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

Electronic Supporting Information

The effect of hydration on the stability of Ionic Liquid Crystals: MD simulations of $[C_{14}C_1im]Cl$ and $[C_{14}C_1im]Cl{\cdot}H_2O$

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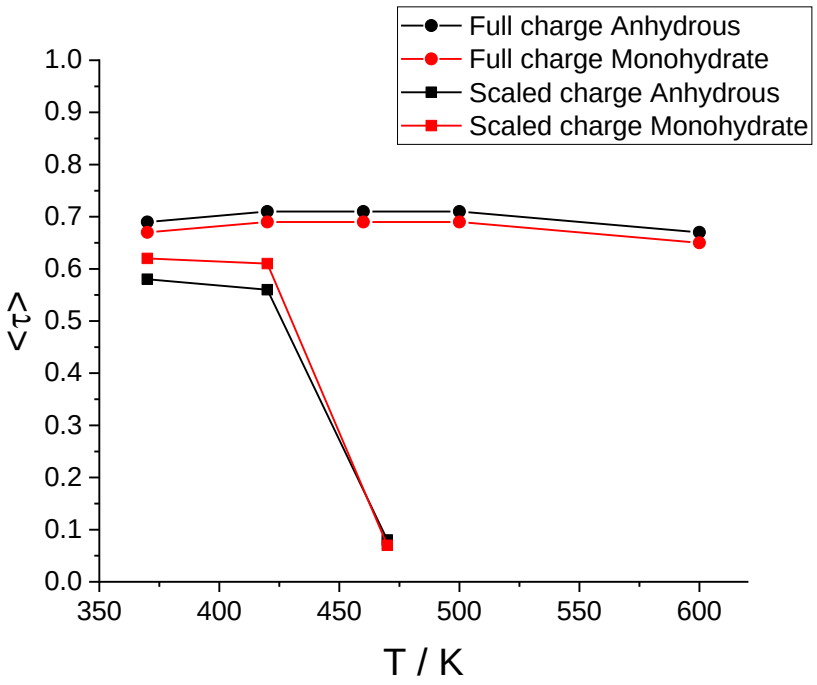

Figure S1. Translational order parameter, <τ> as a function of the temperature for the anhydrous and monohydrate box using the two versions of the FF, full-charge and scaled by a factor of 0.80. The translational order parameter is calculated as $\langle\tau\rangle = |\langle exp(2i\pi z/d)\rangle|$, following Bates&Luckhurst *J. Chem. Phys.* **1999**, 110, 7087,where *d* is the layer thickness and *z* is the position of a selected particle species showing a density modulation along *z* (that is along the director). Here we arbitrarily selected the chloride anion as the reference particle. As for all other average quantities discussed in this work, <τ> is calculated over the last 40 ns of production run, which follow the 60 ns of equilibration, except for the two points at 470 K using the scaled FF, where it is calculated over the last 10 ns after the melting.

