

Electronic Supplementary Information

Effect of Salts on the Solubility of Ionic Liquids in Water: Experimental and Electrolyte Perturbed- Chain Statistical Associating Fluid Theory

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Table S1. Experimental solubility, in weight and molal units, of [C₄C₁im][NTf₂] in aqueous salt solutions at 298.15 K.

(mol·kg ⁻¹)				(g/g)			
[K₃C₆H₅O₇]	[IL] × 10² ± σ	[K₃PO₄]	[IL] × 10² ± σ	[K₃C₆H₅O₇]	[IL] × 10³ ± σ	[K₃PO₄]	[IL] × 10³ ± σ
0	1.69 ± 0.01	0	1.69 ± 0.01	0	7.09 ± 0.02	0	7.09 ± 0.02
0.100	1.64 ± 0.05	0.100	1.48 ± 0.02	2.58 × 10 ⁻²	6.89 ± 0.20	2.12 × 10 ⁻²	6.19 ± 0.10
0.200	1.40 ± 0.02	0.200	1.12 ± 0.01	5.17 × 10 ⁻²	5.89 ± 0.07	4.25 × 10 ⁻²	4.68 ± 0.04
0.500	0.898 ± 0.048	0.500	0.868 ± 0.011	1.29 × 10 ⁻¹	3.77 ± 0.20	1.06 × 10 ⁻¹	3.64 ± 0.05
1.00	0.354 ± 0.014	1.00	0.390 ± 0.026	2.58 × 10 ⁻¹	1.48 ± 0.06	2.12 × 10 ⁻¹	1.63 ± 0.11
1.50	0.126 ± 0.090	1.50	0.221 ± 0.012	3.88 × 10 ⁻¹	0.53 ± 0.38	3.18 × 10 ⁻¹	0.929 ± 0.051
[K₂HPO₄]	[IL] × 10² ± σ	[KH₂PO₄]	[IL] × 10² ± σ	[K₂HPO₄]	[IL] × 10³ ± σ	[KH₂PO₄]	[IL] × 10³ ± σ
0	1.69 ± 0.01	0	1.69 ± 0.01	0	7.09 ± 0.02	0	7.09 ± 0.02
0.100	1.95 ± 0.02	0.100	1.74 ± 0.02	1.74 × 10 ⁻²	8.19 ± 0.09	1.36 × 10 ⁻²	7.29 ± 0.08
0.200	1.91 ± 0.01	0.200	1.83 ± 0.02	3.48 × 10 ⁻²	7.99 ± 0.04	2.72 × 10 ⁻²	7.69 ± 0.07
0.500	1.20 ± 0.02	0.500	1.53 ± 0.01	8.71 × 10 ⁻²	5.05 ± 0.08	6.80 × 10 ⁻²	6.40 ± 0.03
1.00	0.560 ± 0.011	1.00	1.10 ± 0.02	1.74 × 10 ⁻¹	2.35 ± 0.04	1.36 × 10 ⁻¹	4.60 ± 0.09
1.50	0.270 ± 0.008	1.50	0.733 ± 0.006	2.61 × 10 ⁻¹	1.13 ± 0.04	2.04 × 10 ⁻¹	3.07 ± 0.03
[KNaC₄H₄O₆]	[IL] × 10² ± σ	[KCH₃CO₂]	[IL] × 10² ± σ	[KNaC₄H₄O₆]	[IL] × 10³ ± σ	[KCH₃CO₂]	[IL] × 10³ ± σ
0	1.69 ± 0.01	0	1.69 ± 0.01	0	7.09 ± 0.02	0	7.09 ± 0.02
0.100	1.61 ± 0.03	0.100	1.59 ± 0.01	1.88 × 10 ⁻²	6.75 ± 0.13	1.88 × 10 ⁻²	6.66 ± 0.02
0.200	1.53 ± 0.02	0.200	1.60 ± 0.02	3.76 × 10 ⁻²	6.40 ± 0.07	3.76 × 10 ⁻²	6.72 ± 0.09
0.500	1.02 ± 0.05	0.500	1.54 ± 0.01	9.41 × 10 ⁻²	4.28 ± 0.20	9.41 × 10 ⁻²	6.45 ± 0.06
1.00	0.305 ± 0.070	1.00	1.37 ± 0.05	1.88 × 10 ⁻¹	1.28 ± 0.29	1.88 × 10 ⁻¹	5.76 ± 0.20
1.50	0.137 ± 0.106	1.50	1.05 ± 0.01	2.82 × 10 ⁻¹	0.57 ± 0.44	2.82 × 10 ⁻¹	4.39 ± 0.05
[Mg(CH₃CO₂)₂]	[IL] × 10² ± σ	[MgSO₄]	[IL] × 10² ± σ	[Mg(CH₃CO₂)₂]	[IL] × 10³ ± σ	[MgSO₄]	[IL] × 10³ ± σ

