

The Effect of the Cation on the Interactions between Alkyl Methyl Imidazolium Chloride Ionic Liquids and Water

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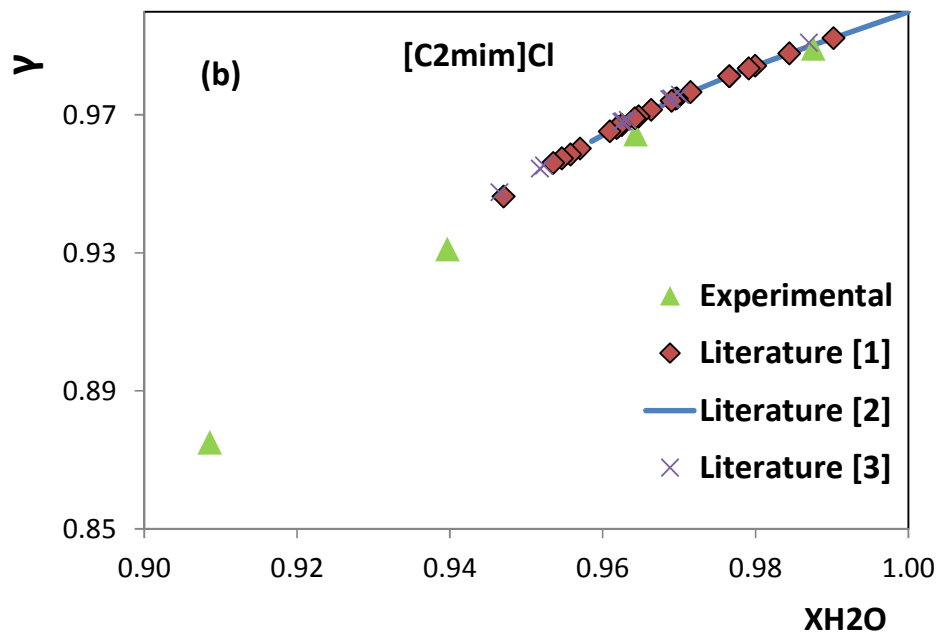
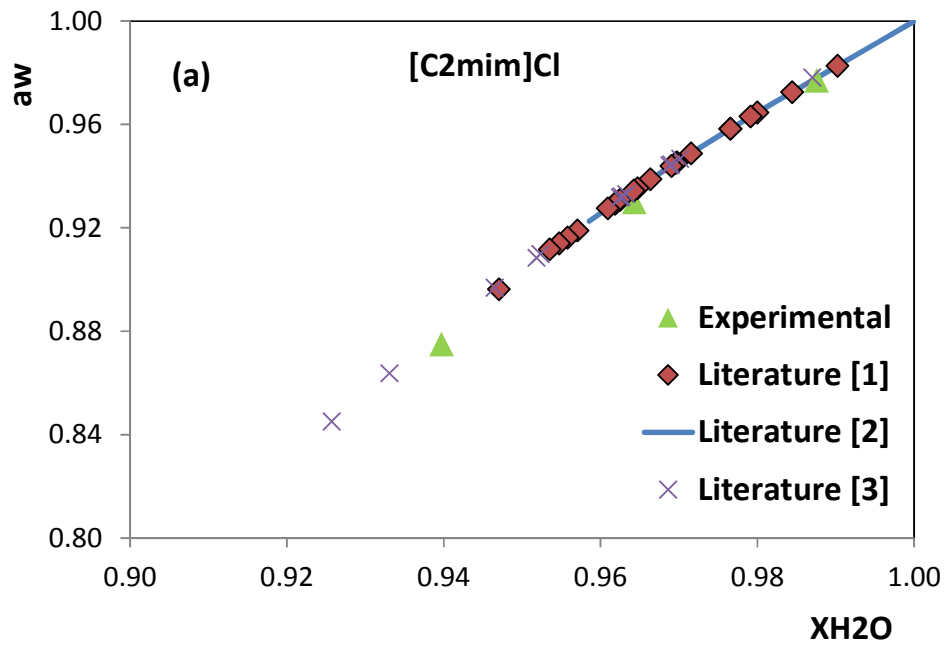
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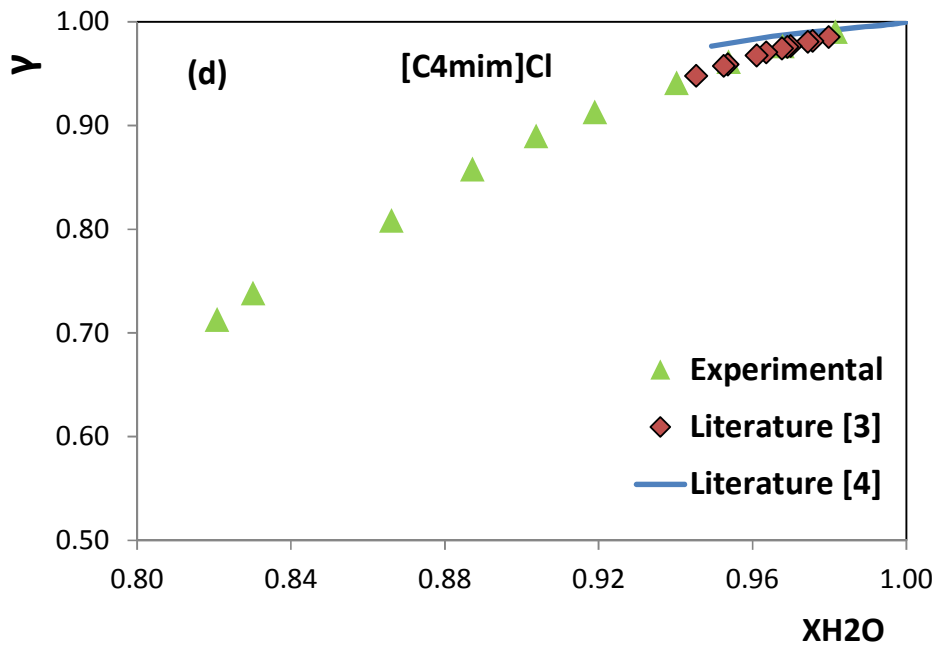
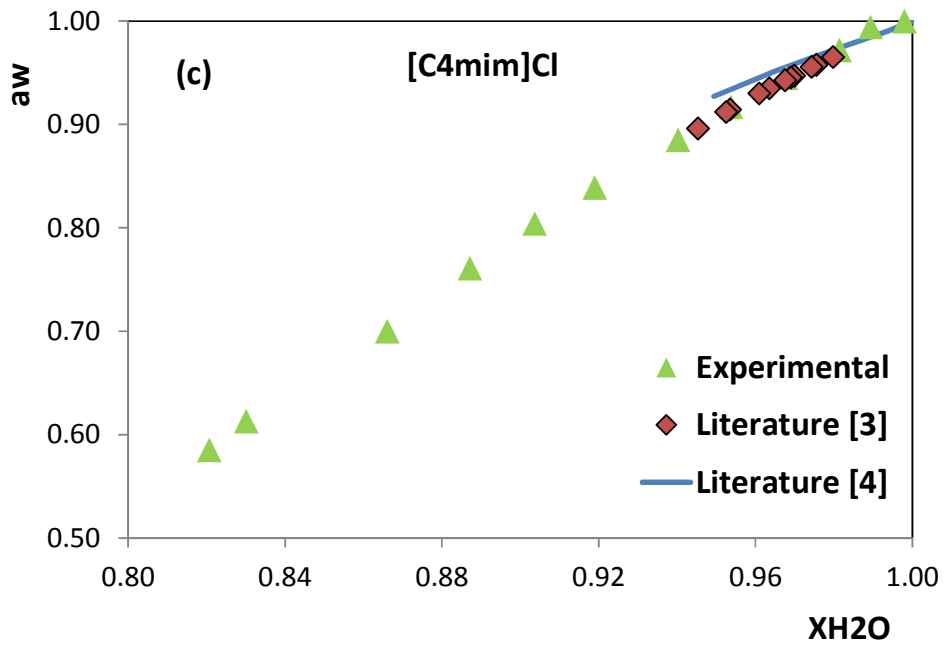
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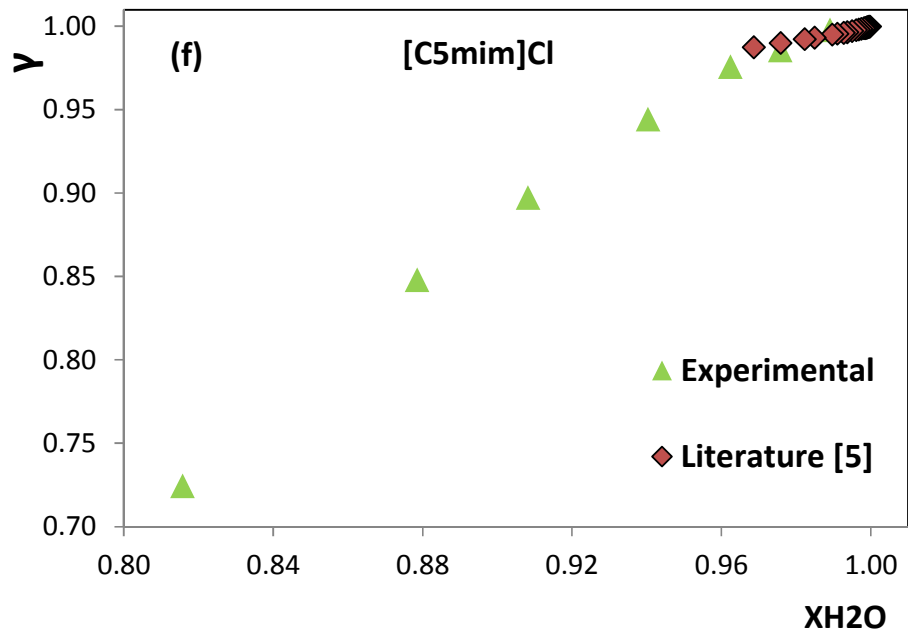
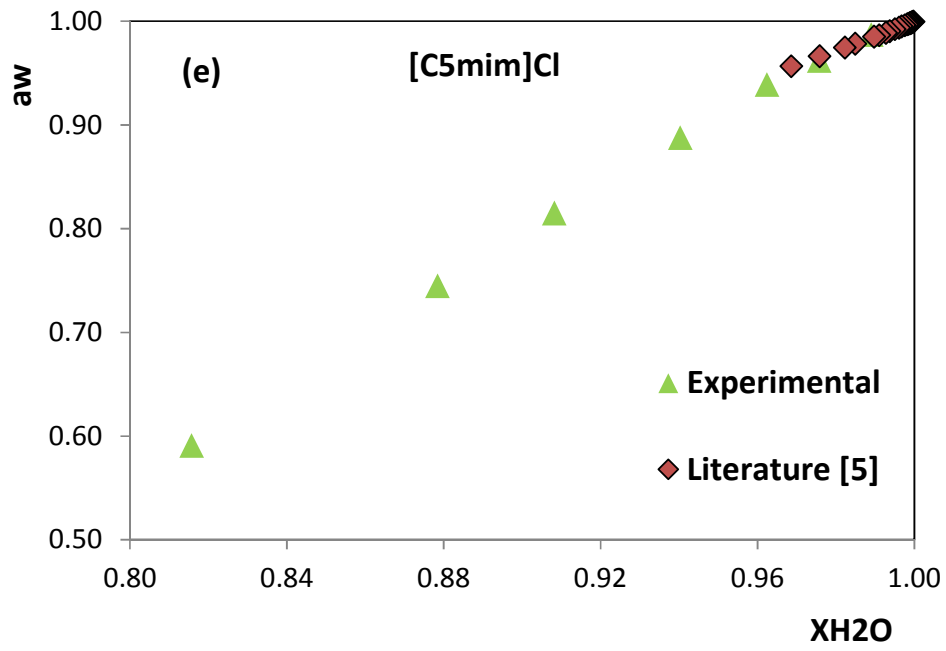
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SUPPORTING INFORMATION