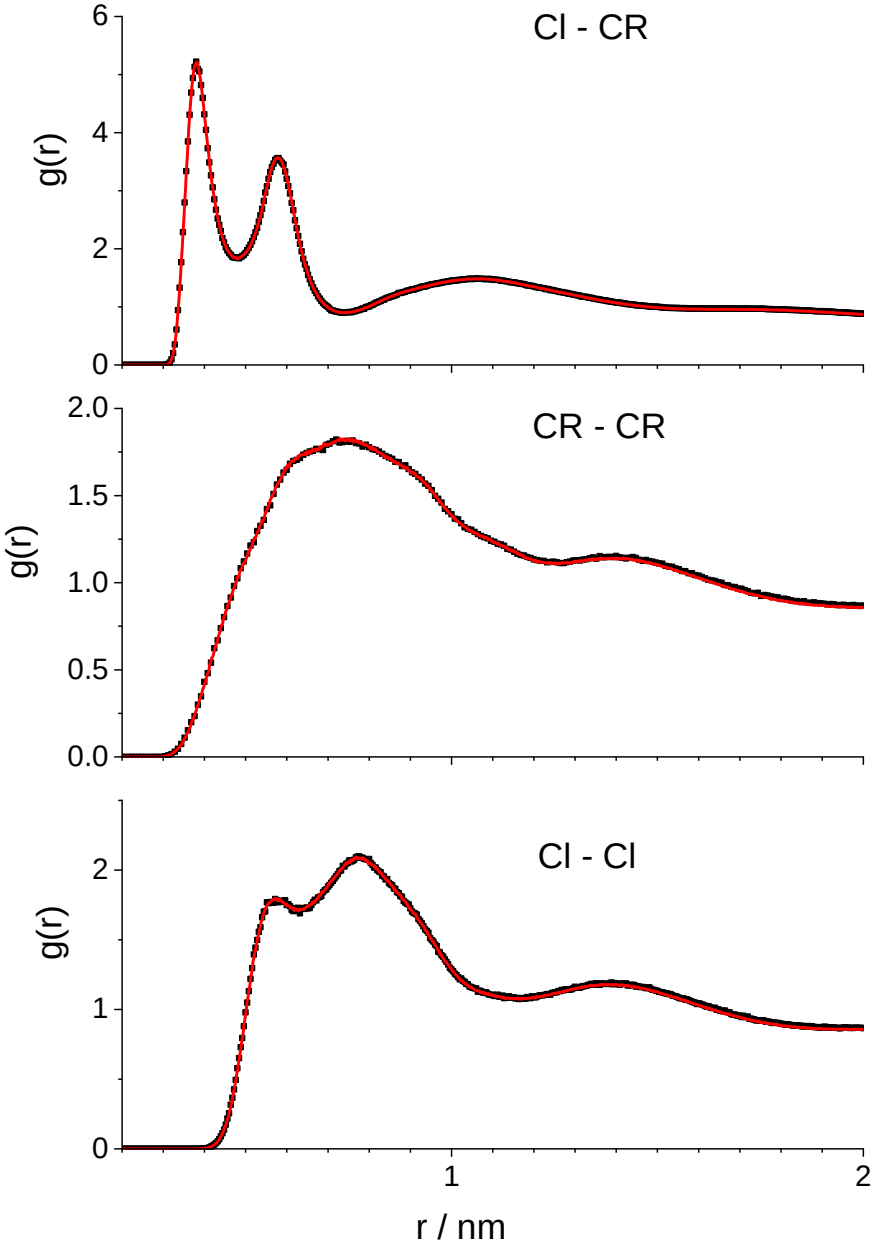

Figure S2. Comparison of the RDF of Figure 5 of the main text for the monohydrate sample at 420 K (scaled charge FF) with different values of the cut-off for the van der Waals interactions. (Solid red line): cut-off of 10 Å. (Black points): cut-off of 14 Å. Simulations with cut-off of 14 Å were started from the last configuration of the run with a cut-off of 10 Å; the system was simulated for 50 ns and the last 25 ns used to calculate the properties.

