Electronic Supporting Information for :

A Combined LX-NMR and Molecular Dynamics Investigation of the Bulk and Local Structure of Ionic Liquid Crystals

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(12) Table S2: $\Delta\nu_2$, T_{CD2}, D_{CD2} (J_{CD2} = 32 Hz) values extracted from the ^{2}H and ^{13}C-{^{1}H} NMR spectra of $[C_{12}C_1im][BF_4]$ tri-deuterated (d_3) imidazolium ring and corresponding values of S_{CD2} (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures.
(13) Table S3: $\Delta\nu_5$ values extracted from the ^{2}H NMR spectra of $[C_{12}C_1im][BF_4]$ tri-deuterated (d_3) imidazolium ring and corresponding S_{CD5} values (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures.
(14) Table S4: . $\Delta\nu_2$ value extracted from the ^{2}H NMR spectrum of $[C_{12}C_1im]Cl$ tri-deuterated (d_3) imidazolium ring and corresponding values of S_{CD2} (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures. Note that the sign of $\Delta\nu_2$ (then, of S_{CD2}) has been obtained only at the temperature of 305 K (T_{red} = 0.866); then, the same sign has been assumed for the other temperatures.

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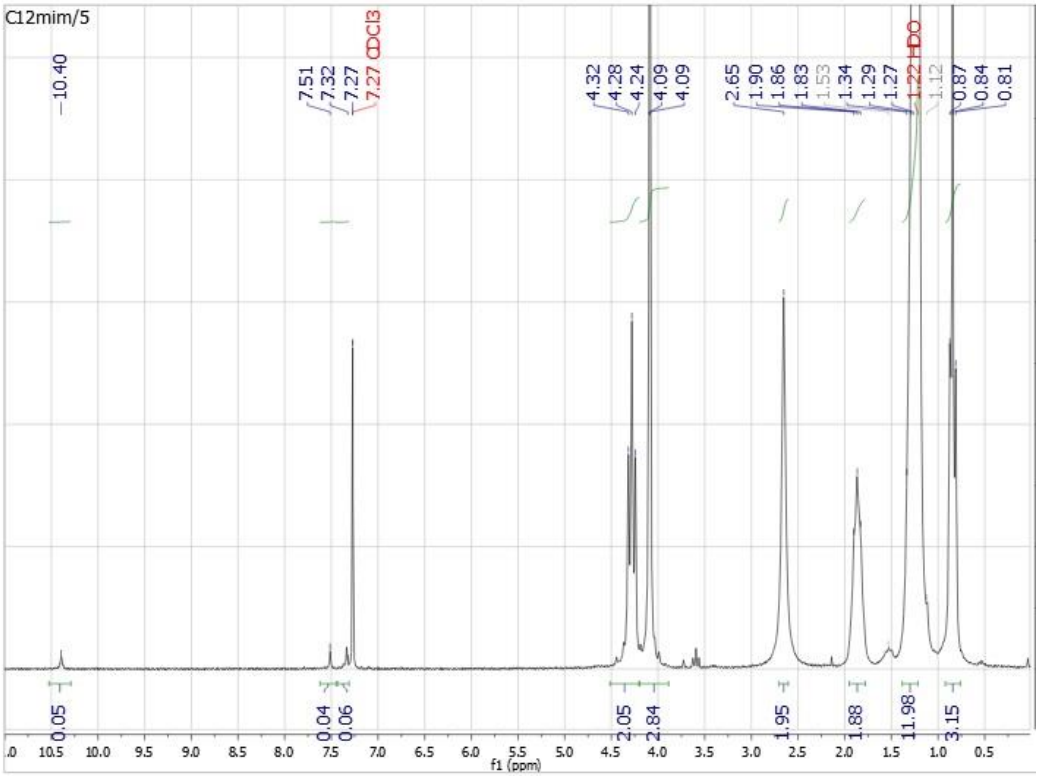

Figure S1: ^{1}H NMR spectrum of $[C_{12}C_1im]Cl$ after the deuteration reaction.