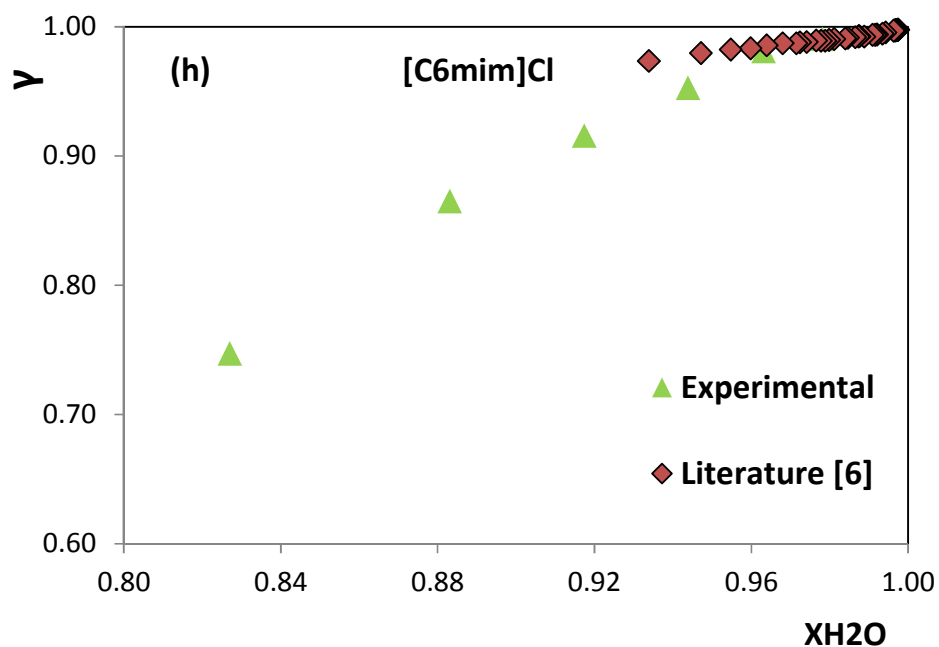
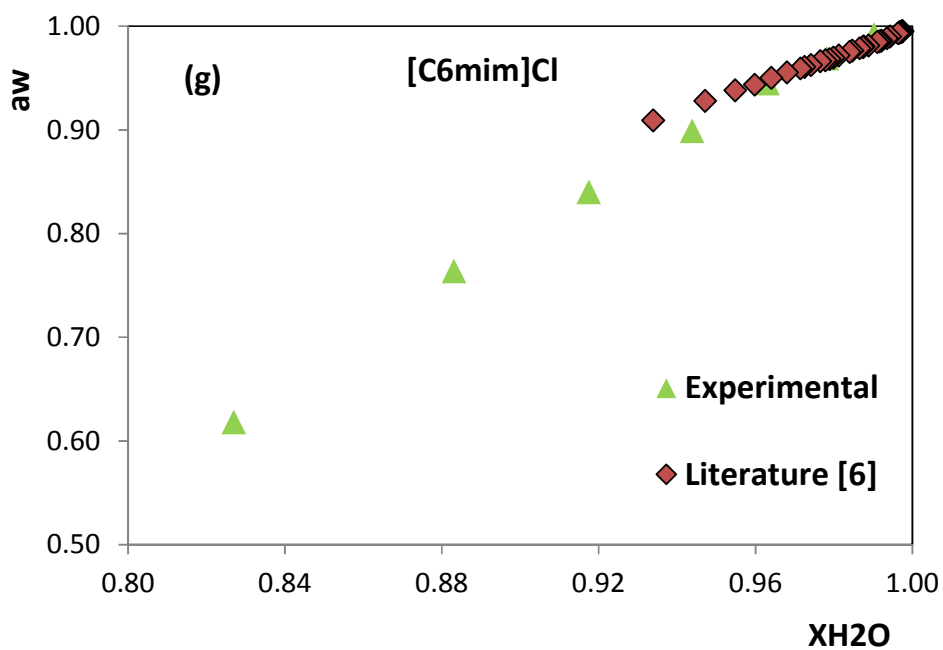


