

ESI for:  
Local order and long range correlations in  
imidazolium halide ionic liquids: a combined  
molecular dynamics and XAS study

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	R( $\text{\AA}$ )	N	cutoff( $\text{\AA}$ )
Br-Cat	4.73	3.7	5.60
Br-HCR	2.79	1.5	4.47
Br-HCW1	2.80	2.2	4.20
Br-HCW2	2.80	2.2	4.20
Br-H1	2.97	6.3	4.09
Br-H2	3.08	1.9	4.23
Br-CR	3.63	1.5	4.50
Br-CW	3.70	2.5	4.34
Br-C1	3.76	6.9	6.21
Br-C2	3.92	1.3	4.56
Br-N	4.16	6.6	5.51

Table S1. Structural parameters of the radial distribution functions,  $g(r)$ 's, calculated from the MD simulations of  $[\text{C}_6\text{mim}]\text{Br}$ . R is the position of the  $g(r)$  first peak, and N is the coordination number calculated by integration of the  $g(r)$  up to the cutoff distance. The cutoff distances used in the calculation of N are also reported.

	R( $\text{\AA}$ )	N	cutoff( $\text{\AA}$ )
I-Cat	5.21	4.2	6.13
I-HCR	3.34	1.8	5.00
I-HCW1	3.35	1.4	4.75
I-HCW2	3.37	1.6	4.86
I-H1	3.53	7.6	4.60
I-H2	3.60	2.2	4.70
I-CR	4.10	1.8	5.06
I-CW	4.22	3.4	4.94
I-C1	4.25	8.1	6.82
I-C2	4.43	4.0	6.98
I-N	4.69	6.9	6.10

Table S2. Structural parameters of the radial distribution functions,  $g(r)$ 's, calculated from the MD simulations of  $[\text{C}_6\text{mim}]\text{I}$ . R is the position of the  $g(r)$  first peak, and N is the coordination number calculated by integration of the  $g(r)$  up to the cutoff distance. The cutoff distances used in the calculation of N are also reported.

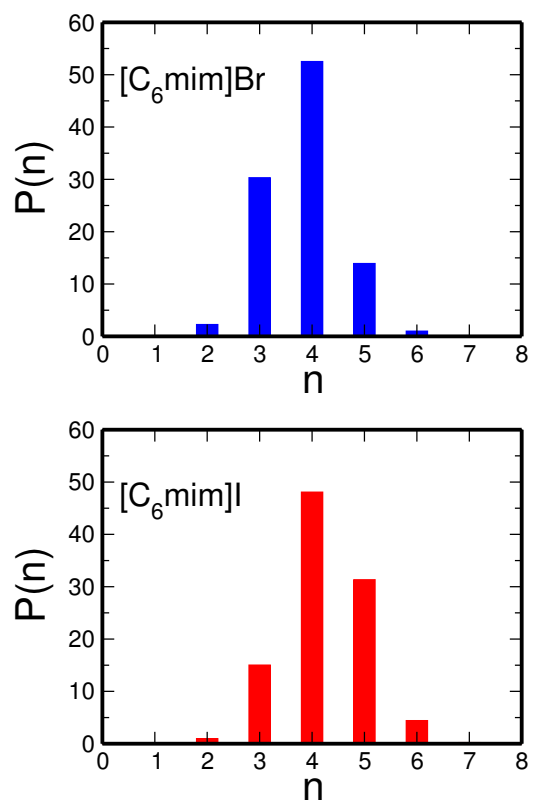


Figure S1. Instantaneous cation-anion coordination number ( $n$ ) distribution, expressed in percentage, calculated from the MD simulations of [C<sub>6</sub>mim]Br and [C<sub>6</sub>mim]I.