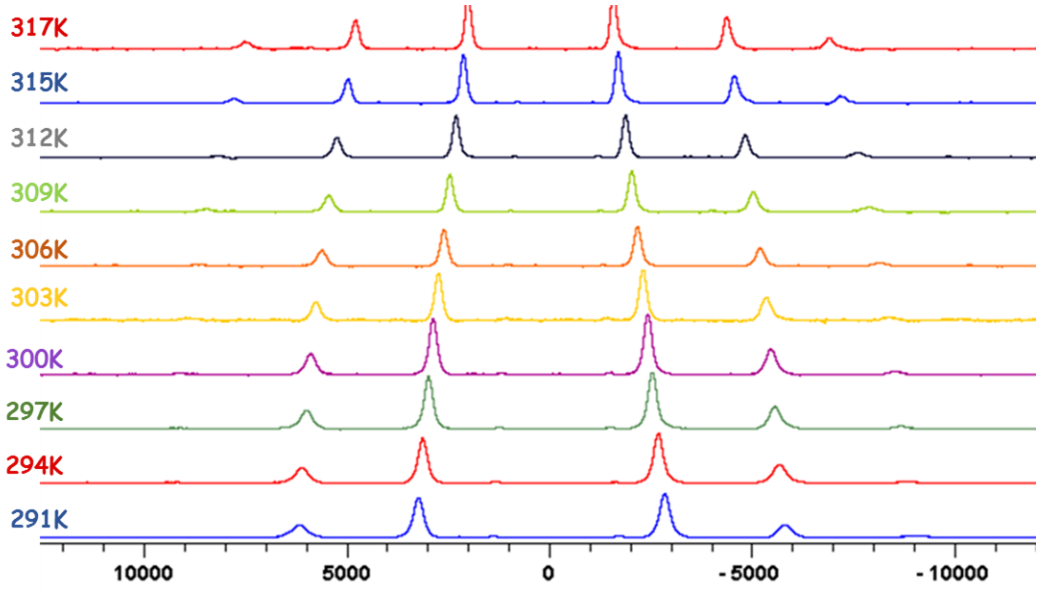

Figure S2: Experimental ^{2}H-NMR spectra of $[C_{12}C_1im][BF_4]$ tri-deuterated (d_3) imidazolium ring at different temperatures.

