	p_i /kPa	158.5	159.6	158.5	158.2	158.5	157.7
	p_o /kPa	98.5	99.6	98.5	98.2	98.5	97.7
Pentan-2-one	\bar{p} /kPa	130.8	131.9	130.9	130.5	130.9	130.0
	p_i /kPa	158.5	159.6	158.5	158.2	158.5	157.7
	p_o /kPa	98.5	99.6	98.5	98.2	98.5	97.7
Pentan-3-one	\bar{p} /kPa	130.1	131.9	131.6	130.5	130.2	130.0
	p_i /kPa	157.8	159.6	159.3	158.2	157.8	157.7
	p_o /kPa	97.8	99.6	99.3	98.2	97.8	97.7
Butanal	\bar{p} /kPa	130.2	131.9	130.8	130.5	130.9	130.0
	p_i /kPa	157.8	159.6	158.5	158.2	158.5	157.7
	p_o /kPa	97.8	99.6	98.5	98.2	98.5	97.7
Acetonitrile	\bar{p} /kPa	144.5	143.7	130.9	142.9	130.9	141.6
	p_i /kPa	180.7	179.8	158.5	179.1	158.5	177.8
	p_o /kPa	100.7	99.8	98.5	99.1	98.5	97.8
1-Nitropropane	\bar{p} /kPa	144.5	143.7	143.1	143.0	130.3	141.6
	p_i /kPa	180.7	179.8	179.3	179.1	158.0	177.8
	p_o /kPa	100.7	99.8	99.3	99.1	98.0	97.8

^a Standard uncertainties u are $u(T) = 0.02$ K, $u(\bar{p}) = 0.06$ kPa, $u(p_i) = 0.1$ kPa, $u(p_o) = 0.07$ kPa.

	p_i /kPa	157.6	158.2	158.8	158.1	158.9	158.2
	p_o /kPa	97.6	98.2	98.8	98.1	98.9	98.2
Pentan-2-one	\bar{p} /kPa	129.9	130.5	131.1	130.5	131.2	130.5
	p_i /kPa	157.6	158.2	158.8	158.1	158.9	158.2
	p_o /kPa	97.6	98.2	98.8	98.1	98.9	98.2
Pentan-3-one	\bar{p} /kPa	129.9	130.5	130.8	130.5	130.3	130.5
	p_i /kPa	157.6	158.2	158.5	158.1	158.0	158.2
	p_o /kPa	97.6	98.2	98.5	98.1	98.0	98.2
Butanal	\bar{p} /kPa	129.9	130.5	131.1	130.5	131.2	130.5
	p_i /kPa	157.6	158.2	158.8	158.1	158.9	158.2
	p_o /kPa	97.6	98.2	98.8	98.1	98.9	98.2
Acetonitrile	\bar{p} /kPa	129.9	130.5	131.1	130.5	131.2	130.5
	p_i /kPa	157.6	158.2	158.8	158.1	158.9	158.2
	p_o /kPa	97.6	98.2	98.8	98.1	98.9	98.2
1-Nitropropane	\bar{p} /kPa	129.9	130.5	130.8	130.5	130.5	130.5
	p_i /kPa	157.6	158.2	158.5	158.1	158.1	158.2
	p_o /kPa	97.6	98.2	98.5	98.1	98.1	98.2

^a Standard uncertainties u are $u(T) = 0.02 \text{ K}$, $u(\bar{p}) = 0.06 \text{ kPa}$, $u(p_i) = 0.1 \text{ kPa}$, $u(p_o) = 0.07 \text{ kPa}$