Figure S1. Comparison of experimental water activity (a_w); (a), (c), (e) & (g) and activity coefficient (γ); (b), (d), (f) & (h) of some alkyl methyl imidazolium chloride ($[\text{C}_2\text{mim}]\text{Cl}^{1-3}$; $[\text{C}_4\text{mim}]\text{Cl}^{3-4}$; $[\text{C}_5\text{mim}]\text{Cl}^5$; $[\text{C}_6\text{mim}]\text{Cl}^6$) in aqueous solution at 298.2 K with reported values in literature

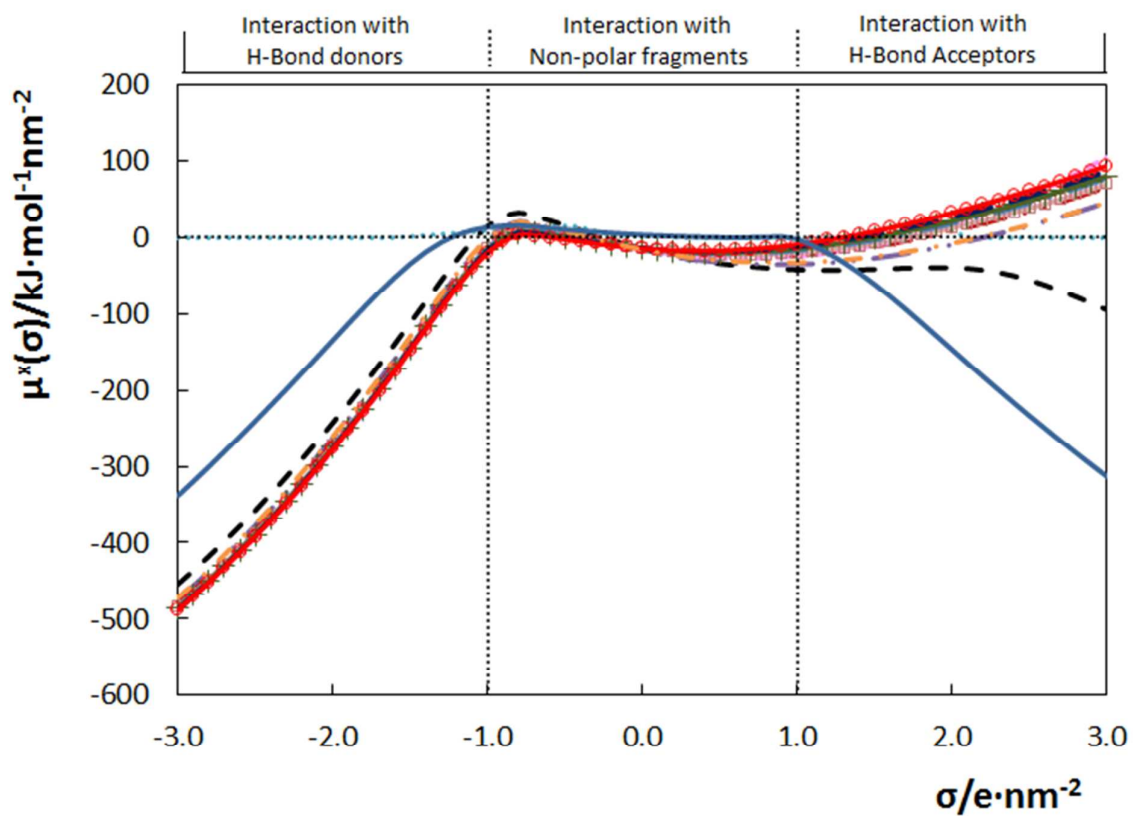
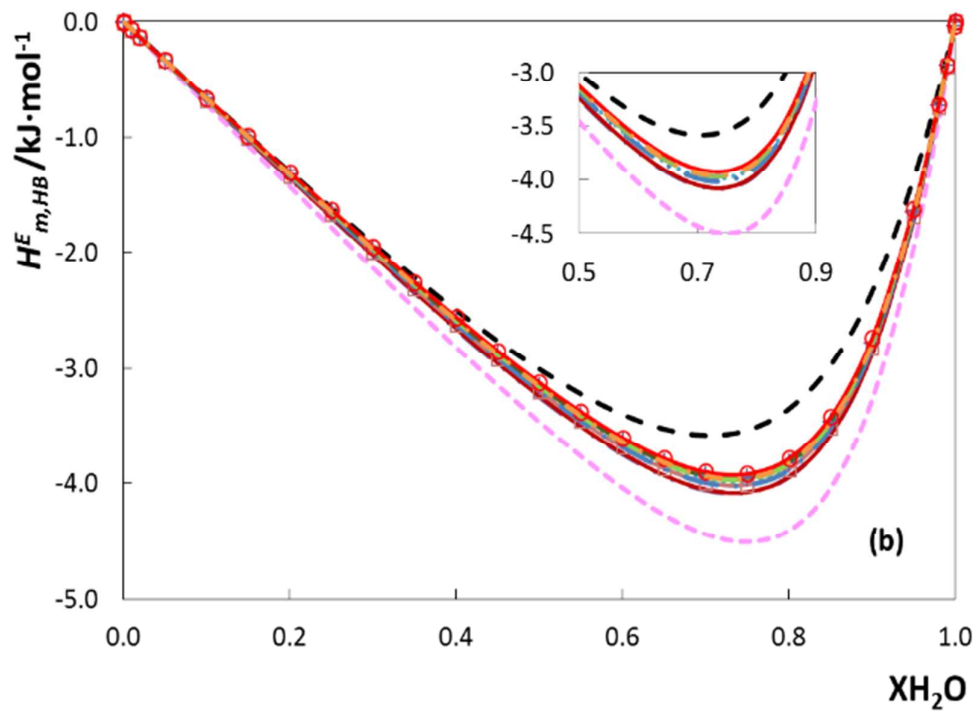
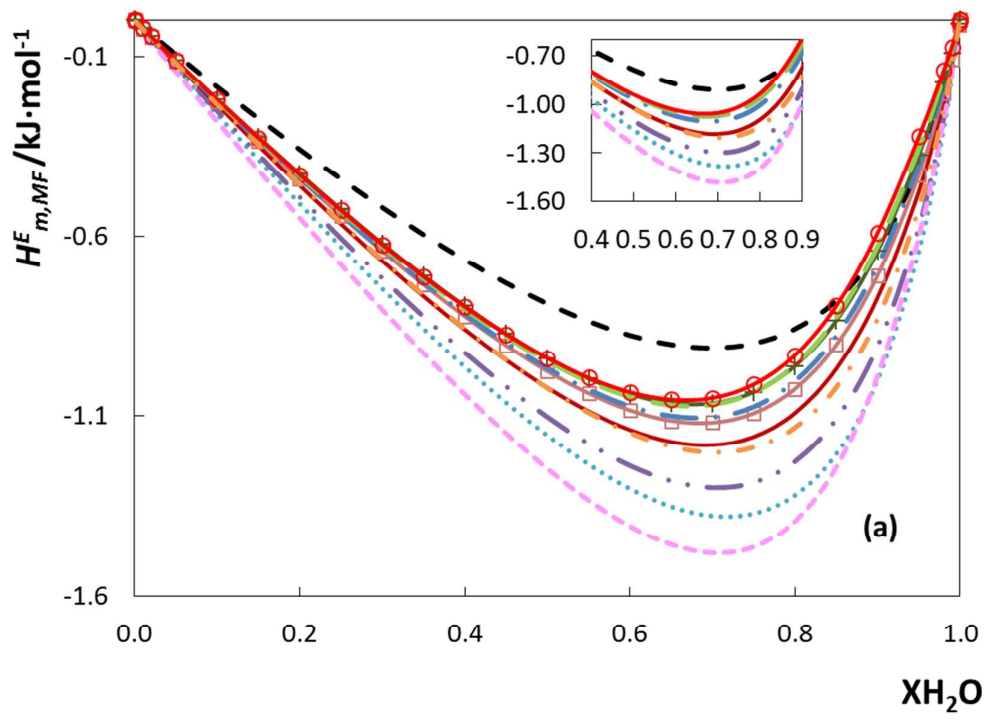


