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

Structuring Effect of the Alkyl Domains on the Polar Network of Ionic Liquids Mixtures: a Molecular Dynamics Study

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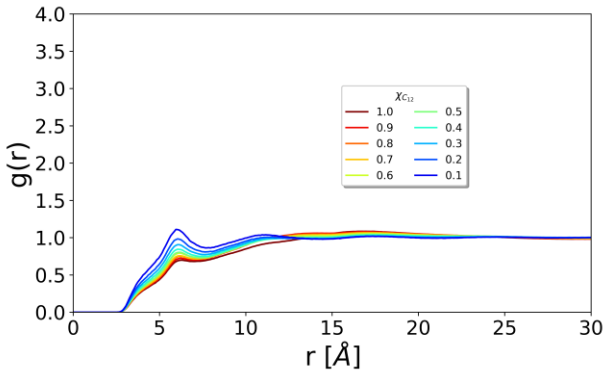
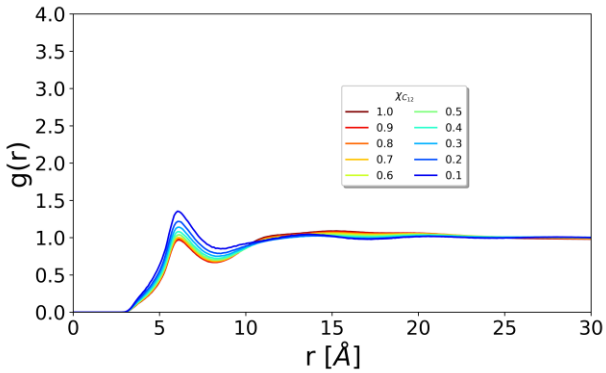
Supporting Information



a)



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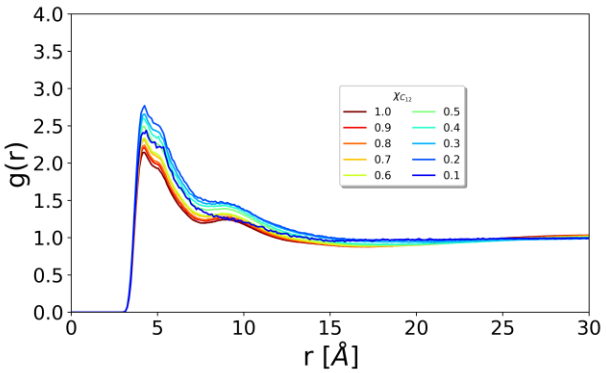
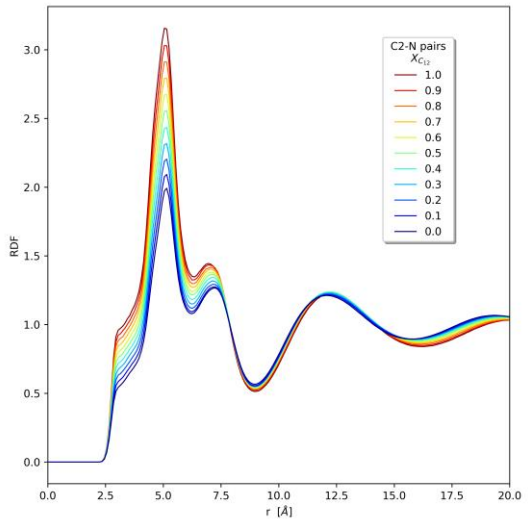