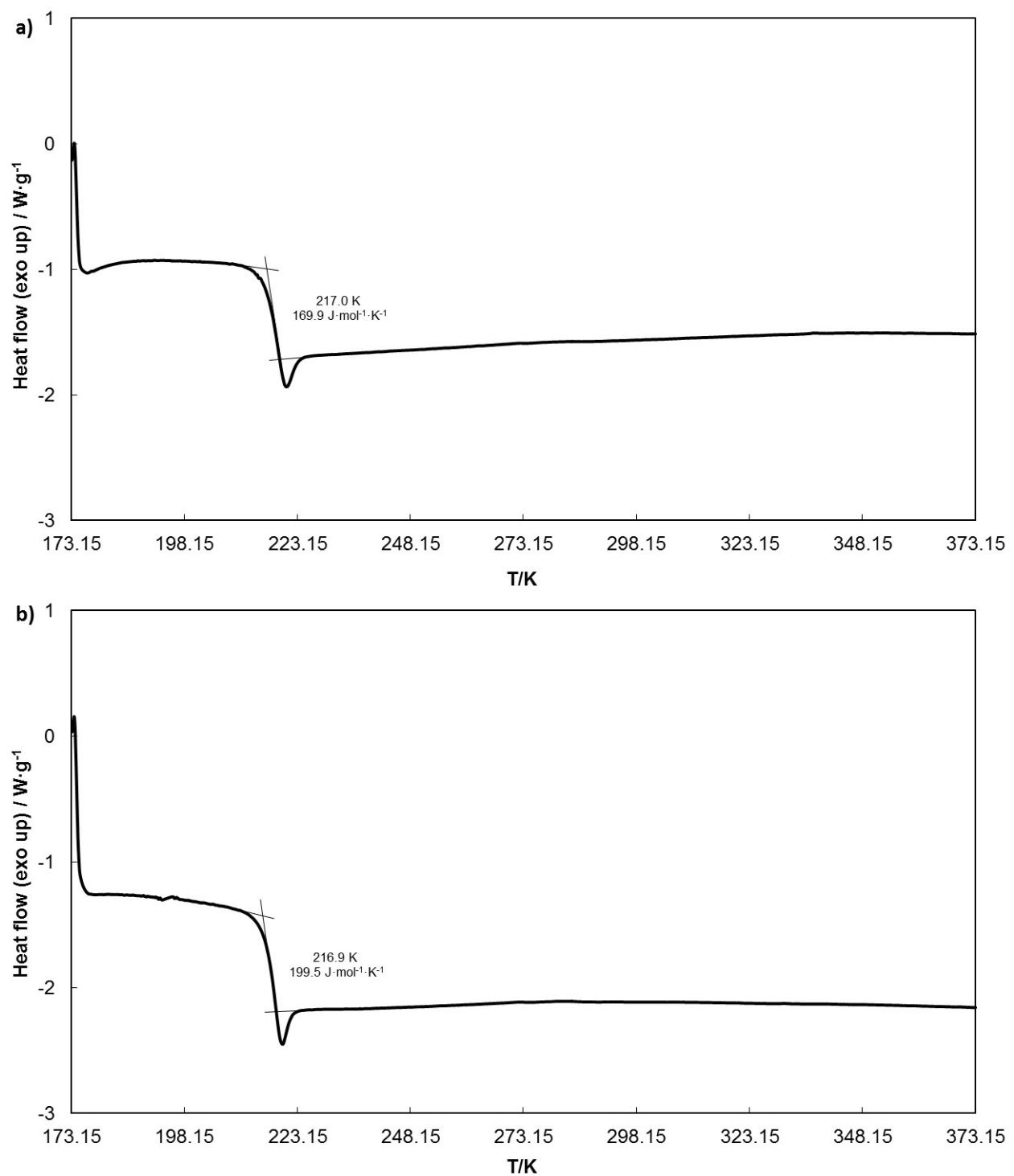


Fig. 1S DSC of a) [BzMIM][DCA]; b) [BzMIM][NTf₂].