Figure S2. σ -potential of H₂O (—), [C₁im]Cl (---), [C₁mim]Cl (.....), [C₂mim]Cl (— · · —), [C₄mim]Cl (—), [C₄C₁mim]Cl (---), [C₅mim]Cl (—□—), [C₆mim]Cl (— · —), [C₇mim]Cl (—++—), [C₈mim]Cl (— —), [C₁₀mim]Cl (—○—) and [a₁C₁mim]Cl (— · —).



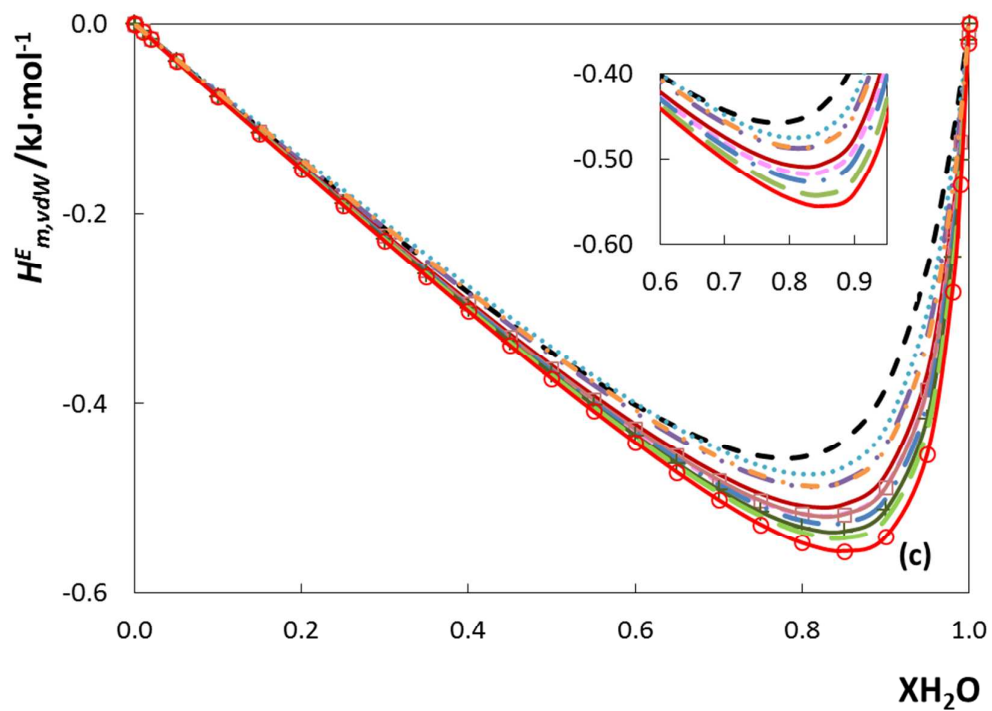


Figure S3. Contribution of (a) electrostatic-misfit interaction; (b) hydrogen bonds interaction; (c) van der Waals forces to the excess enthalpy of binary mixtures of ionic liquids and water at 298.2 K predicted by COSMO-RS. [C₁im]Cl (---), [C₁mim]Cl (.....), [C₂mim]Cl (- · - · -), [C₄mim]Cl (—), [C₄C₁mim]Cl (- · · · -), [C₅mim]Cl (□-□-), [C₆mim]Cl (- · - · -), [C₇mim]Cl (+ + +), [C₈mim]Cl (—), [C₁₀mim]Cl(○-○) and [a₁C₁mim]Cl (- · - · -).