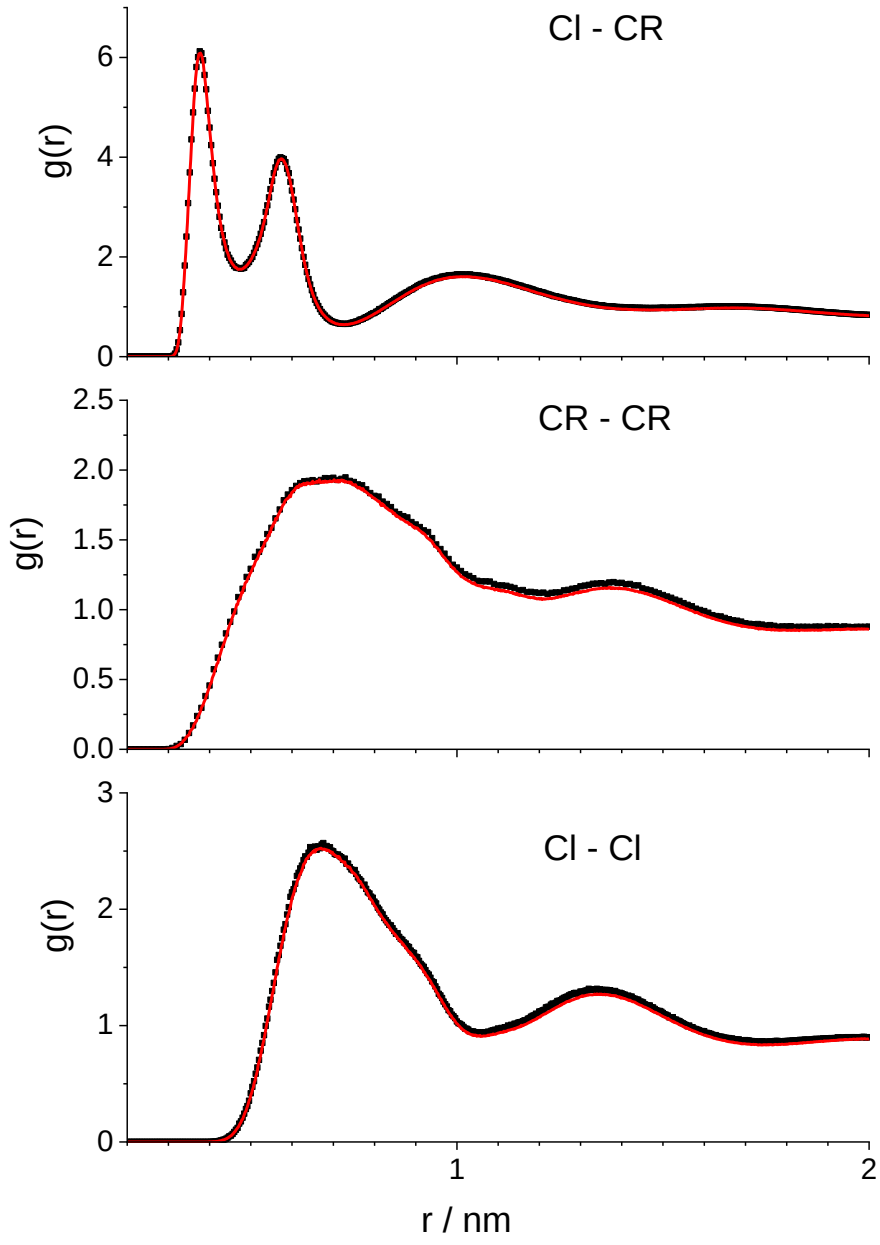

Figure S3. Comparison of the RDF of Figure 5 of the main text for the anhydrous sample at 420 K (scaled charge FF) with different values of the cut-off for the van der Waals interactions. (Solid red line): cut-off of 10 Å. (Black points): cut-off of 14 Å. Simulations with cut-off of 14 Å were started from the last configuration of the run with a cut-off of 10 Å; the system was simulated for 50 ns and the last 25 ns used to calculate the properties.

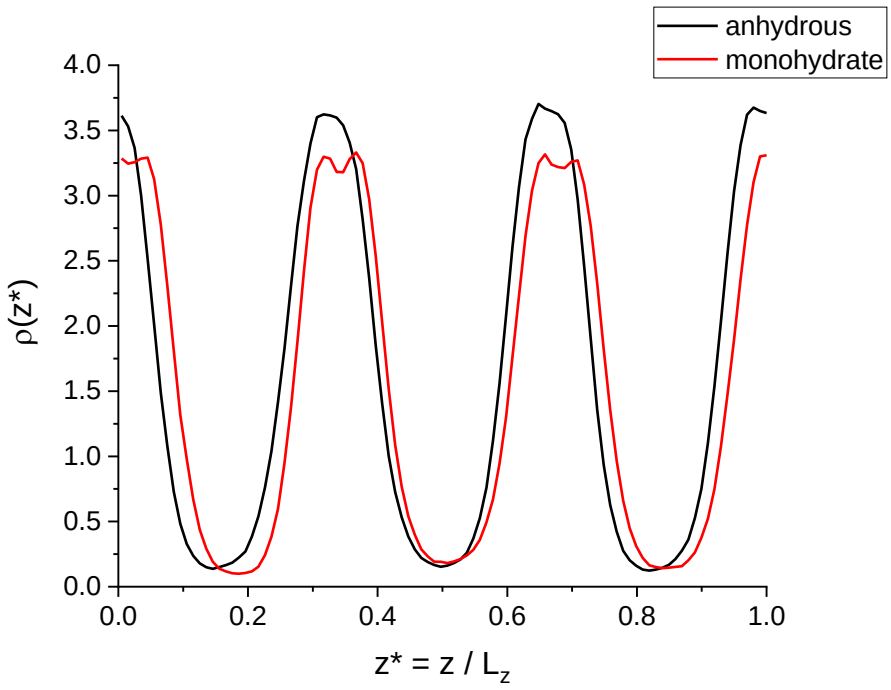

Figure S4. Comparison of the density profiles of the cation head for the (black) anhydrous sample and (red) monohydrate sample at 420 K (scaled charge FF) obtained with a values of the cut-off for the van der Waals interactions of 14 Å. Simulations with cut-off of 14 Å were started from the last configuration of the run with a cut-off of 10 Å; the systems were simulated for 50 ns and the last 25 ns used to calculate the properties.