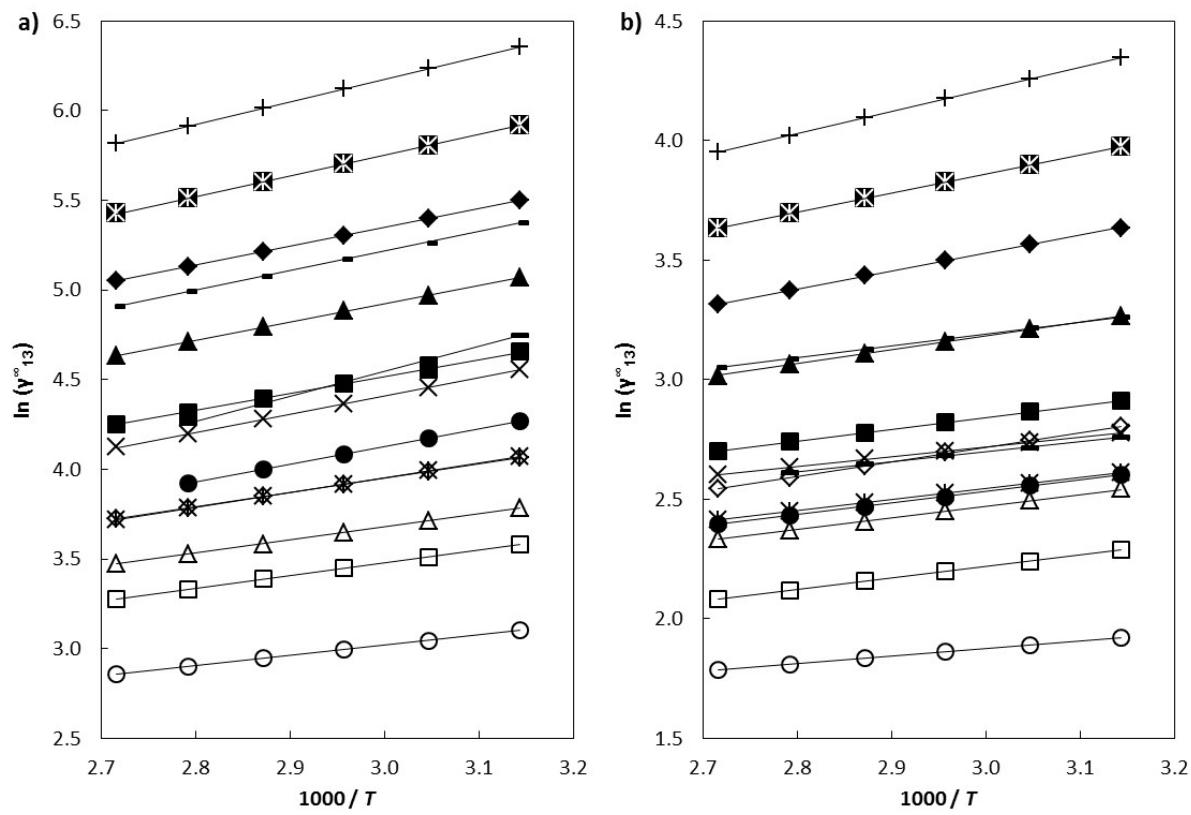


Fig. 2S Plot of $\ln(\gamma_{13}^{\infty})$ for ionic liquid a) [BzMIM][DCA]; b) [BzMIM][NTf₂] versus $1/T$ for the solutes: (●) pentane; (■) hexane; (×) 3-methylpentane; (—) 2,2,-dimethylbutane; (▲) heptane; (✳) octane; (-) 2,2,4-trimethylpentane; (▼) nonane; (△) decane; (○) cyclopentane; (□) cyclohexane; (▽) methylcyclohexane; (Δ) cycloheptane; (◊) cyclooctane.