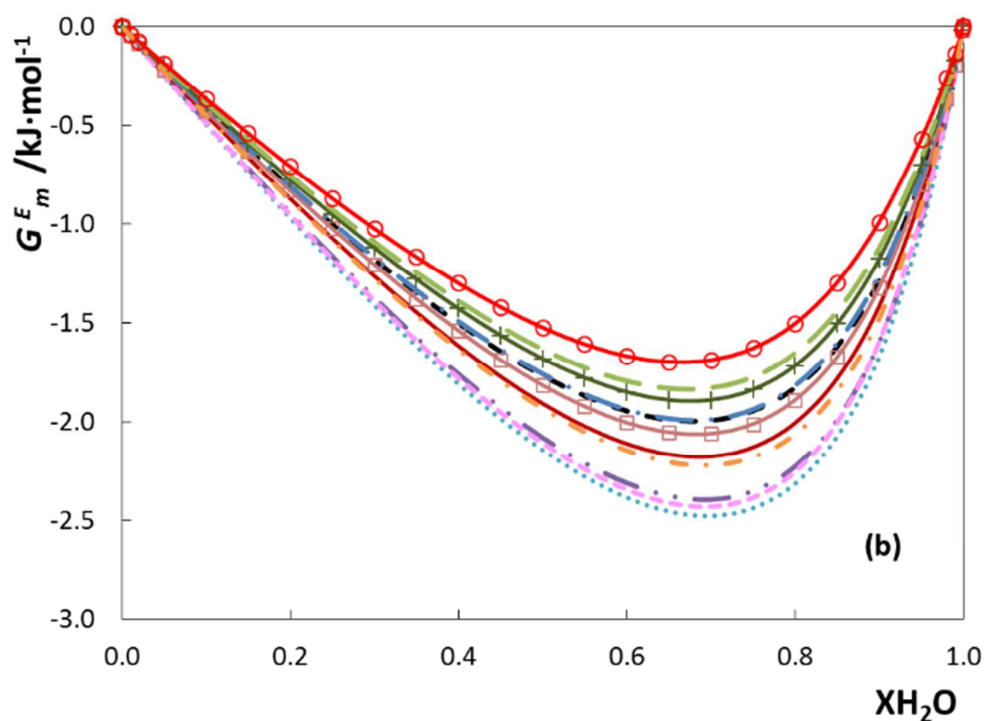
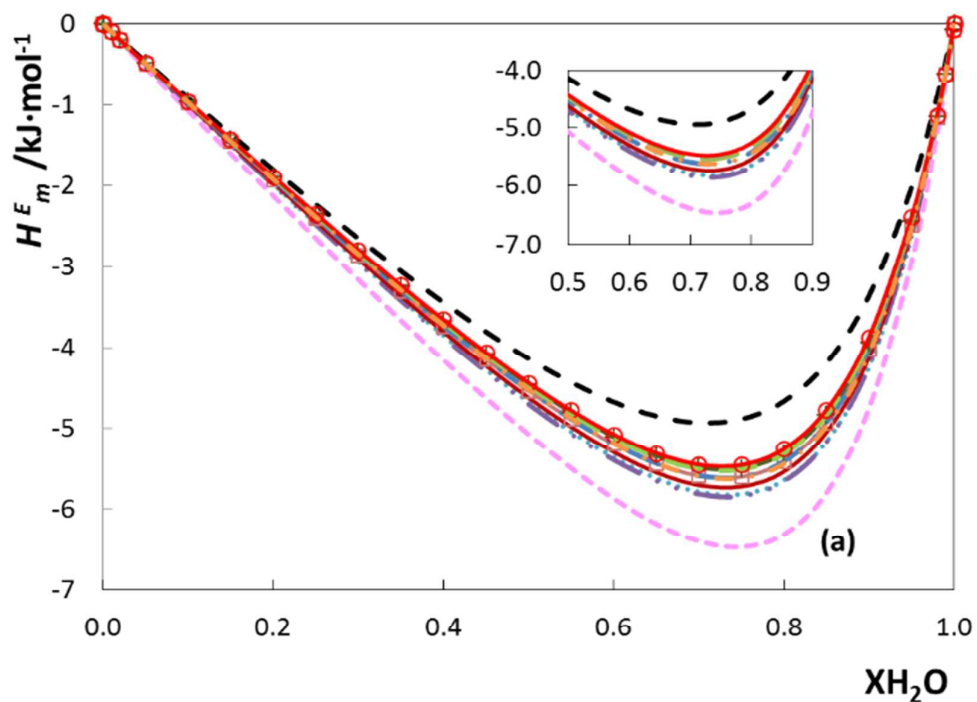
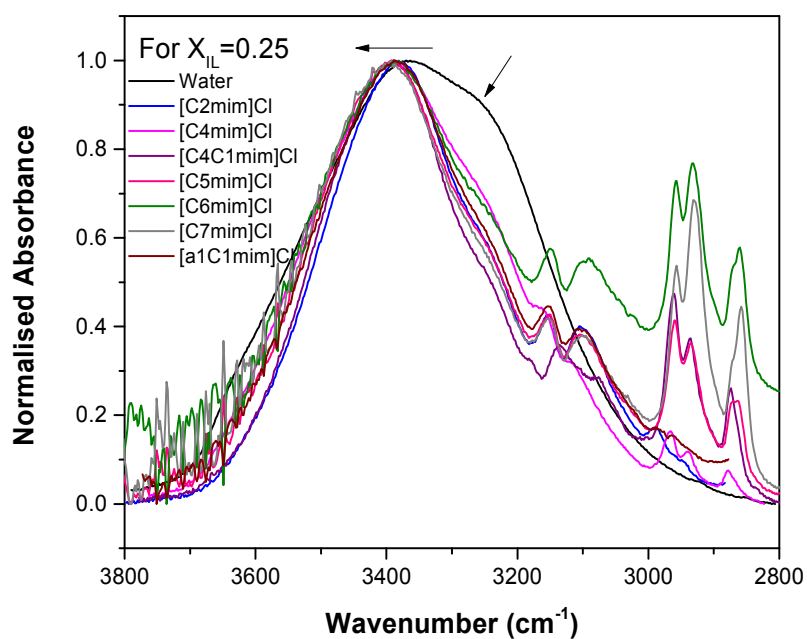
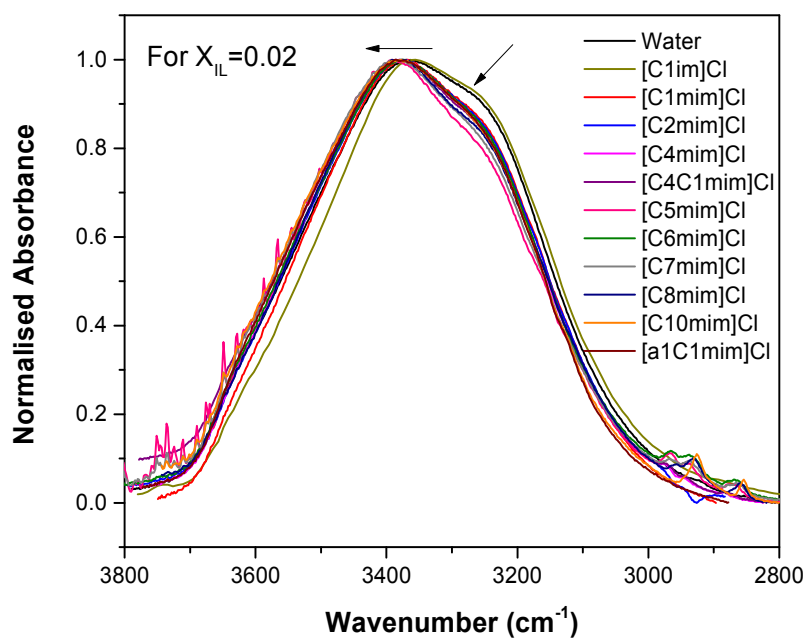


Figure S4. (a) Estimated total excess enthalpies; (b) Estimated excess Gibbs Free energy of binary mixture of ionic liquids and water at 298.2 K predicted by COSMO-RS. [C₁mim]Cl (---), [C₁mim]Cl (.....), [C₂mim]Cl (— · · —), [C₄mim]Cl (—), [C₄C₁mim]Cl (---), [C₅mim]Cl (—□—□—), [C₆mim]Cl (— · —), [C₇mim]Cl (+ +), [C₈mim]Cl (— —), [C₁₀mim]Cl (—○—) and [a1C₁mim]Cl (— · —).



