Effect of water on the thermo-physical properties of Reline: An

experimental and molecular simulation based approach

Supplementary Material

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Figure S1: Number of hydrogen bonds in Reline at 310 K for a 1 ns run (x axis showing time in ps). In comparison with the values at 298 K (Figure 3) the change is marginal. Likewise, the analysis remains the same at the experimental temperature of 303 K.



Figure S2: Coordination number evaluated based on the carbon atom of urea. First coordination shell in pure urea has approximately 8 molecules, whereas in Reline the number is around 4. The shell diameter is almost the same in Reline as of pure urea. The results are shown between 2 to 8 Angstrom to represent the data clearly. We also note herein that the rdf shown in figure 3 is based on all atom calculations, whereas coordination number is calculated based on carbon atom (so that the number provides average number of urea molecules in the shell and not the number of atoms).



Figure S3: All atom rdf between urea-urea at 30% water. Distance is in Angstrom.



Figure S4: Coordination number with respect to the anion vs. distance for 10% water system. The results indicate the first anion prefers water more than urea. Coordination number is calculated based on carbon atom of urea and oxygen atom of water. Distance is in Angstrom.



Figure S5: Urea-anion rdf at 30% and 50% aqueous Reline solution (extension to figure 7b), indicating a significant loss in urea-anion interactions beyond 25% of water.

	Urea	Deviation	Choline	deviation	Chloride	Deviation	Water	deviation
PURE								
COMPONENTS	0.0546	0.0023	0.002541	0.0004351	0.001308	0.0004338	2.6127	0.022
Reline	0.0004881	0.00006339	0.001412	0.0004175	0.0003479	0.00004908		
1% Water	0.004612	0.0007552	0.004763	0.000413	0.00292	0.0001578	0.0227	0.0001
10% Water	0.097	0.0095	0.0867	0.006	0.0852	0.0087	0.1104	0.0323
30% Water	0.0602	0.0029	0.041	0.0025	0.0799	0.0064	0.2096	0.0032
50% Water	0.3039	0.0004	0.1866	0.0153	0.3322	0.0159	0.7152	0.02
70% Water	0.7736	0.0118	0.5056	0.0432	0.754	0.0658	1.4932	0.0074
90% Water	1.3618	0.0293	0.8741	0.0195	1.2463	0.0326	2.2745	0.005

Table S1: Diffusion coefficient with standard deviation (in support of figure 9). All values in 10^{-9} m²/s

Water fraction (wt %)	Water-Urea	Water-Anion
1	30	35
10	270	350
30	790	850
50	1250	1070
70	1570	1210
90	1870	1310

Table S2: Increasing number of hydrogen bonds between water-urea and water-anion in Reline revealing hydration of urea and the anion in the presence of water.