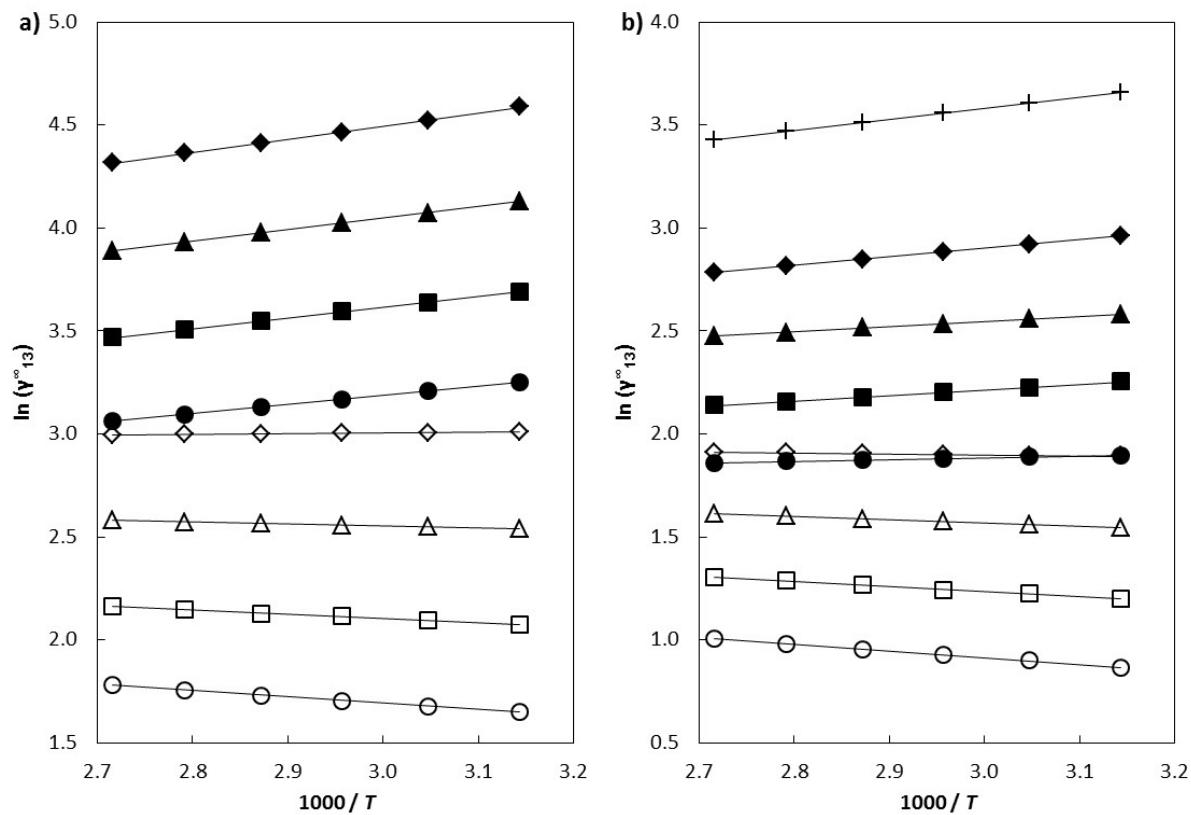


Fig. 3S Plot of $\ln(\gamma_{13}^\infty)$ for ionic liquid a) $[\text{BzMIM}][\text{DCA}]$; b) $[\text{BzMIM}][\text{NTf}_2]$ versus $1/T$ for the solutes: (●) pent-1-ene; (■) hex-1-ene; (×) cyclohexene; (▲) hept-1-ene; (✳) oct-1-ene; (◆) dec-1-ene; (○) pent-1-yne; (□) hex-1-yne; (Δ) hept-1-yne; (◊) oct-1-yne.