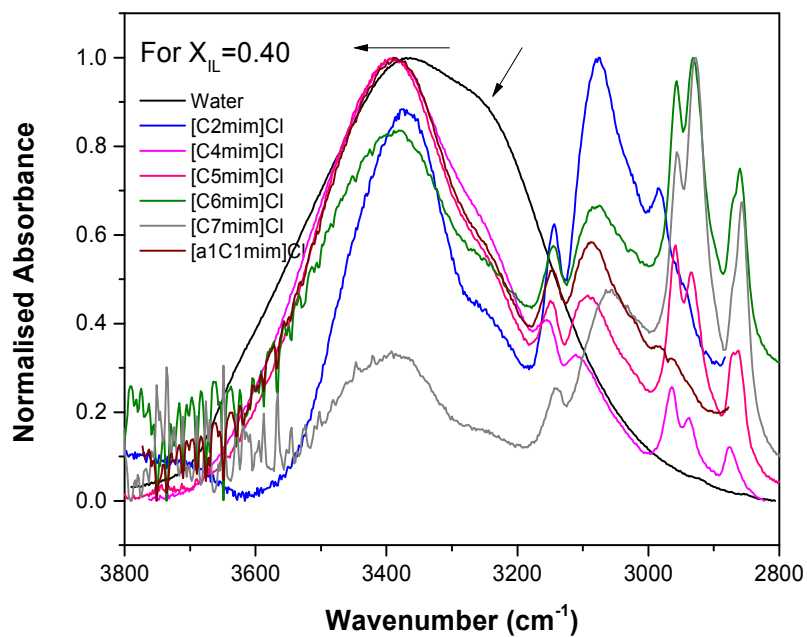
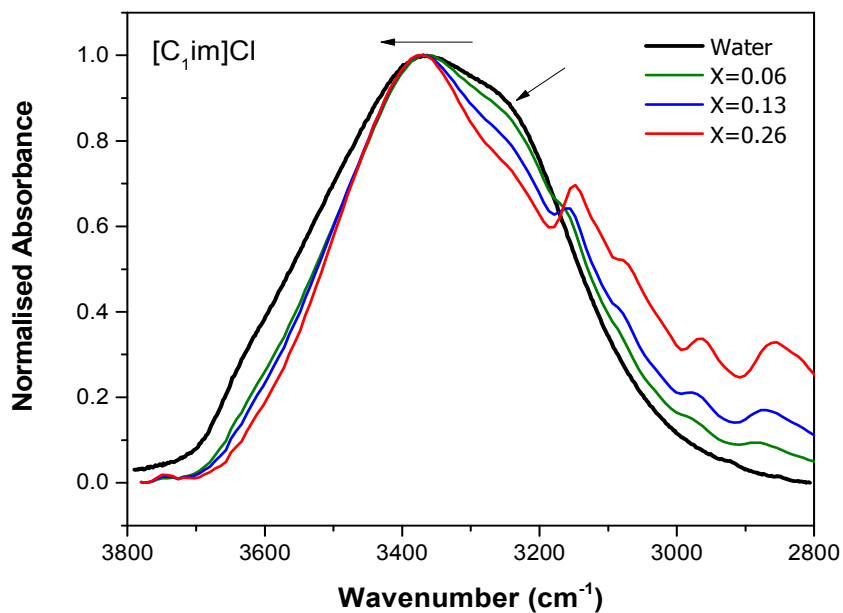
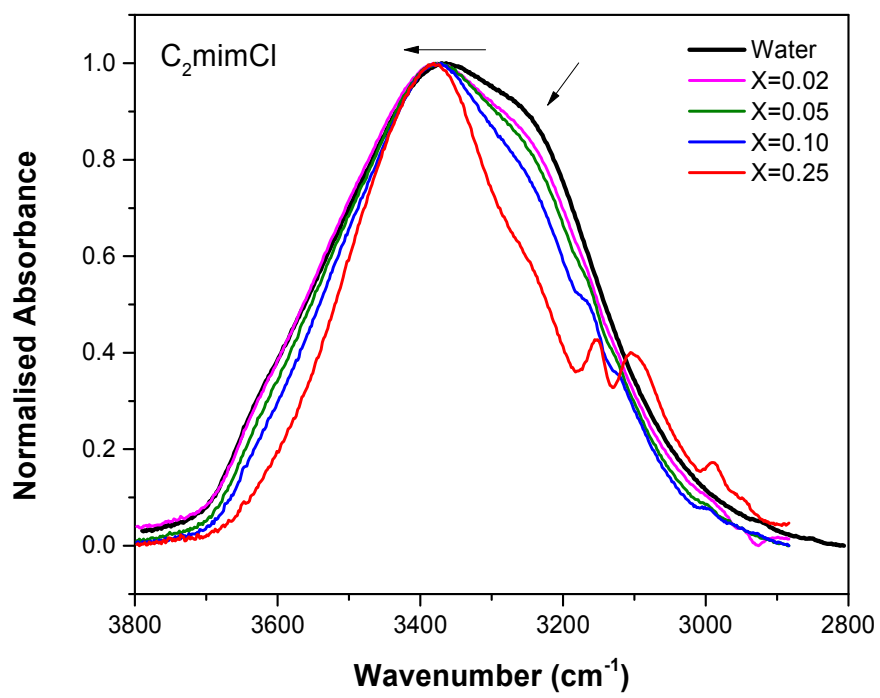
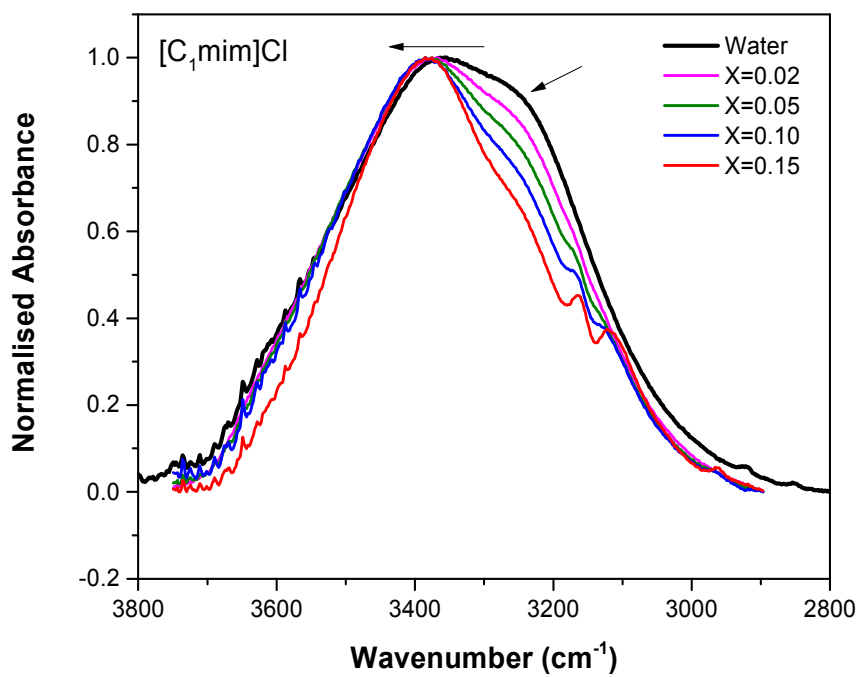
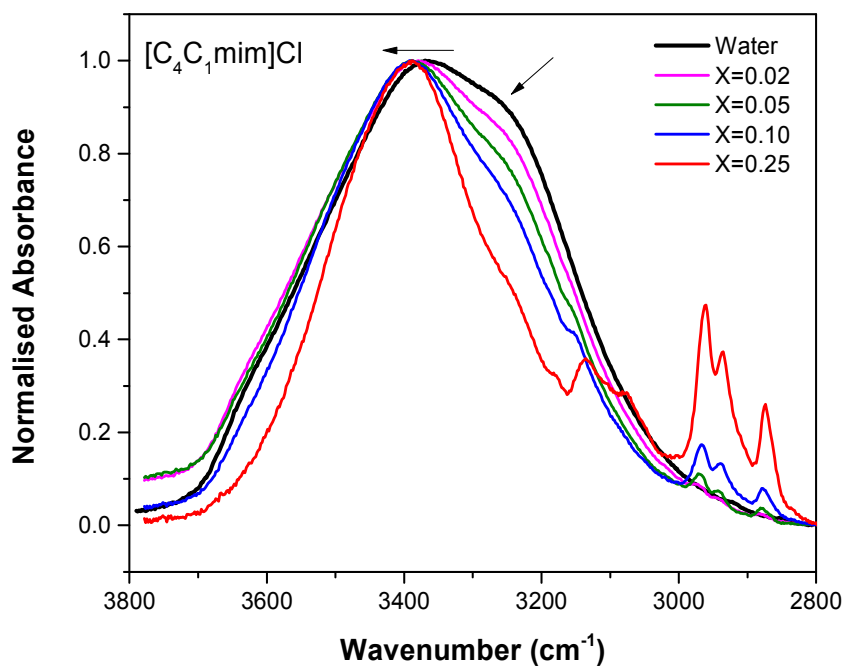
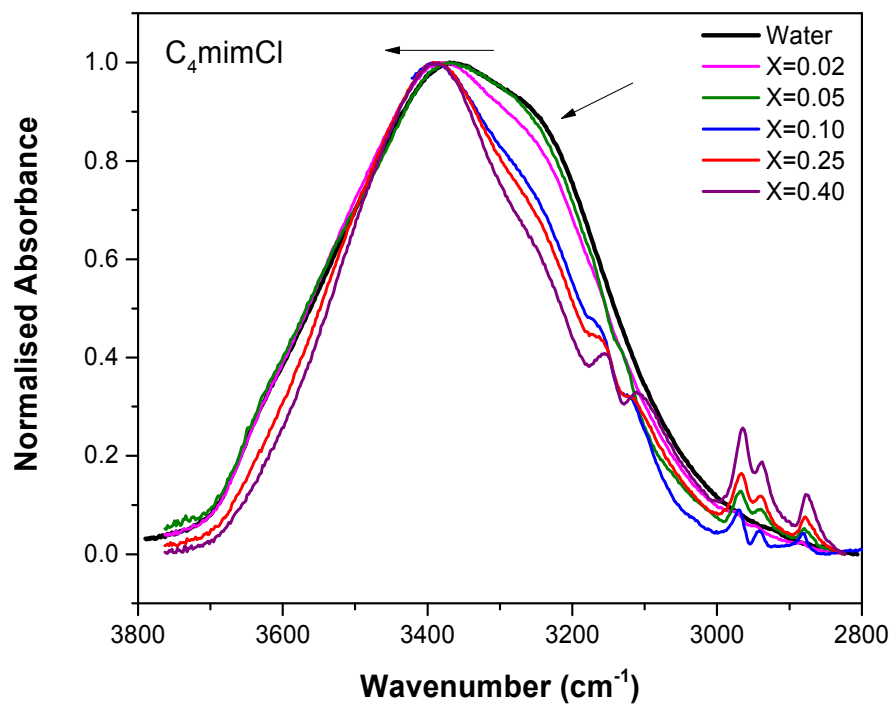
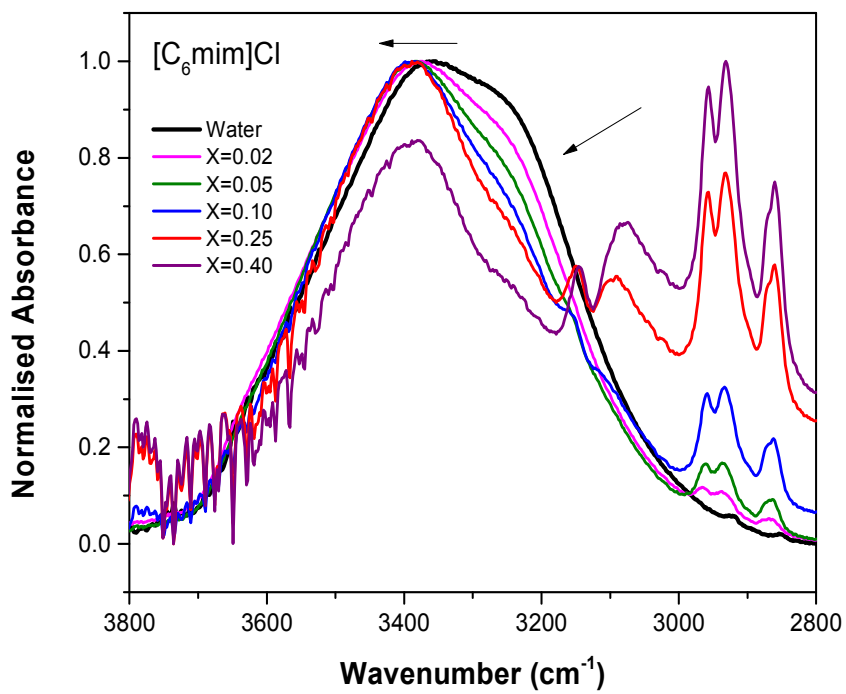
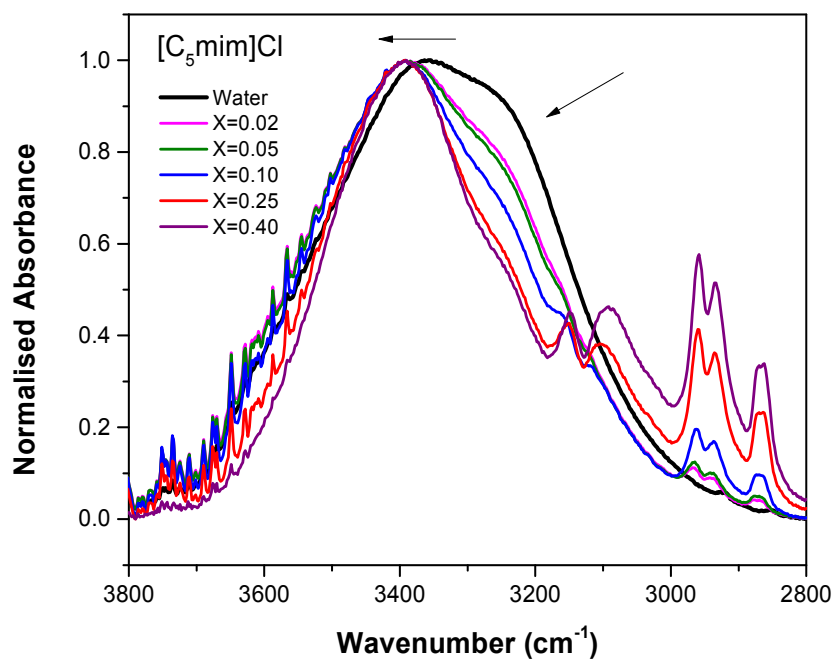