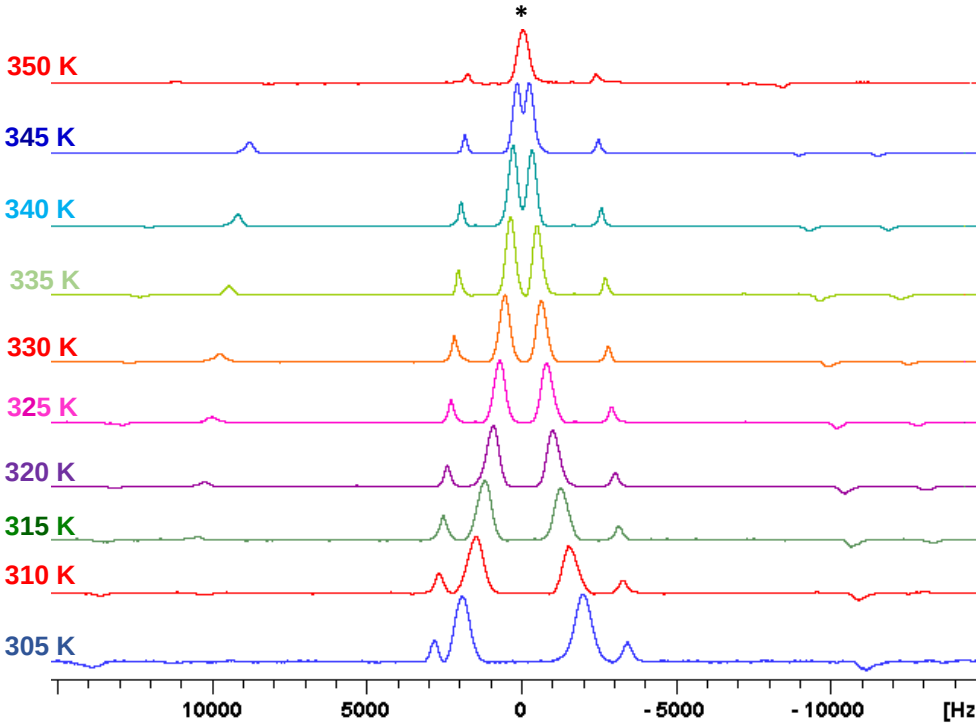

Figure S3: Experimental ^{2}H-NMR spectra of [$C_{12}C_1$im]Cl tri-deuterated (d_3) imidazolium ring at different temperatures. The symbol * refers to the D_2O present in the sample.

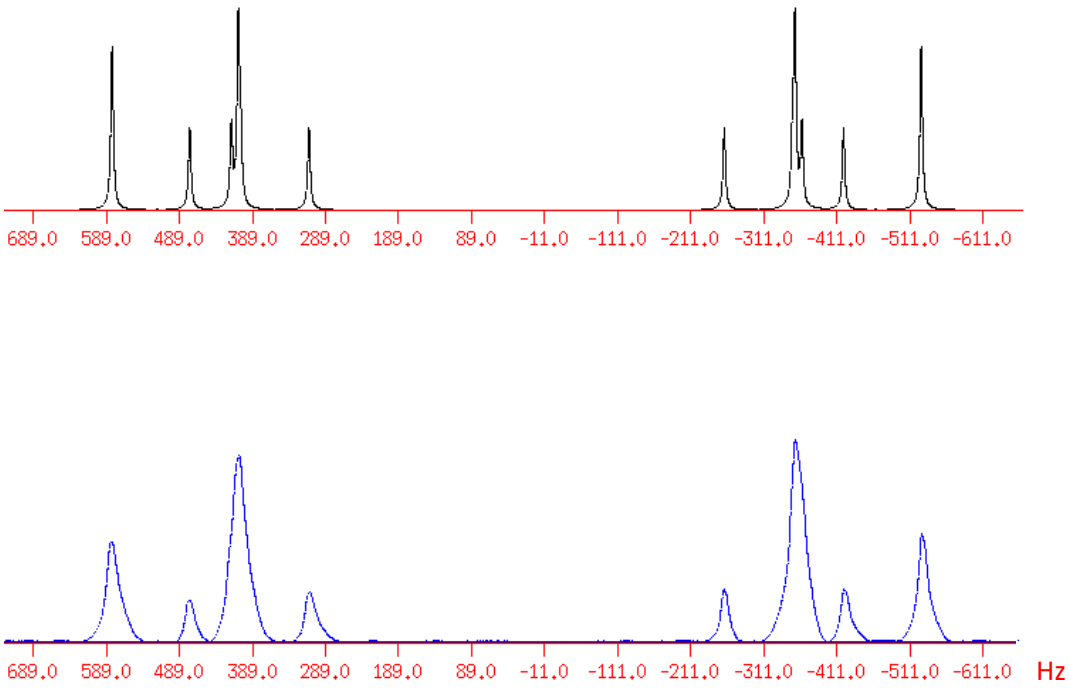

Figure S4: Experimental (bottom) and simulated (top) ^{1}H-NMR spectrum of DBB in [$C_{12}C_1$im][BF_4] at T = 309 K (T_{red} = 0.97)