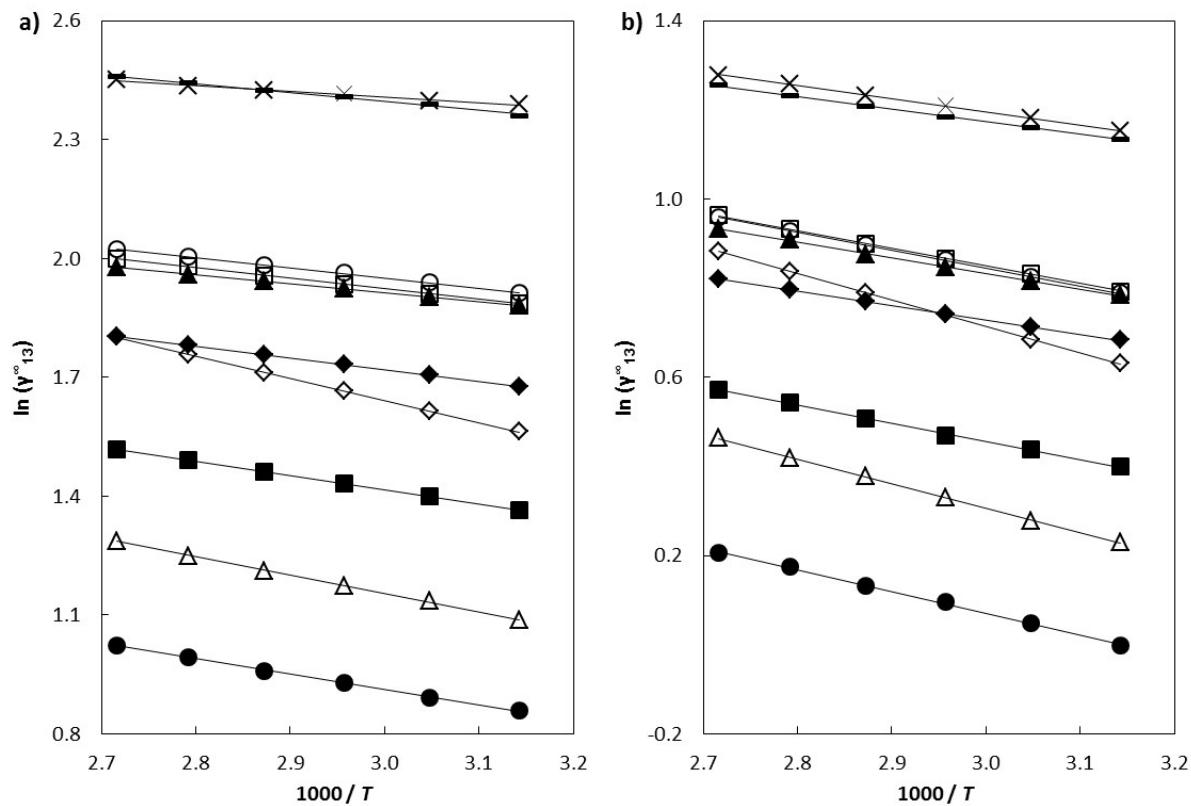


Fig. 4S Plot of $\ln(\gamma_{13}^{\infty})$ for ionic liquid a) [BzMIM][DCA]; b) [BzMIM][NTf₂] versus 1/T for the solutes: (●) benzene; (■) toluene; (▲) ethylbenzene; (◆) o-xylene; (○) m-xylene; (□) p-xylene; (×) propylbenzene; (—) iso-propylbenzene; (Δ) styrene; (◊) α-methylstyrene.