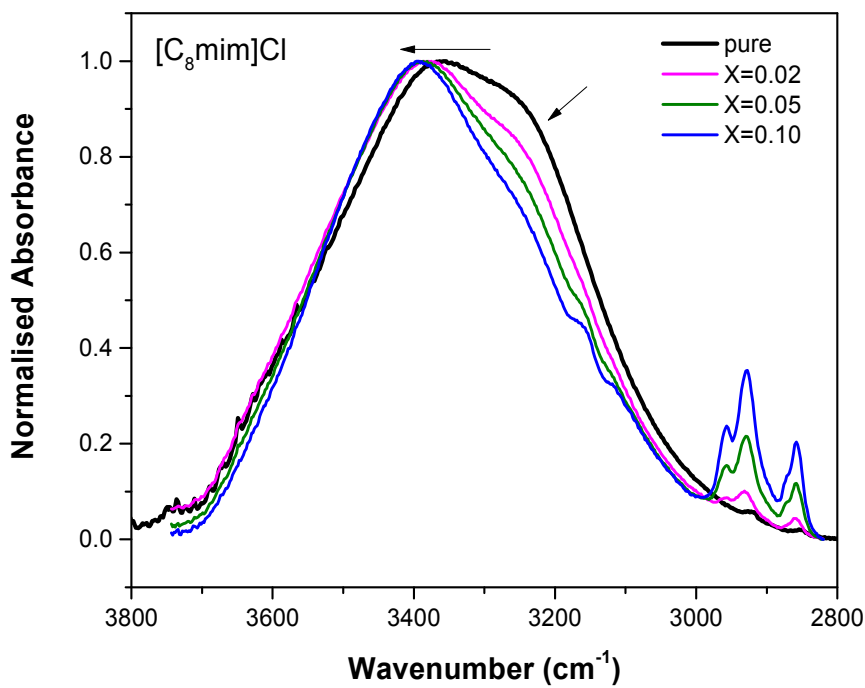
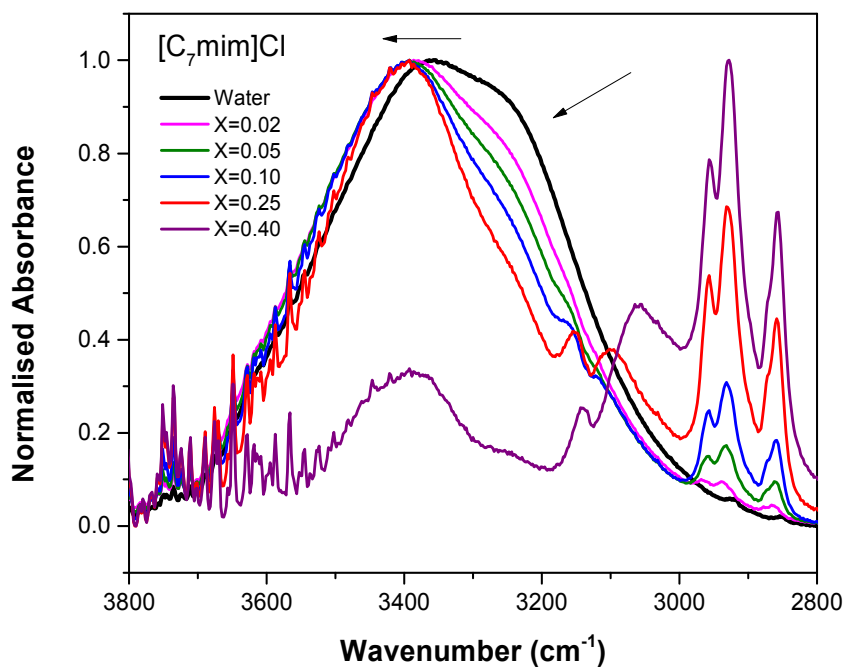
Figure S5. FTIR normalized absorbance spectra of water in the OH stretch regions in the range 2800–3800 cm^{-1} at fixed concentrations of ILs for the various studied water-ILs mixtures.