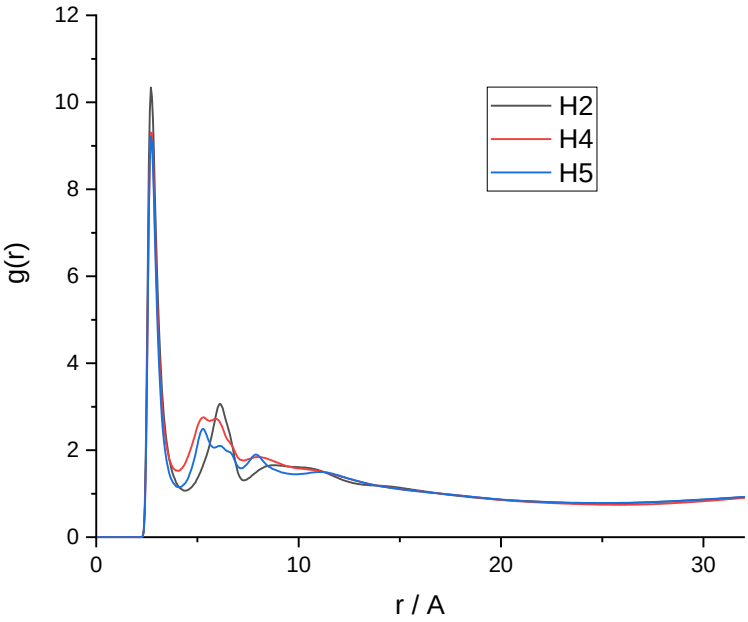

Figure S5: RDF of the distance between the imidazolium ring hydrogens and the chlorine anion in $[C_{12}C_1im]Cl$.

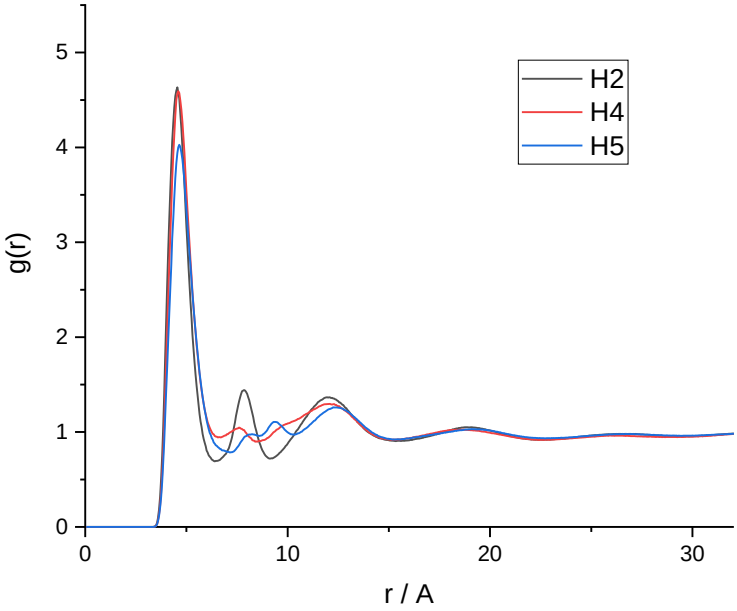

Figure S6: RDF of the distance between the imidazolium ring hydrogens and the boron atom of the anion in $[C_{12}C_1im][BF_4]$.

