Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Dissolved chloride markedly changes the nanostructure of the protic ionic liquids propylammonium and ethanolammonium nitrate - Supporting Information

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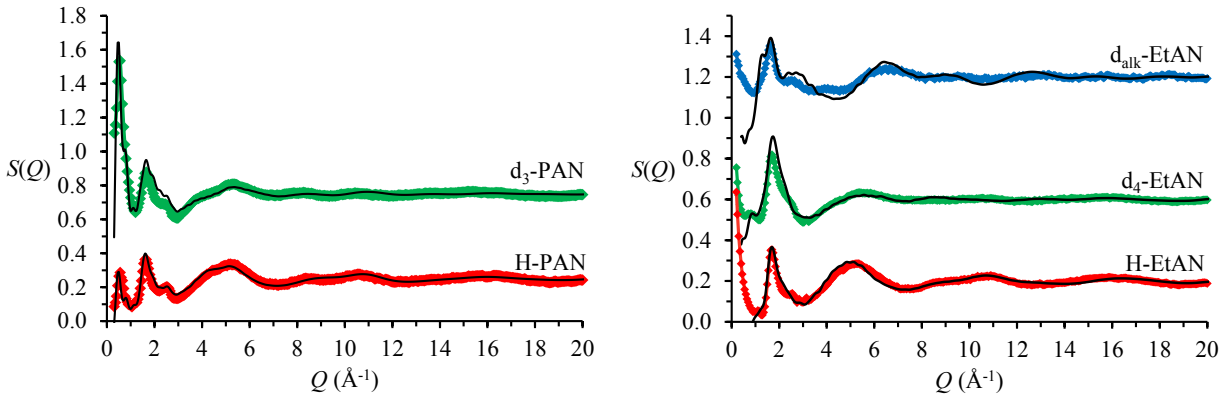

Figure S1. Measured (coloured diamonds) and EPSR fits (black lines) for pure propylammonium nitrate, PAN, (left) and pure ethanolammonium nitrate, EtAN, (right).

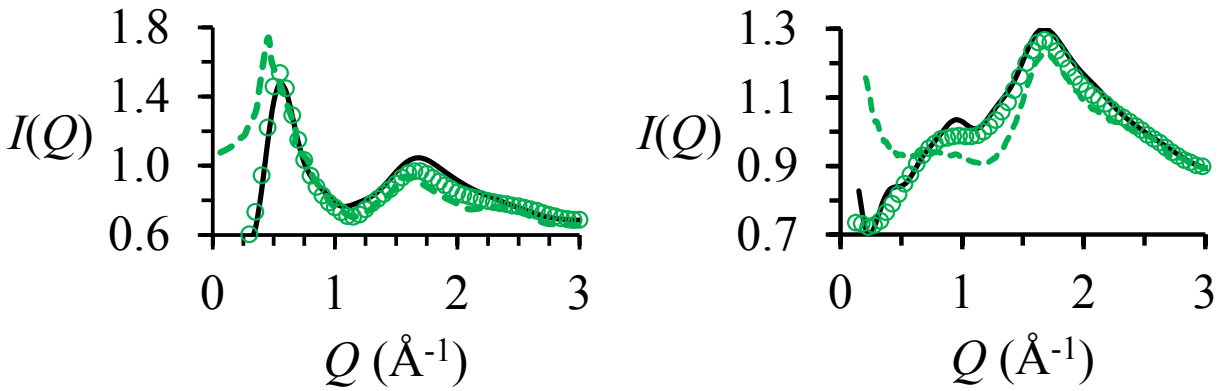

Figure S2. Expanded view of the low$Q$ region (0 – 3 Å) for the d_3-PAN:PACl contrast (left) and d_4-EtAN:EtACl contrast (right). Open circles give the measured diffraction data, Solid lines give the EPSR fits and dashed lines give the diffraction data for the respective pure ILs.

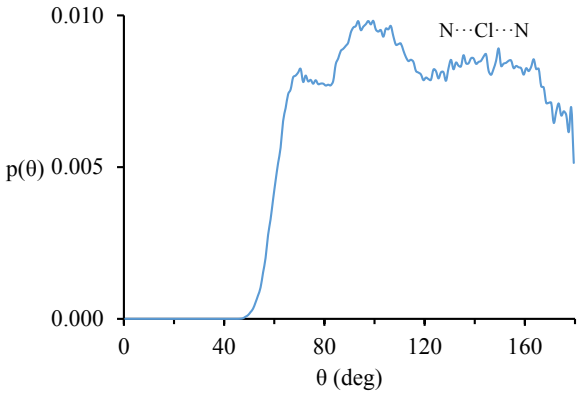

Figure S3. Normalized angle probability distribution (p(θ)) for N···Cl···N triplets. The separation between N and Cl atoms were constrained to only consider atoms within distances closer than the first local minimum in the corresponding N···Cl $g_{ij}(r)$ data.