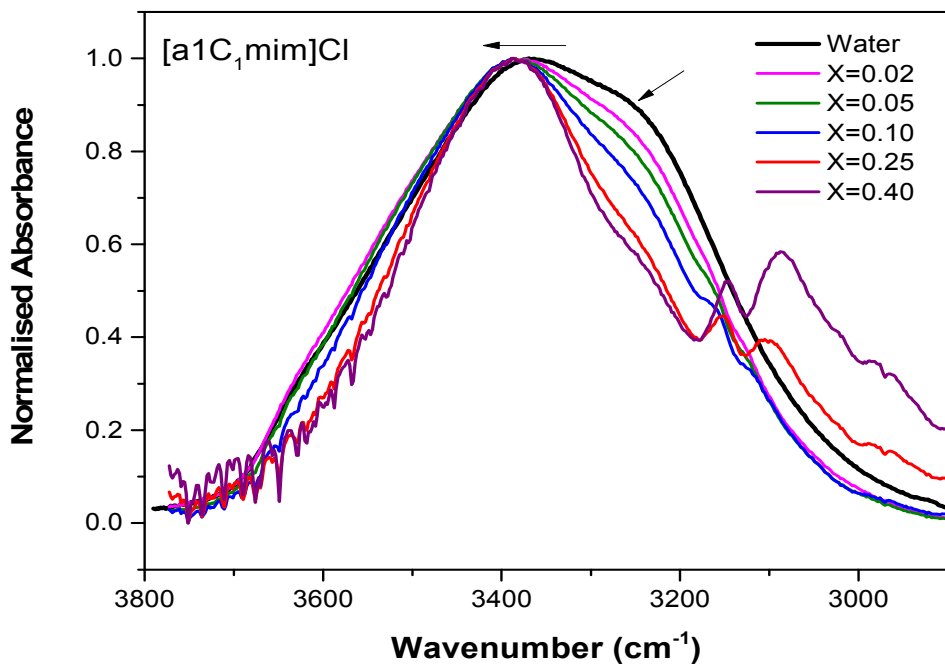
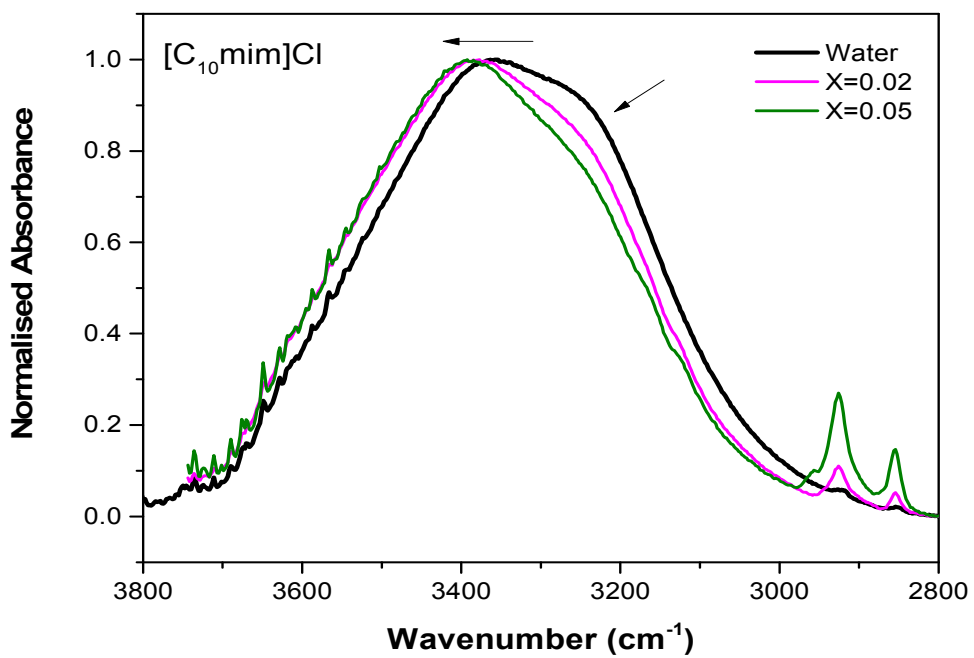


Figure S6. FTIR normalized absorbance spectra of water in the OH stretch region in the range 2800–3800 cm^{-1} for various studied water-ILs mixtures at different water ($x_{\text{H}_2\text{O}}=0.02, 0.05, 0.10, 0.25, 0.40$) mole fractions.

References

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