

# Effect of Alkyl Chain Length on the Structure and Thermodynamics of Protic-Aprotic Ionic Liquid Mixtures: A Molecular Dynamics Study

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Supporting information

Table 1: Experimental conductivities for [EMIM][BF<sub>4</sub>]+EAN mixtures

$x_{EAN}$	$\sigma/\text{mS}\cdot\text{cm}^{-1}$
0	15.85
0.033	16.31
0.066	16.55
0.1	16.62
0.1333	16.48
0.1666	16.38
0.2	16.23
0.25	15.82
0.3	14.75
0.4	14.6
0.5	14.88
0.6	15.64
0.7	16.69
0.8	18.58
0.9	21.5
1	24.8

Table 2: Experimental conductivities for [EMIM][BF<sub>4</sub>]+PAN mixtures

$x_{PAN}$	$\sigma/\text{mS}\cdot\text{cm}^{-1}$
0	15.85
0.1	15.58
0.2	14.39
0.3	13.31
0.4	12
0.5	11.09
0.6	10.21
0.7	9.74
0.8	9.67
0.9	9.81
1	10.32

Table 3: Experimental conductivities for [EMIM][BF<sub>4</sub>]+BAN mixtures

$x_{BAN}$	$\sigma/\text{mS}\cdot\text{cm}^{-1}$
0	15.85
0.1	15.18
0.2	12.79
0.3	10.99
0.4	9.28
0.5	7.78
0.6	6.96
0.7	5.78
0.8	5.25
0.9	5.11
1	5.35

Table 4: Experimental conductivities for [BMIM][BF<sub>4</sub>]+EAN mixtures

$x_{EAN}$	$\sigma/\text{mS}\cdot\text{cm}^{-1}$
0.0000	4.41
0.0348	4.05
0.0673	4.12
0.1015	4.22
0.1035	4.09
0.2021	4.54
0.2957	4.96
0.3975	4.7
0.5339	5.52
0.6124	6.01
0.7114	6.65
0.8089	7.77
0.9056	12.6
1	24.8

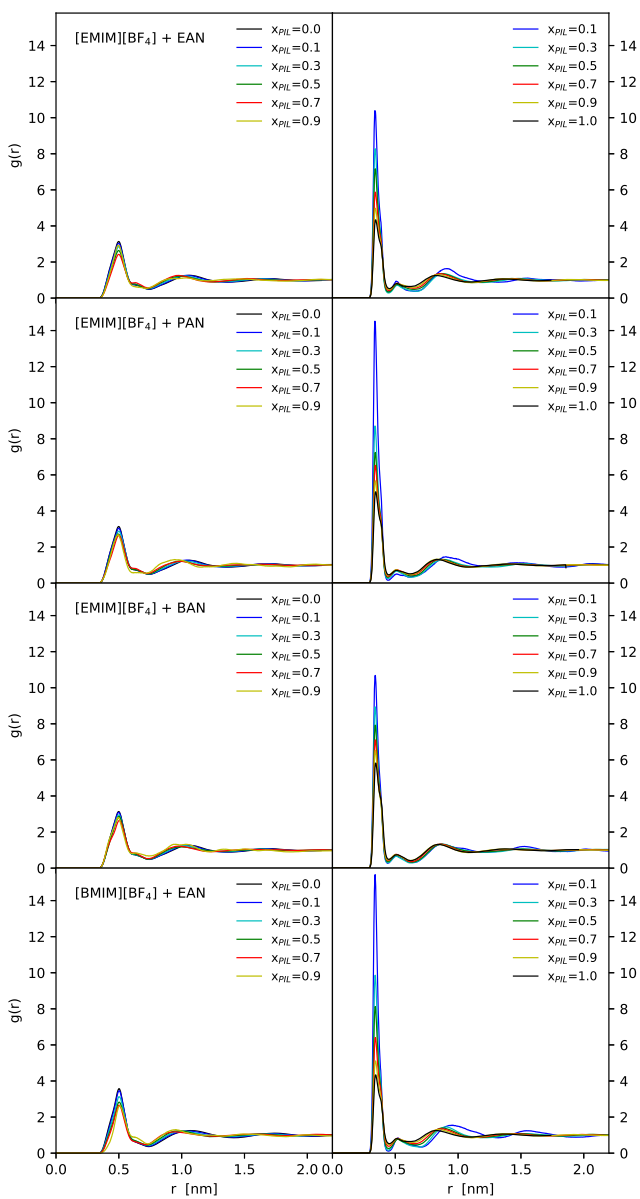


Figure 1:  $[\text{EMIM}]^+ / [\text{BMIM}]^+ - [\text{BF}_4]^-$  (left) and EAN/PAN/BAN -  $[\text{NO}_3]^-$  (right) RDFs for selected concentrations in the systems studied.

