

# Supporting Information

## Effect of Side-Chain Length on Structural and Dynamic Properties of Ionic Liquids with Hydroxyl Cationic Tails

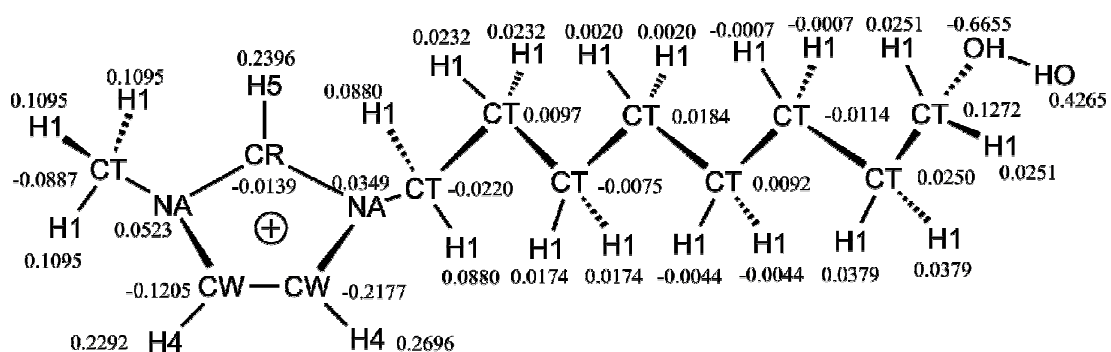
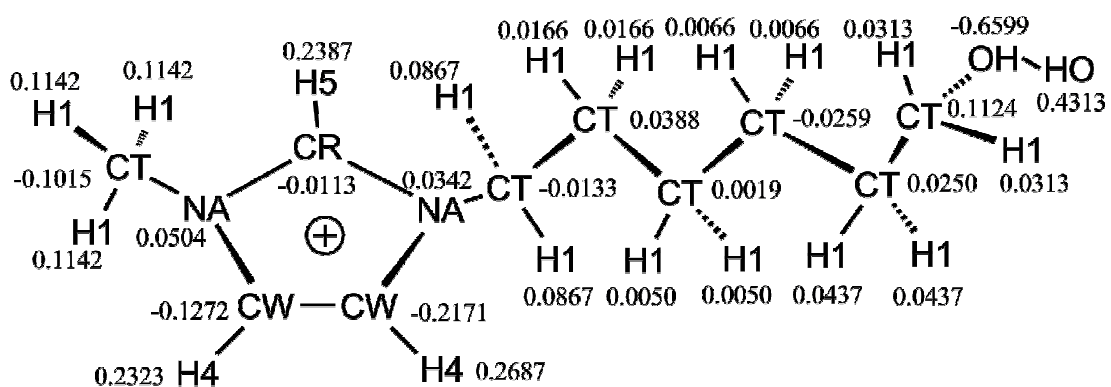
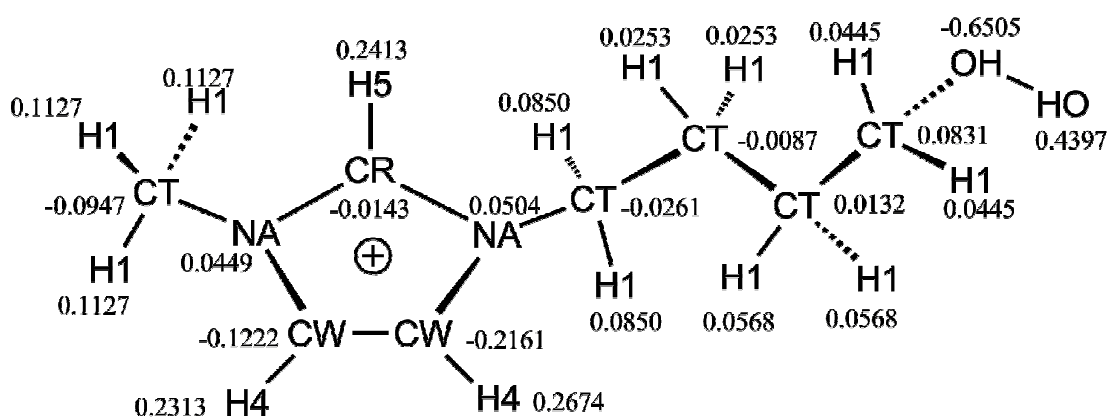
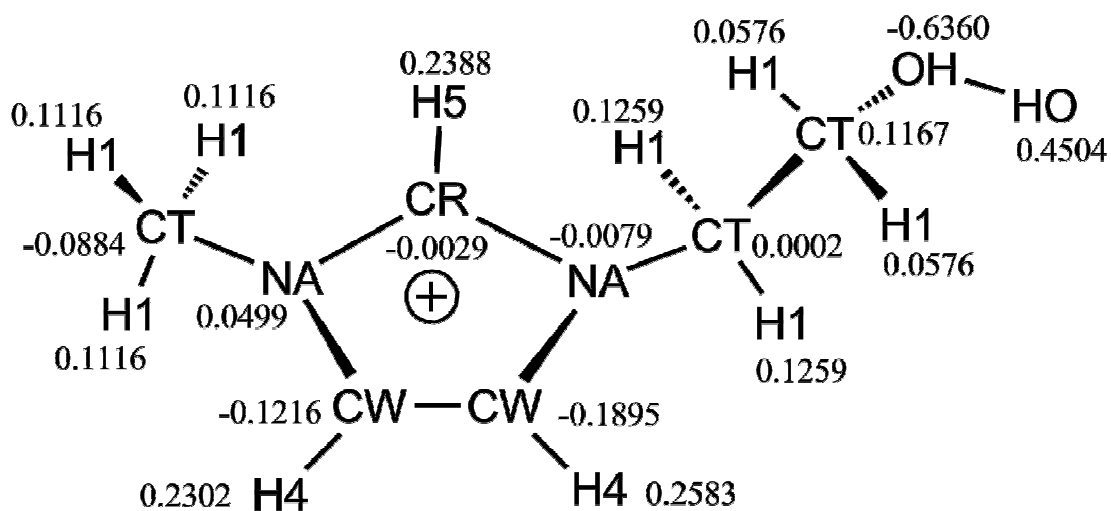
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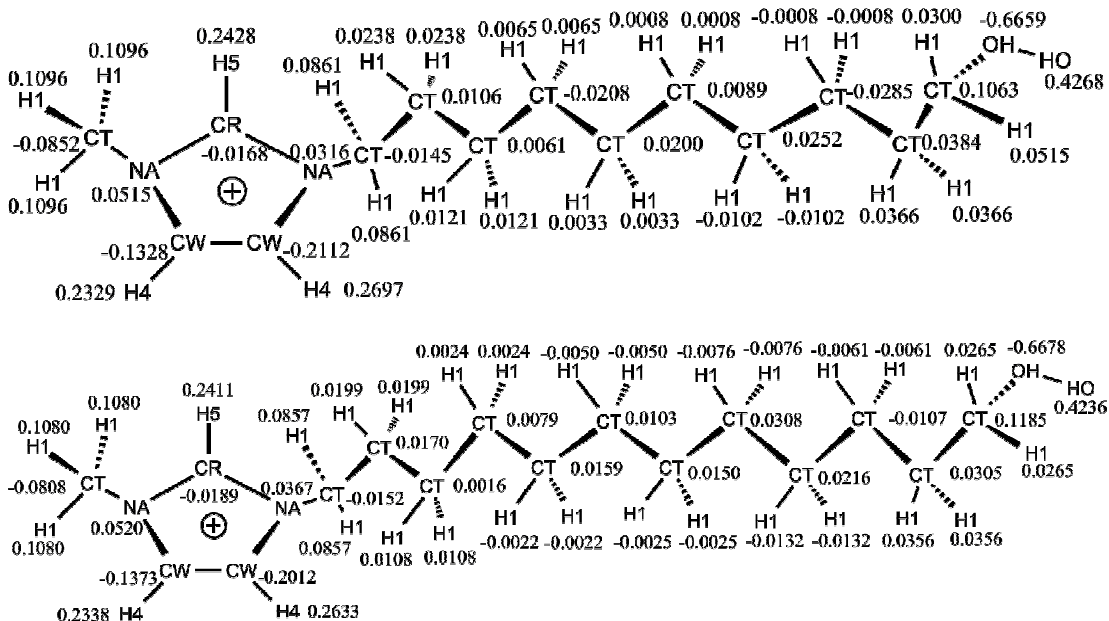
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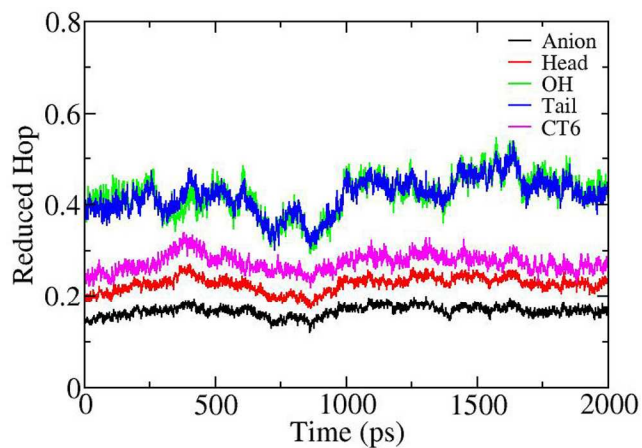