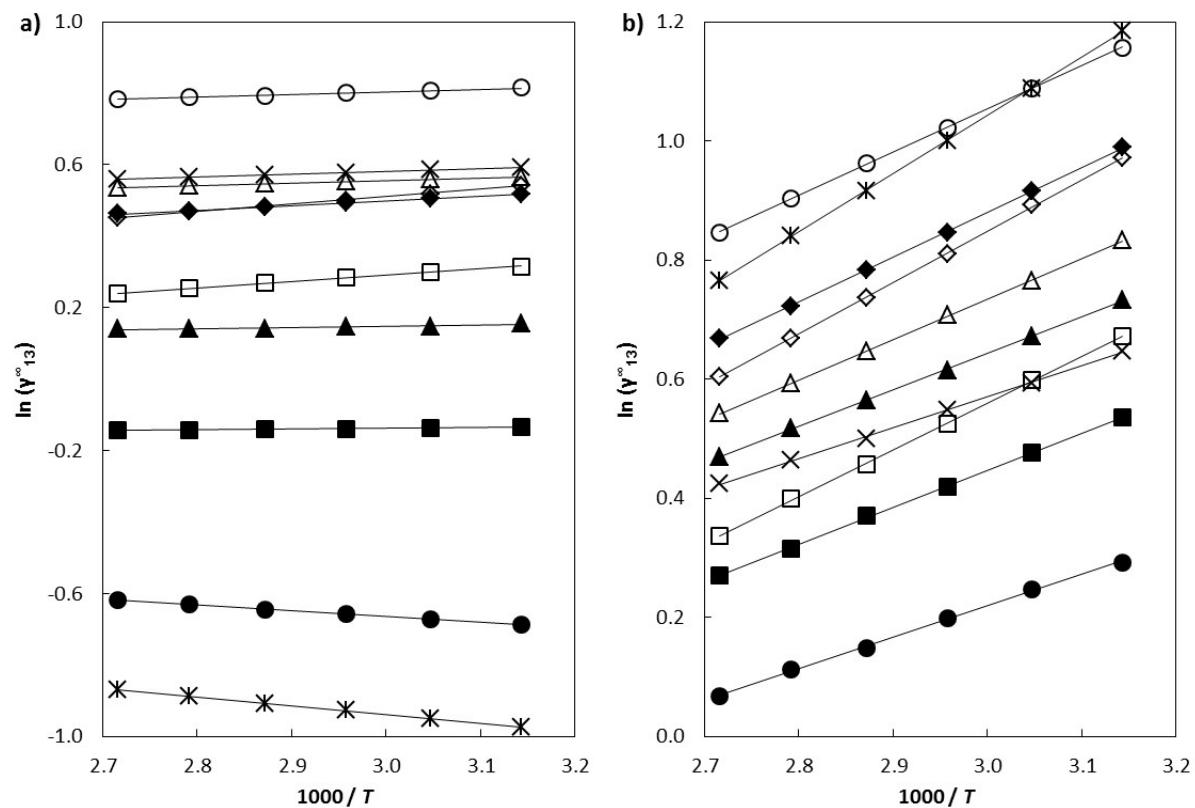


Fig. 5S Plot of $\ln(\gamma_{13}^\infty)$ for ionic liquid a) [BzMIM][DCA]; b) [BzMIM][NTf₂] versus $1/T$ for the solutes: (●) methanol; (■) ethanol; (▲) propan-1-ol; (●) butan-1-ol; (□) propan-2-ol; (△) butan-2-ol; (◊) 2-methyl-1-propanol; (×) *tert*-butanol; (○) pentan-1-ol; (✗) water.