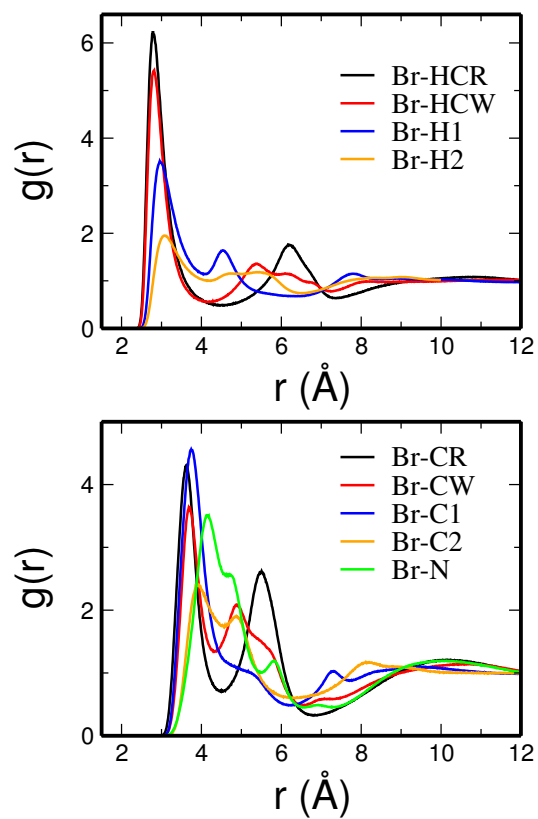


Figure S2. Radial distribution functions,  $g(r)$ 's, calculated from the MD simulation of  $[\text{C}_6\text{mim}]\text{Br}$ . In the upper panel the Br-H  $g(r)$ 's are reported, while in the lower panel the Br-C and Br-N  $g(r)$ 's.

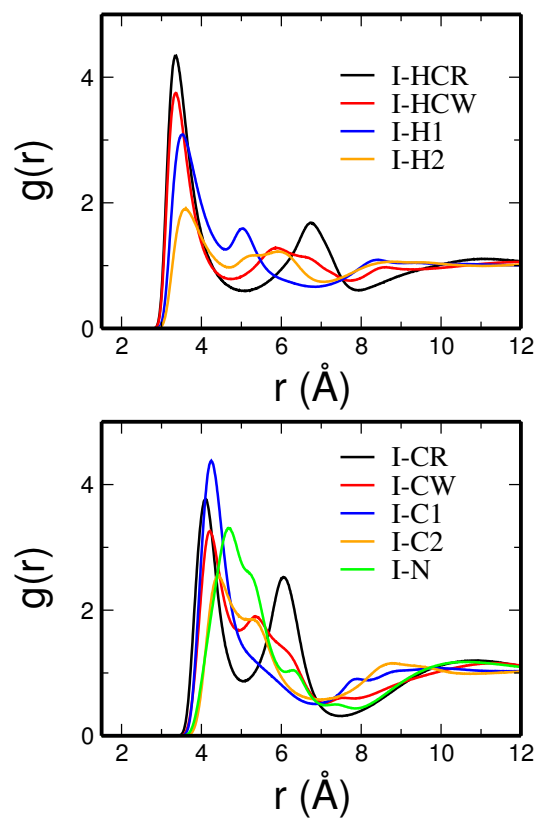


Figure S3. Radial distribution functions,  $g(r)$ 's, calculated from the MD simulation of  $[\text{C}_6\text{mim}]\text{I}$ . In the upper panel the I-H  $g(r)$ 's are reported, while in the lower panel the I-C and I-N  $g(r)$ 's.

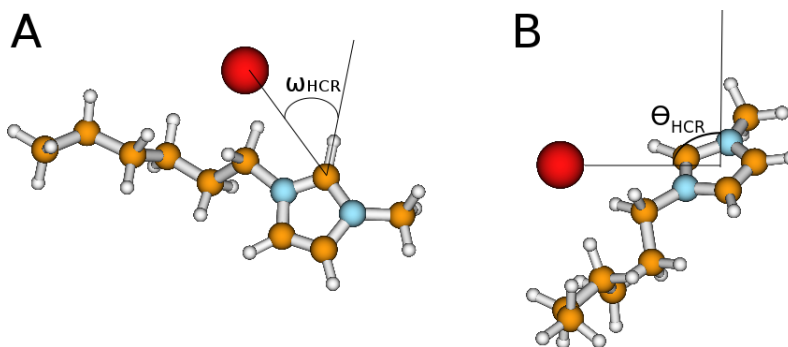


Figure S4. Definition of the  $\omega_{HCR}$  and  $\theta_{HCR}$  angles. (A)  $\omega_{HCR}$ : angle formed between the CR-HCR and the CR-X vectors. (B)  $\theta_{HCR}$ : angle between the normal vector to the ring plane and the ring center-X vector.