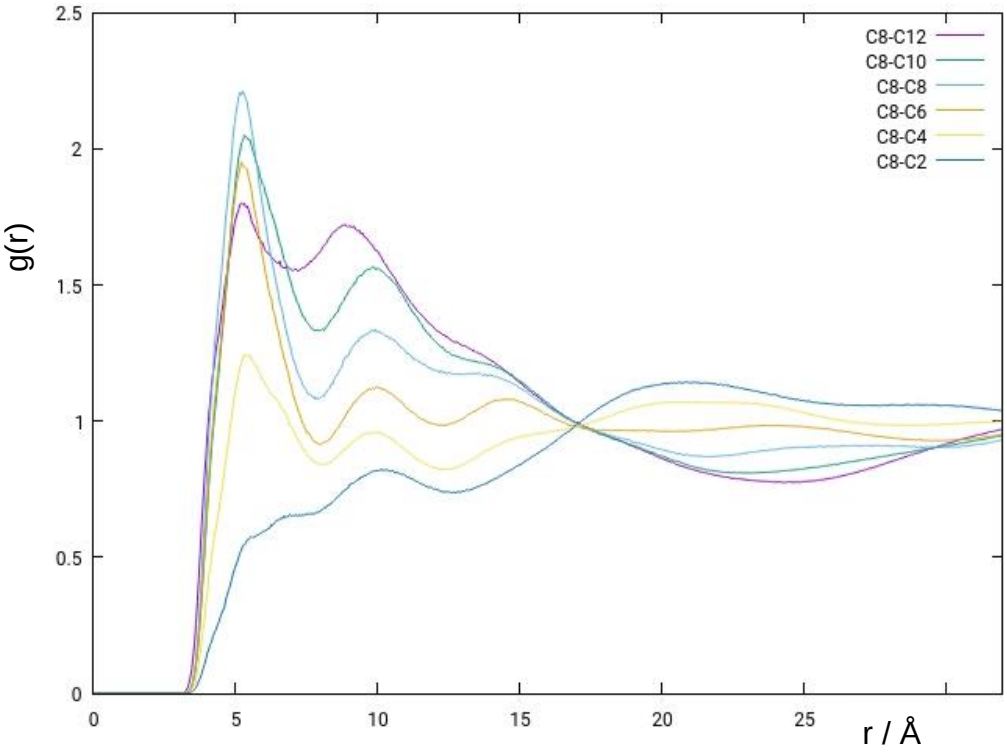

Figure S7: RDF of the distance between carbon C8 of the alkyl chain and some other carbons along the alkyl chain in $[C_{12}C_1im][Cl]$.

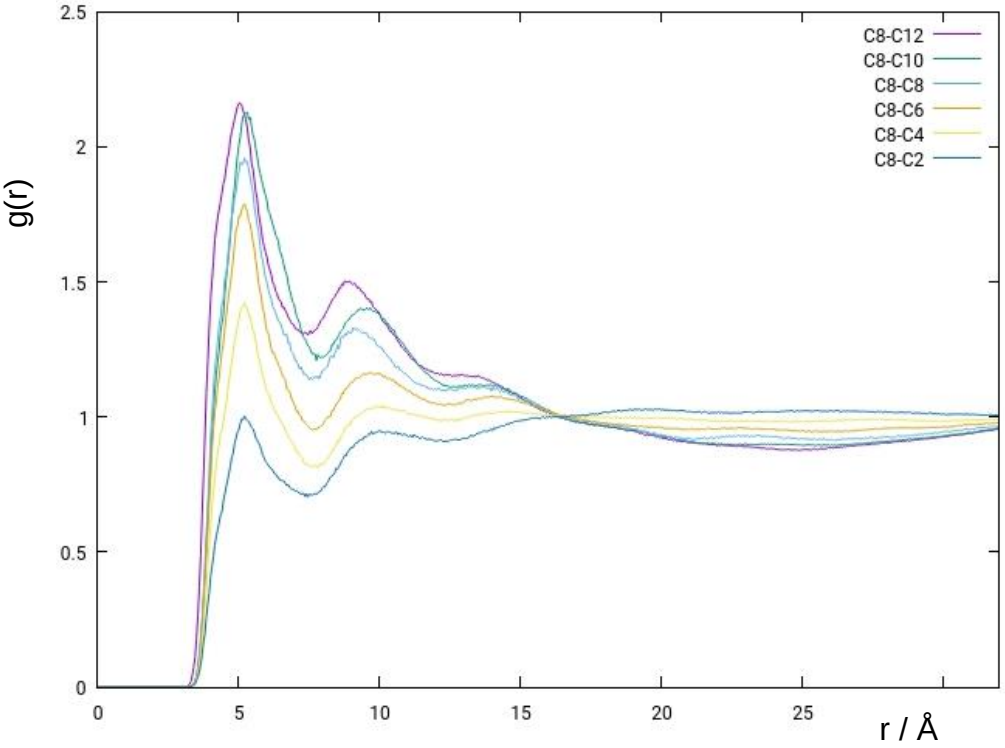

Figure S8: RDF of the distance between carbon C8 of the alkyl chain and some other carbons along the alkyl chain in $[C_{12}C_1im][BF_4]$.

