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

Highlighting the difference in nanostructure between domain-forming and domainless protic ionic liquids

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Supplementary Table. Parameters of the ionic liquids models used in MD simulations.

Atom type	σ / nm	ε / kJ·mol^{-1}	q (full charges)	q (scaled charges)
HC	0.250	0.125520	0.060	0.048
HM	0.250	0.125520	0.030	0.024
CT	0.350	0.276144	–0.180	–0.144
			0.130 (MAN)	0.104 (MAN)
			0.110 (2MEAN)	0.088 (2MEAN)
C1	0.350	0.276144	0.190	0.152
			0.170 (PyrrN)	0.136 (PyrrN)
			0.190 (EOAN, 2MEAN)	0.152 (EOAN, 2MEAN)
C2	0.350	0.276144	–0.120	–0.096
			0.145 (EOAN)	0.116 (EOAN)
			0.140 (2MEAN)	0.112 (2MEAN)
C3	0.350	0.276144	–0.120	–0.096
NH	0.325	0.711280	–0.300	–0.24
			–0.200 (PyrrN)	–0.16 (PyrrN)
HN	0.250	0.125520	0.330	0.264
			0.310 (PyrrN)	0.248 (PyrrN)
OH	0.312	0.711280	–0.683	–0.5464
HO	0.000	0.000000	0.418	0.3344
OT	0.290	0.585760	–0.400	–0.32
NN	0.306	0.338000	0.950	0.76
ON	0.277	0.610000	–0.650	–0.52
S	0.356	1.046000	1.250	1.00008
O	0.296	0.878640	–0.658	–0.52672
OS	0.296	0.878640	–0.435	–0.34808
HS	0.000	0.000000	0.160	0.12816
NK	0.325	0.711280	–0.720	–0.576
CK	0.340	0.359800	0.440	0.352
SK	0.355	1.046000	–0.720	–0.576