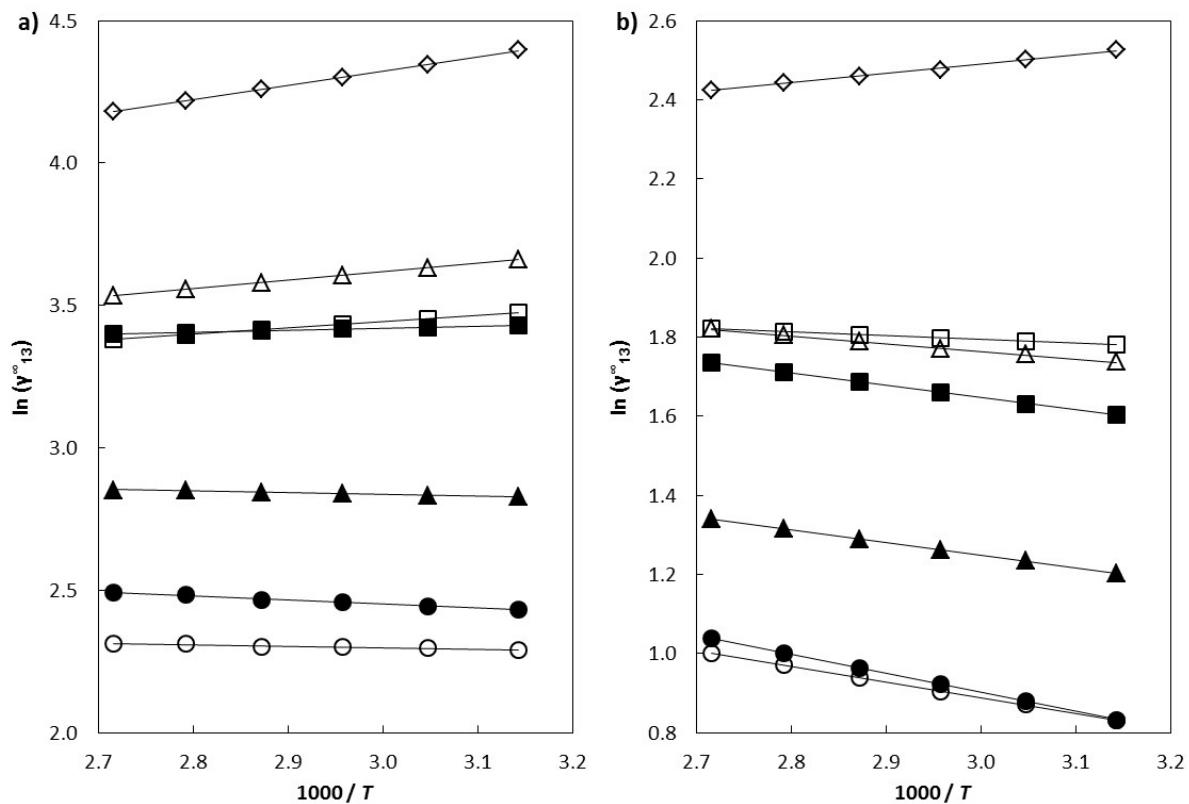


Fig. 6S Plot of $\ln(\gamma_{13}^\infty)$ for ionic liquid a) [BeMIM][DCA]; b) [BeMIM][NTf₂] versus 1/T for the solutes: (○) diethyl ether; (□) di-*n*-propyl ether; (Δ) di-*iso*-propyl ether; (◊) di-*n*-butyl ether; (●) MTBE; (■) ETBE; (▲) TAME.

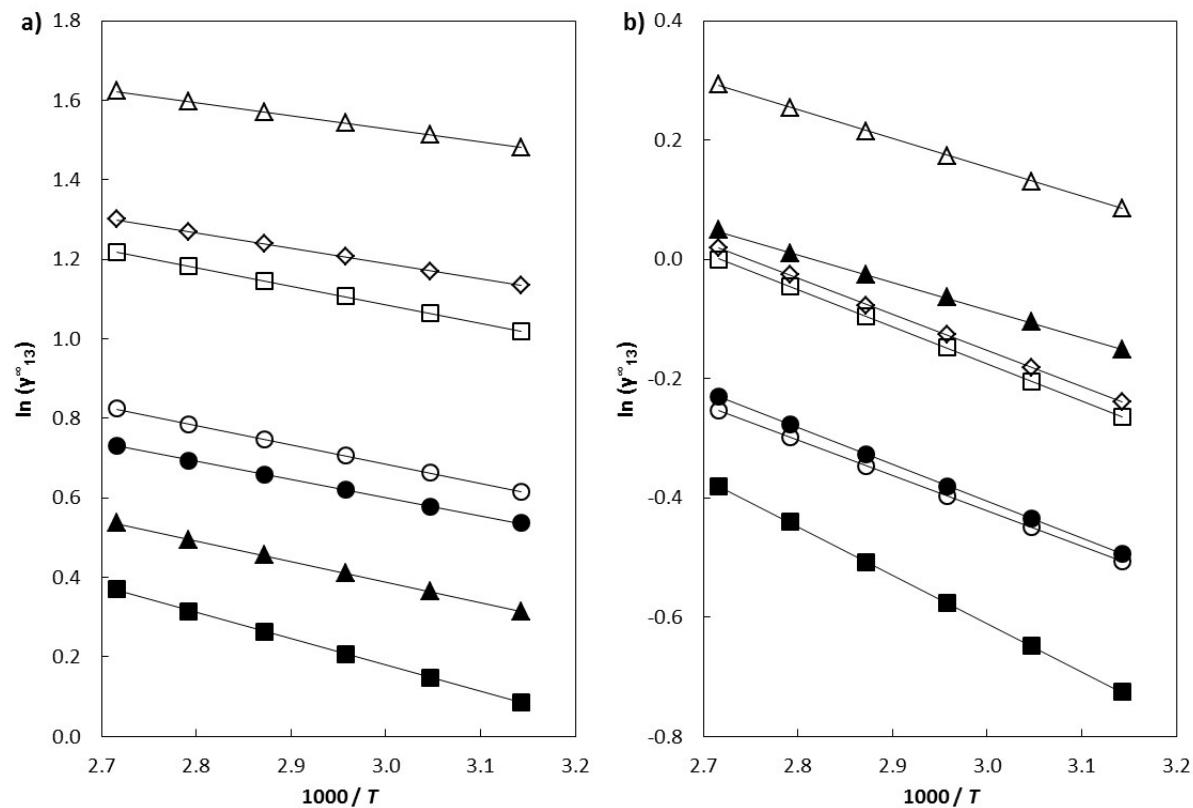


Fig. 7S Plot of $\ln(\gamma_{13}^{\infty})$ for ionic liquid a) [BzMIM][DCA]; b) [BzMIM][NTf₂] versus $1/T$ for the solutes: (○) methyl acetate; (□) methyl propanoate; (Δ) methyl butanoate; (◊) ethyl acetate; (●) THF; (■) 1,4-dioxane; (▲) thiophene.