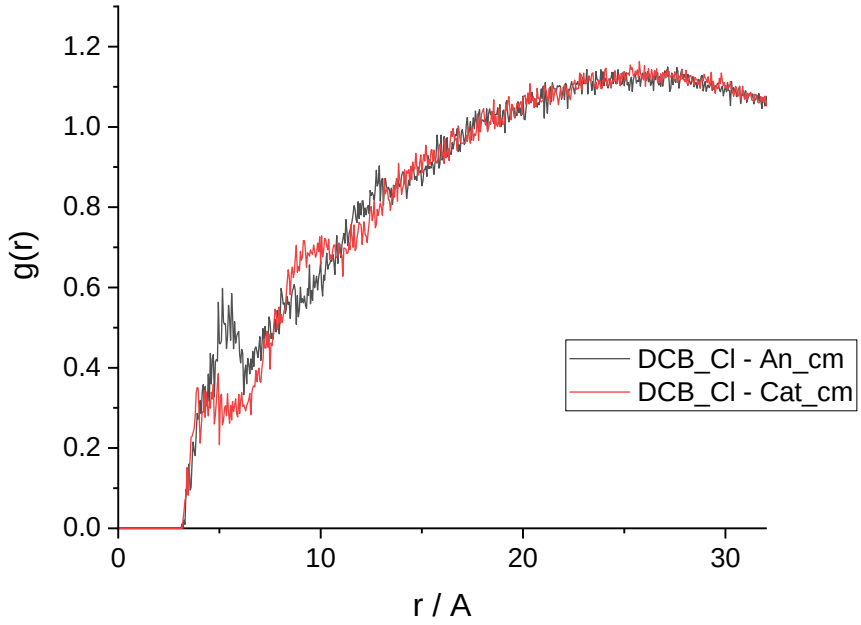

Figure S9: RDF of the distance between the chlorine atom of DCB and the center of mass of the cation and the chloride anion in $[C_{12}C_1im]Cl$.

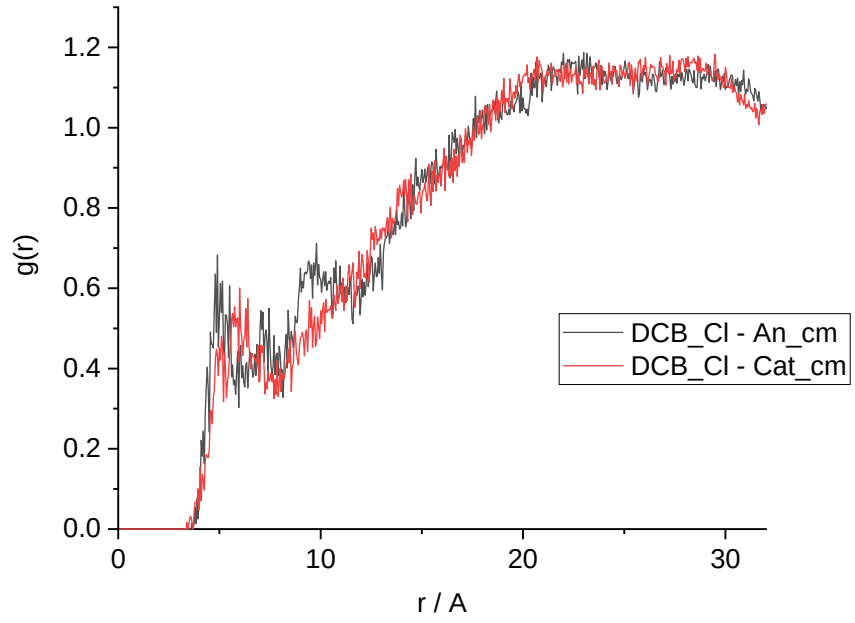

Figure S10: RDF of the distance between the chlorine atom of DCB and the center of mass of the cation and the boron atom of the anion in $[C_{12}C_1im][BF_4]$.