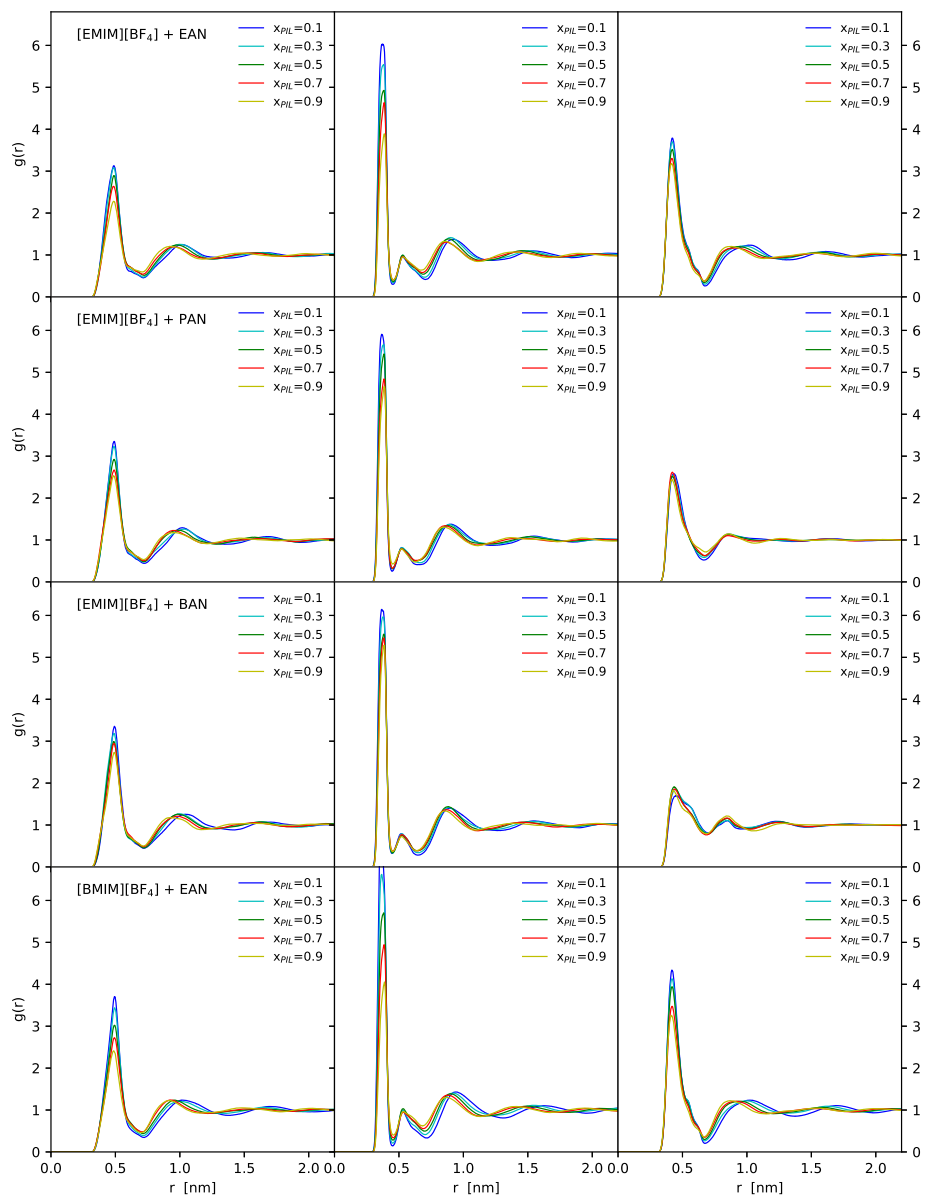


Figure 2: [EMIM]<sup>+</sup>/[BMIM]<sup>+</sup> - [NO<sub>3</sub>]<sup>-</sup> (left) and EAN/PAN/BAN - [BF<sub>4</sub>]<sup>-</sup> (polar head, middle; and terminal carbon atom, right) RDFs for selected concentrations in the systems studied.