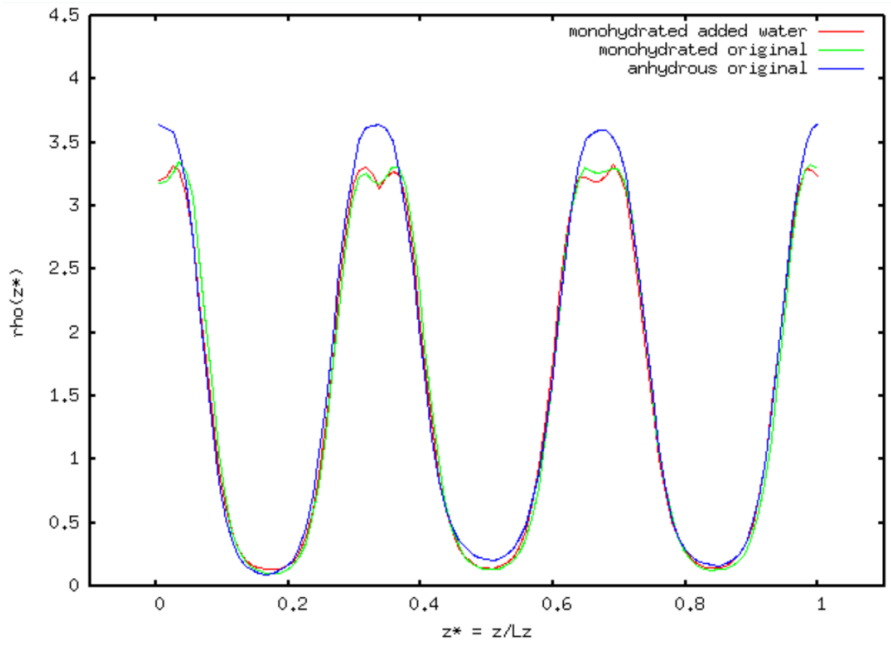

Figure S5: number density of the imidazolium carbon CR (see Figure 3) along the director of the phase, z axis at 420 K (scaled charge FF). The position is scaled with respect to the length of the box, L_z, to better compare the monohydrated and anhydrous boxes. The red line is the result obtained from the monohydrated box, which is built from the anhydrous box by adding a 1:1 amount of water molecules. It overlaps with the original monohydrated box (green line) and it is markedly different from the anhydrous box (blue line) from which it originates.

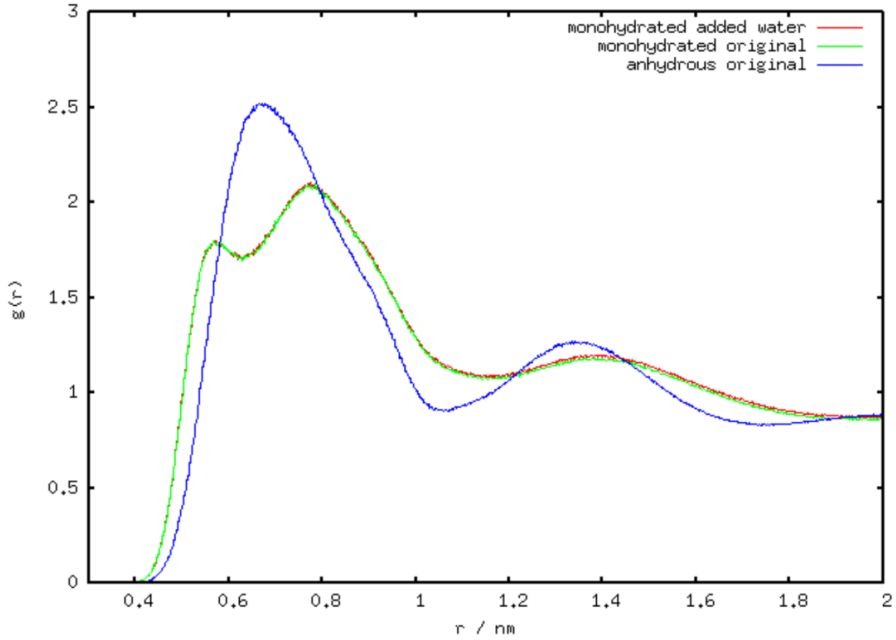

Figure S6: RDF of the distance between two chlorine atoms at 420 K (scaled charge FF). The red line is the result obtained from the monohydrated box, which is built from the anhydrous box by adding a 1:1 amount of water molecules. It overlaps with the original monohydrated box (green line) and it is markedly different from the anhydrous box (blue line) from which it originates.