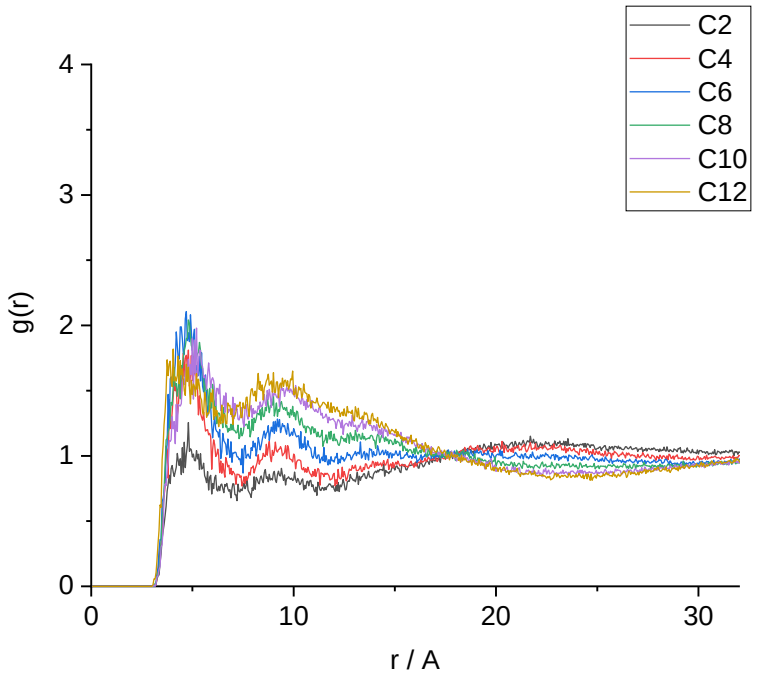

Figure S11: RDF of the distance between the chlorine atom of DCB and the various carbon atoms of the alkyl chain of the cation in $[C_{12}C_1im]Cl$.

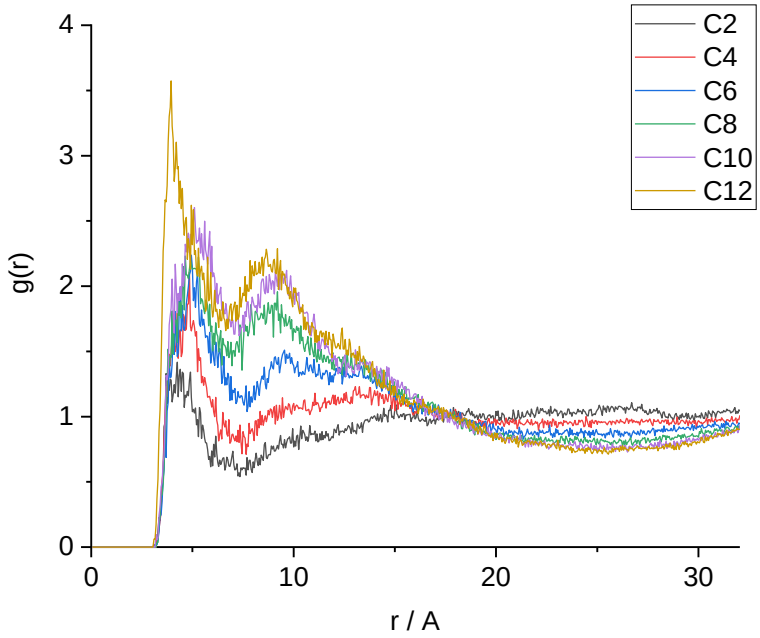

Figure S12: RDF of the distance between the chlorine atom of DCB and the various carbon atoms of the alkyl chain of the cation in $[C_{12}C_1im][BF_4]$.