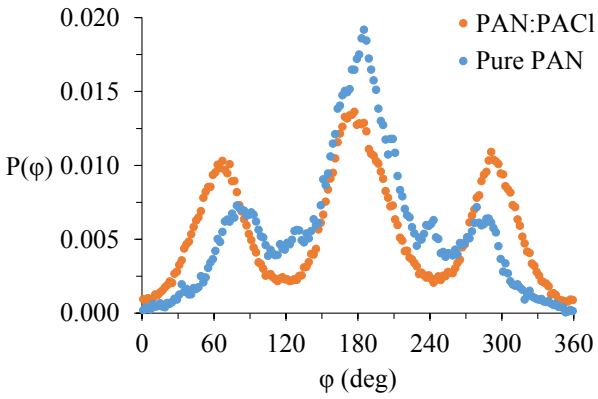

Figure S4. Dihedral angle distributions for the propylammonium cation (considering rotation about the C_E–C_P bond) for cations in a 15 mol% PAN:PACl mixture (blue data) and pure PAN (red data)

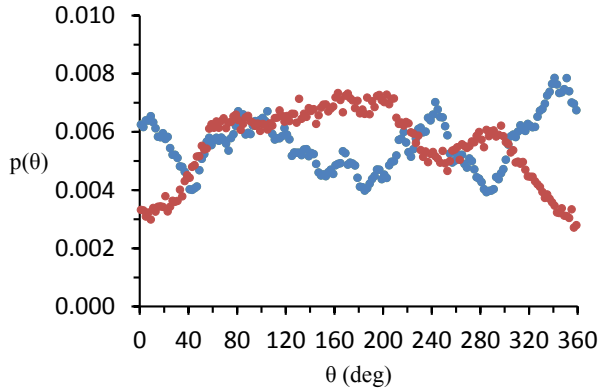

Figure S5. Dihedral angle distributions for the ethanolammonium cation (considering rotation about the C_1–C_2 bond) for cations in a 15 mol% EtAN:EtACl mixture (blue data) and pure EtAN (red data)

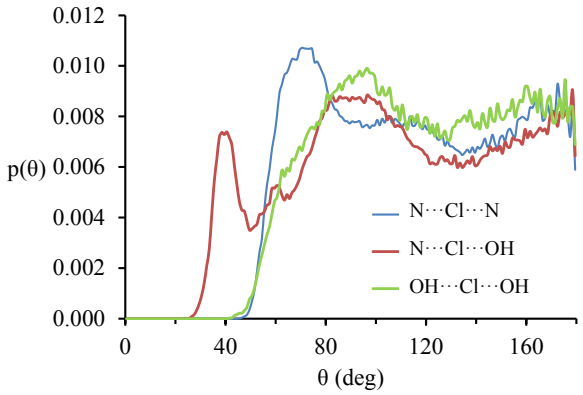

Figure S6. Normalized angle probability distribution (p(θ)) for atom cation-chloride-cation atom triplets involving the cation hydroxyl (OH) and ammonium (N) groups. The atom-atom separations were constrained to only consider atoms within distances lower than the first local minima in the corresponding $g_{ij}(r)$ data.

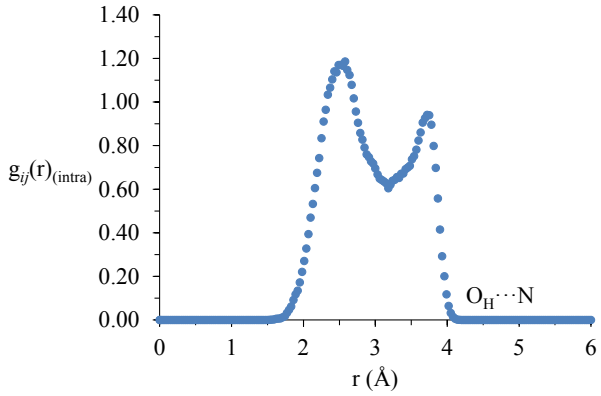

Figure S7. Intramolecular $g_{ij}(r)$ function for the hydroxyl O atom and ammonium N atom correlation for ethanolammonium cations in a 15 mol% EtACl in EtAN mixture.