0	1.69 ± 0.01	0	1.69 ± 0.01	0	7.09 ± 0.02	0	7.09 ± 0.02
0.100	1.76 ± 0.02	0.100	1.60 ± 0.01	1.42 × 10 ⁻²	7.39 ± 0.08	1.20 × 10 ⁻²	6.70 ± 0.02
0.200	1.44 ± 0.01	0.200	1.40 ± 0.01	2.85 × 10 ⁻²	6.03 ± 0.06	2.41 × 10 ⁻²	5.89 ± 0.02
0.500	0.969 ± 0.033	0.500	1.14 ± 0.01	7.12 × 10 ⁻²	4.06 ± 0.14	6.02 × 10 ⁻²	4.78 ± 0.03
1.00	0.681 ± 0.052	1.00	0.643 ± 0.051	1.42 × 10 ⁻¹	2.85 ± 0.22	1.20 × 10 ⁻¹	2.70 ± 0.21
1.50	0.242 ± 0.014	1.50	0.318 ± 0.006	2.14 × 10 ⁻¹	1.01 ± 0.06	1.81 × 10 ⁻¹	1.33 ± 0.02
[ZnSO₄]	[IL] × 10² ± σ	[Al₂(SO₄)₃]	[IL] × 10² ± σ	[ZnSO₄]	[IL] × 10³ ± σ	[Al₂(SO₄)₃]	[IL] × 10³ ± σ
0	1.69 ± 0.01	0	1.69 ± 0.01	0	7.09 ± 0.02	0	7.09 ± 0.02
0.100	1.66 ± 0.02	0.100	1.80 ± 0.01	1.61 × 10 ⁻²	6.94 ± 0.08	3.42 × 10 ⁻²	7.56 ± 0.02
0.200	1.60 ± 0.01	0.200	1.78 ± 0.01	3.23 × 10 ⁻²	6.72 ± 0.06	6.84 × 10 ⁻²	7.47 ± 0.05
0.500	1.03 ± 0.03	0.500	1.09 ± 0.01	8.07 × 10 ⁻²	4.32 ± 0.07	1.71 × 10 ⁻¹	4.58 ± 0.01
1.00	0.609 ± 0.052	0.750	0.157 ± 0.011	1.61 × 10 ⁻¹	2.56 ± 0.01	2.57 × 10 ⁻¹	6.58 ± 0.04
1.50	0.242 ± 0.014			2.42 × 10 ⁻¹	0.44 ± 0.06		

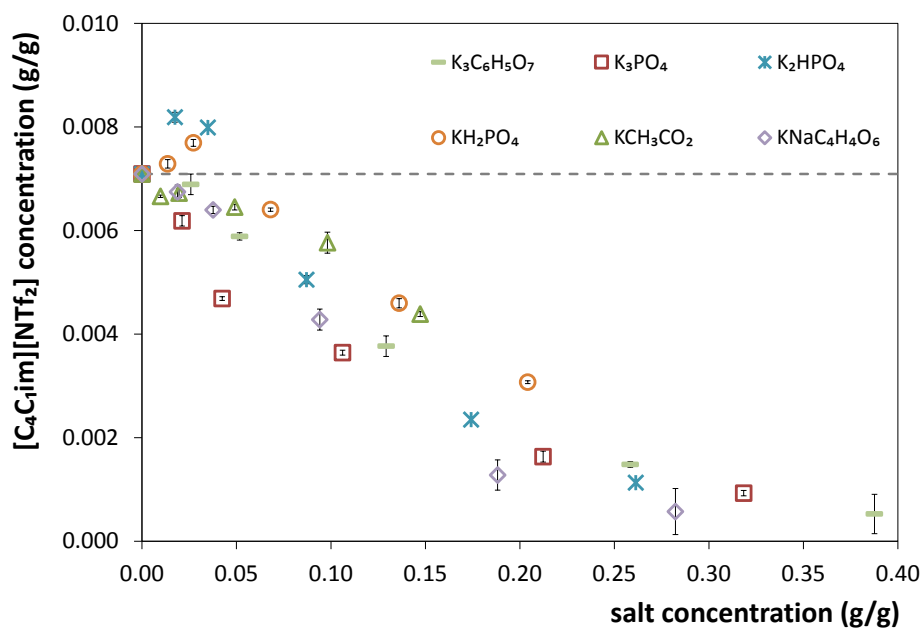


Fig. S1. Solubility of [C₄C₁im][NTf₂] in water for the aqueous potassium-based salt solutions in weight units.