Table S1. $\Delta\nu_4$, T_{CD4}, D_{CD4} (J_{CD4} = 31 Hz) values extracted from the ^2H and ^{13}C-{^1H} NMR spectra of $[C_{12}C_1im][BF_4]$ tri-deuterated (d_3) imidazolium ring and corresponding values of S_{CD4} (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures.

T_{red}	$\Delta\upsilon_4$ (Hz)	T_{CD4} (Hz)	D_{CD4} (Hz)	S_{CD4}
0.994	3583.18	122.9	45.9	-0.0124
0.987	3819.22	124.6	46.8	-0.0133
0.978	4187.13	135.6	52.3	-0.0145
0.967	4487.97	145.3	57.2	-0.0156
0.959	4774.58	150.4	59.7	-0.0166
0.950	5043.55	159.4	64.2	-0.0175
0.940	5298.75	164.3	66.6	-0.0184
0.931	5523.46	168.4	68.7	-0.0192
0.921	5821.18	178.3	73.6	-0.0202
0.912	6082.90	190.2	79.6	-0.0211

Table S2. $\Delta\nu_2$, T_{CD2}, D_{CD2} (J_{CD2} = 32 Hz) values extracted from the ^2H and ^{13}C-{^1H} NMR spectra of $[C_{12}C_1im][BF_4]$ tri-deuterated (d_3) imidazolium ring and corresponding values of S_{CD2} (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures.

T_{red}	$\Delta\upsilon_2$ (Hz)	T_{CD2} (Hz)	D_{CD2} (Hz)	S_{CD2}
0.994	14427.81	-355.0	-193.5	0.0501
0.987	14966.19	-375.0	-203.5	0.0520
0.978	15703.49	-393.5	-212.8	0.0545
0.967	16380.29	-416.3	-224.2	0.0569
0.959	16874.45	-428.9	-230.4	0.0586
0.950	17259.20	-436.9	-234.4	0.0599
0.940	17567.68	-452.0	-242.0	0.0610
0.931	17829.55	-455.5	-243.8	0.0619
0.921	18373.50	-464.1	-248.0	0.0638
0.912	18578.84	-484.7	-258.4	0.0645

Table S3. $\Delta\nu_5$ values extracted from the ^{2}H NMR spectra of $[C_{12}C_1im][BF_4]$ tri-deuterated (d_3) imidazolium ring and corresponding S_{CD5} values (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures.

T_{red}	$\Delta\upsilon_5$ (Hz)	S_{CD5}
0.994	9141.84	0.0317
0.987	9539.62	0.0331
0.978	10082.76	0.0350
0.967	10473.00	0.0364
0.959	10825.40	0.0376
0.950	11090.67	0.0385
0.940	11361.04	0.0394
0.931	11565.68	0.0402
0.921	11765.17	0.0408
0.912	11958.08	0.0415

Table S4. $\Delta\nu_2$ value extracted from the ^{2}H NMR spectrum of $[C_{12}C_1im]Cl$ tri-deuterated (d_3) imidazolium ring and corresponding values of S_{CD2} (referred to the external magnetic field B_0 of the spectrometer) at different reduced temperatures. Note that the sign of $\Delta\nu_2$ (then, of S_{CD2}) has been obtained only at the temperature of 305 K (T_{red} = 0.866); then the same sign has been assumed for the other temperatures.

T_{red}	$\Delta\nu_2$ (Hz)	S_{CD2}
0.99	-4101	-0.01402
0.98	-4320	-0.01476
0.96	-4518	-0.01544
0.95	-4738	-0.01619
0.93	-4952	-0.01692
0.92	-5169	-0.01767
0.90	-5406	-0.01848
0.89	-5668	-0.01937
0.88	-5943	-0.02031
0.86	-6151	-0.02130