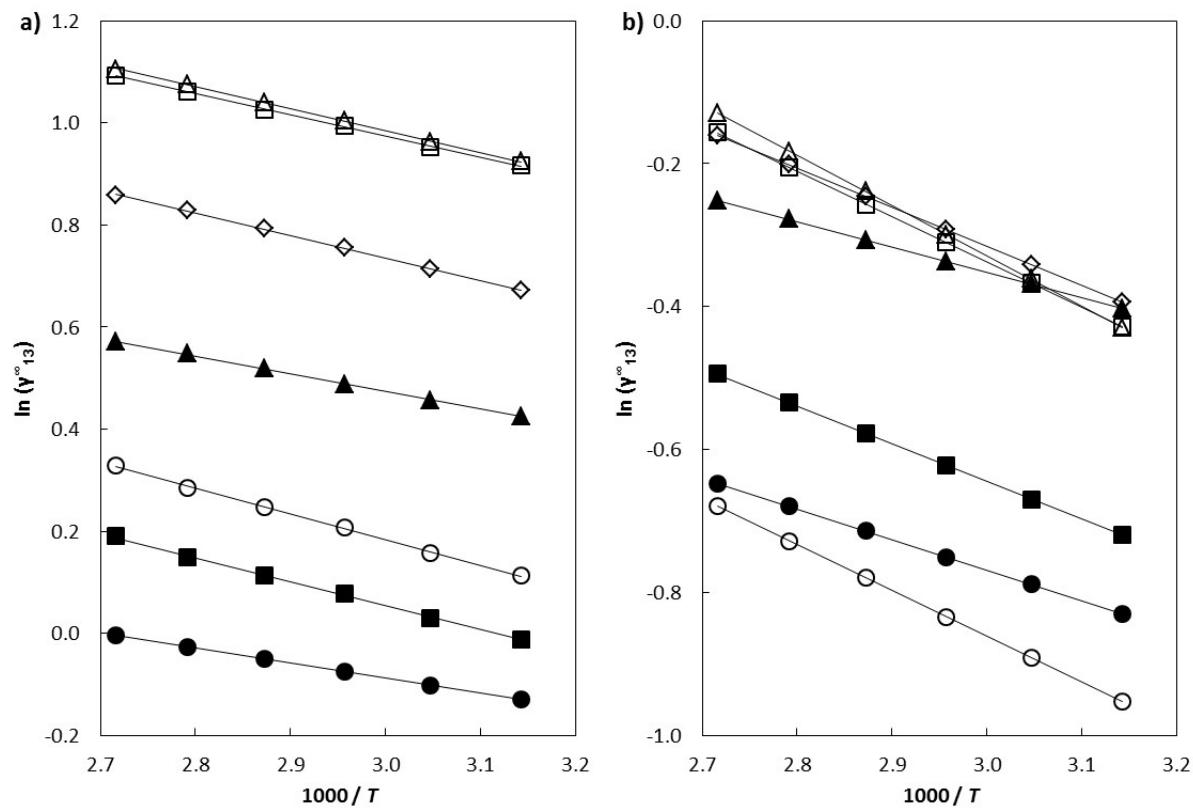


Fig. 8S Plot of $\ln(\gamma_{13}^\circ)$ for ionic liquid a) [BzMIM][DCA]; b) [BzMIM][NTf₂] versus $1/T$ for the solutes: (○) acetone; (□) pentan-2-one; (Δ) pentan-3-one; (●) acetonitrile; (■) pyridine; (▲) 1-nitropropane; (◇) butanal.