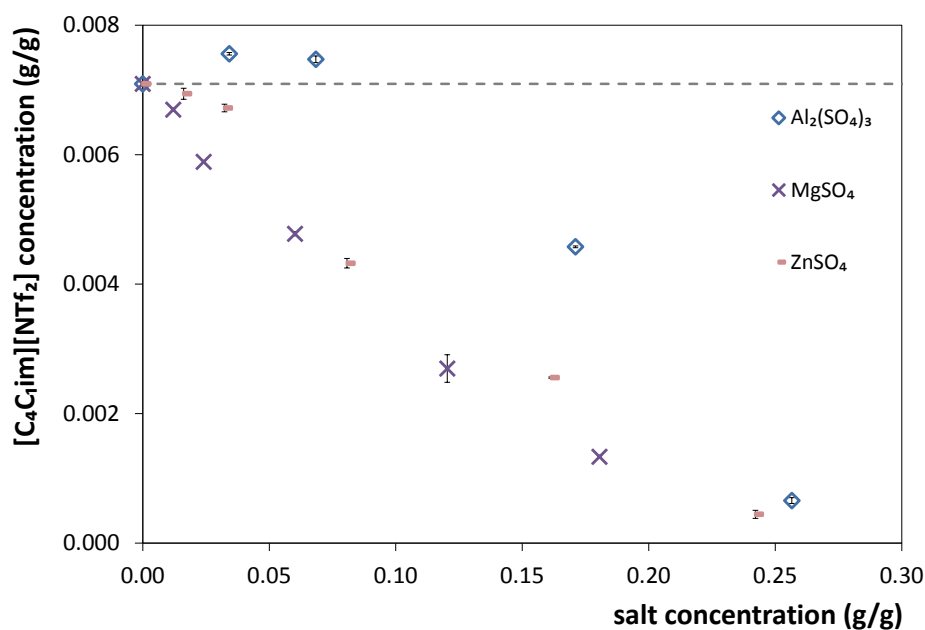


Fig. S2. Solubility of [C₄C₁im][NTf₂] in water for the aqueous sulfate-based salt solutions in weight units.

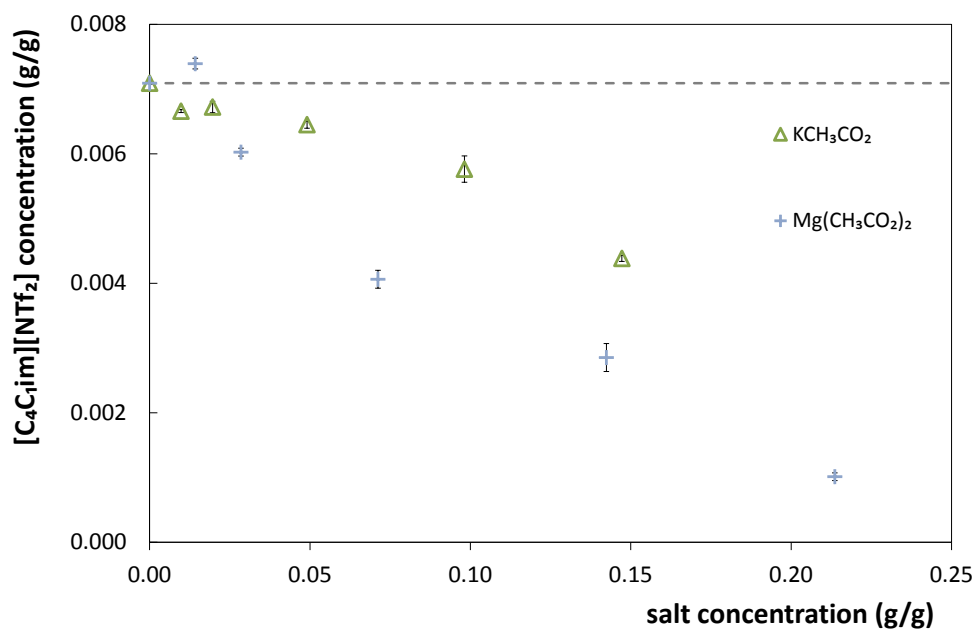


Fig. S3. Solubility of [C₄C₁im][NTf₂] in water for the aqueous acetate-based salt solutions in weight units.