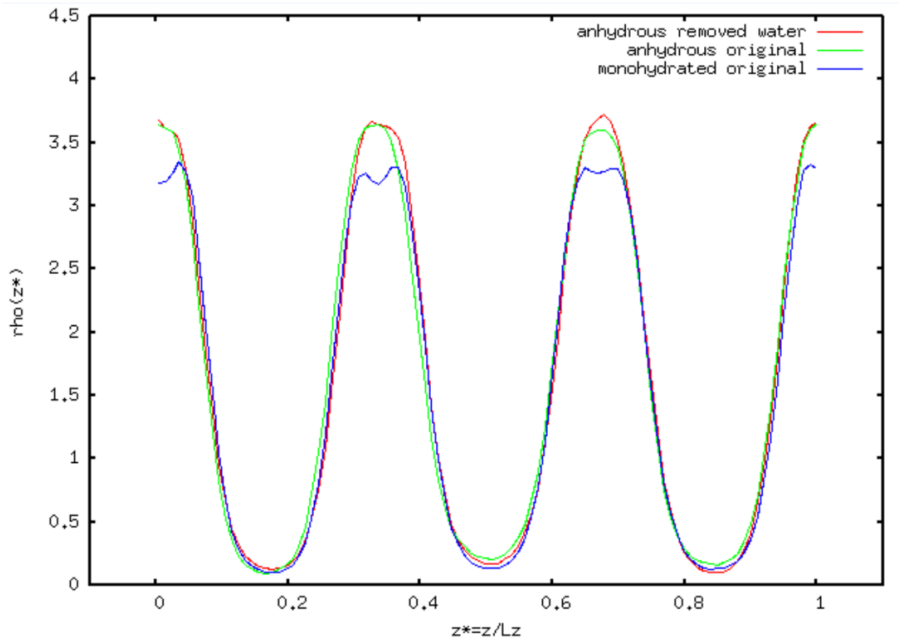

Figure S7: number density of the imidazolium carbon CR (see Figure 3) along the director of the phase, z axis at 420 K (scaled charge FF). The position is scaled with respect to the length of the box, L_z, to better compare the monohydrated and anhydrous boxes. The red line is the result obtained from the anhydrous box, which is built from the monohydrated box by removing all water molecules. It overlaps with the original anhydrous box (green line) and it is markedly different from the monohydrated box (blue line) from which it originates.

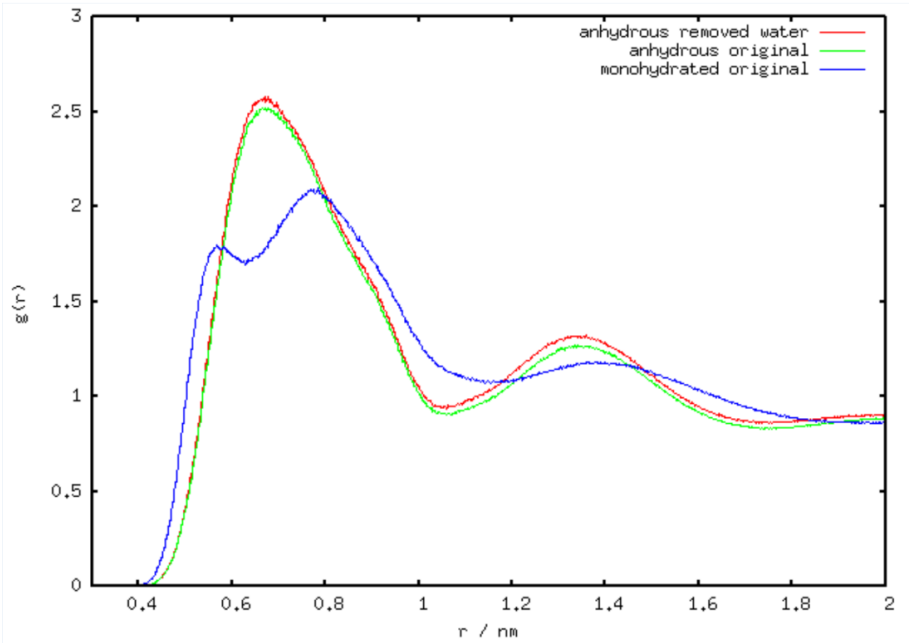

Figure S8: RDF of the distance between two chlorine atoms at 420 K (scaled charge FF). The red line is the result obtained from the monohydrated box, which is built from the anhydrous box by adding a 1:1 amount of water molecules. The red line is the result obtained from the anhydrous box, which is built from the monohydrated box by removing all water molecules. It overlaps with the original anhydrous box (green line) and it is markedly different from the monohydrated box (blue line) from which it originates.