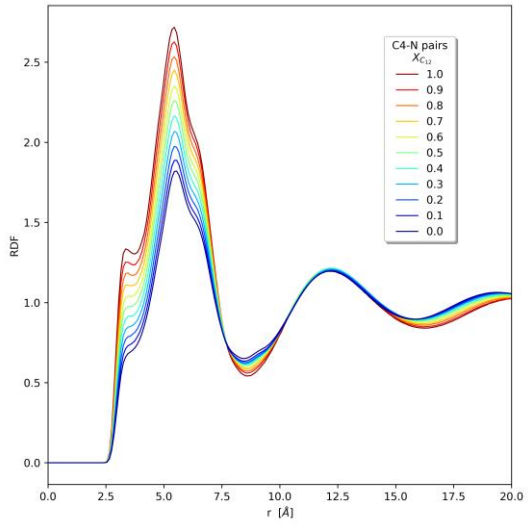
c9

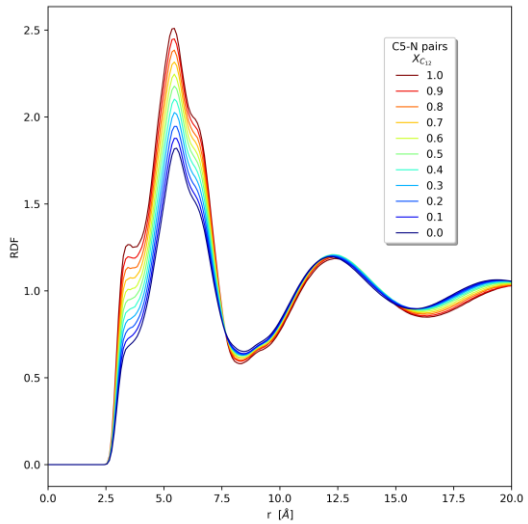
Figure S1. A) RDF of the C_{12}´-N distance between [$C_{12}C_1$im] alkyl chain and anions; b) RDF of the C_{12}´-C_2 distance between [$C_{12}C_1$im] alkyl chain and imidazolium heads (irrespective of being [$C_{12}C_1$im] or [C_1C_1im]); c) RDF of the C_{12}´-C_{12}´ distance between two alkyl chains. (see Figure 1 of the main text for atom numbering).

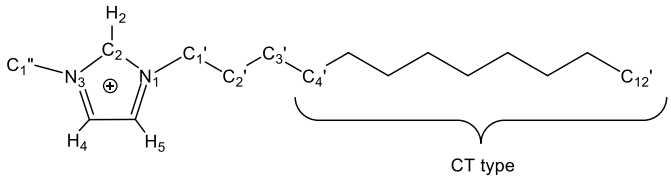
Table S1. Peak position of the RDF in Figure 3a) of the main text. The RDF *x*-axis resolution (that is the discretization of the distance) is 0.1 Å.

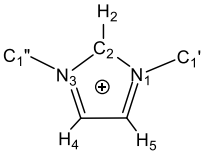
x_{C12}	Peak position (Å)
1.0	6.95 ± 0.05
0.9	6.95 ± 0.05
0.8	7.05 ± 0.05
0.7	7.05 ± 0.05
0.6	7.05 ± 0.05
0.5	7.05 ± 0.05
0.4	7.15 ± 0.05
0.3	7.15 ± 0.05
0.2	7.15 ± 0.05
0.1	7.25 ± 0.05
0.0	7.25 ± 0.05











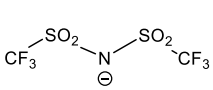


Figure S2. RDF of the distance between the anion's nitrogen and the three carbons of the cationic ring. (Top) N-C2; (middle) N-C4; (bottom) N-C5, see scheme on the right for atom numbering.

Table S2. Diffusion coefficient ratios. C12 = [$C_{12}C_1$im] cation; C1 = [C_1C_1im] cation; Tf_2N = anion.

	D(C12)/D(C1)	D(C12)/D(Tf_2N)	D(C1)/D(Tf_2N)
1.0		0.77	
0.9	0.56	0.71	0.79
0.8	0.54	0.75	0.71
0.7	0.62	0.77	0.80
0.6	0.55	0.69	0.82
0.5	0.50	0.64	0.78
0.4	0.53	0.75	0.71
0.3	0.53	0.76	0.69
0.2	0.52	0.74	0.70
0.1	0.51	0.78	0.65
0.0			0.64