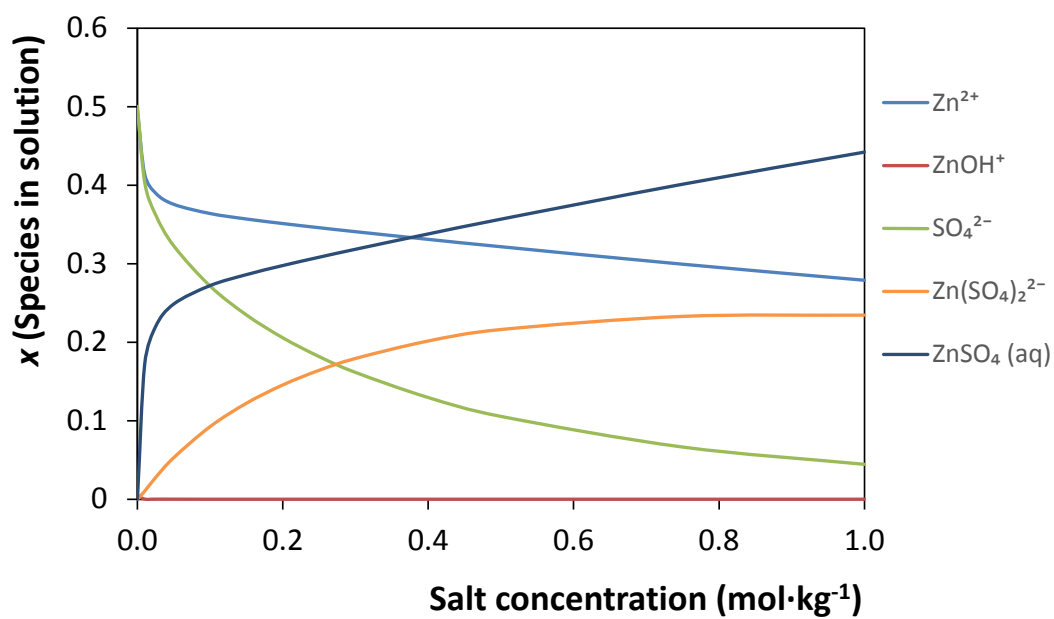


Fig. S4. Ion speciation profile of ZnSO₄ in aqueous solutions at 298 K estimated by Visual MINTEQ.

ePC-SAFT parameter estimation for the citrate anion $\text{C}_6\text{H}_5\text{O}_7^{3-}$

To determine the ePC-SAFT parameters for the citrate anion $\text{C}_6\text{H}_5\text{O}_7^{3-}$ experimental data for potassium citrate solutions were used, including density (293 K, 298 K, 303 K) and osmotic coefficient data (298 K) [S1-S4]. The deviations (ARD) from the experimental data was found to be 0.23 % and 7.02 % for the density and for the osmotic coefficients, respectively.

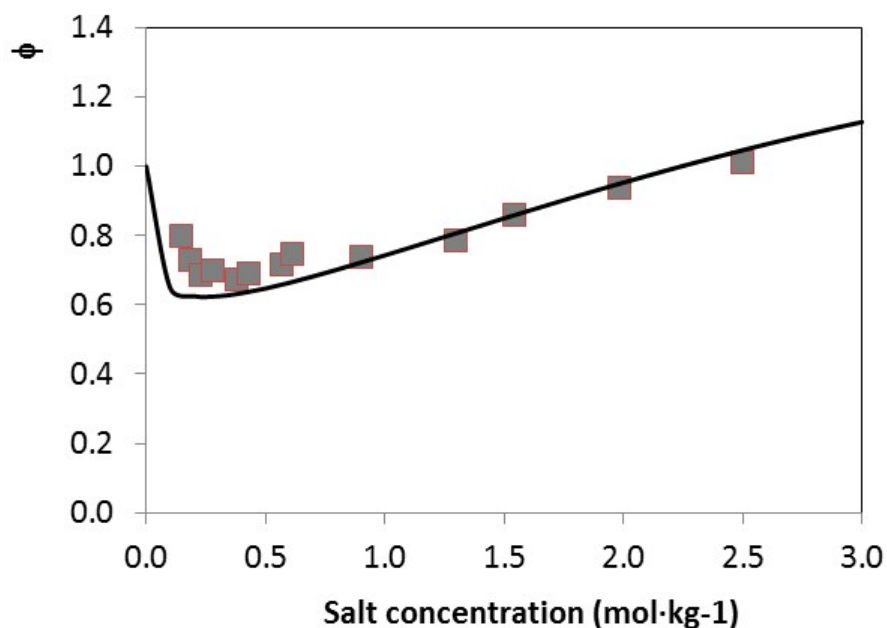


Fig. S5. Osmotic coefficients of binary water/potassium citrate solutions at 298.15 K at 1 bar. Experimental data (symbols) from [S1-S4]. ePC-SAFT (lines) using parameters from Table 1 and 2.

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