**Figure S1.** Partial charges of the cations in  $P_2$ – $P_{12}$  systems. OH and HO denote the oxygen atom and hydrogen atom in a hydroxyl group, respectively.

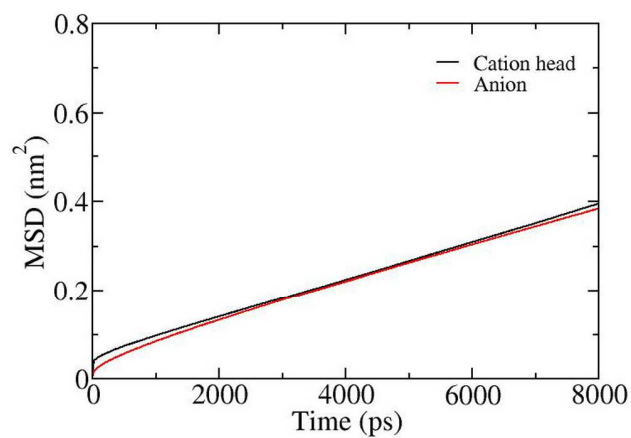
**Table S1.** Numbers of hydrogen bonds in the polar IL systems.

H-bonds	$P_2$	$P_4$	$P_6$	$P_8$	$P_{10}$	$P_{12}$
head-anion	$299.88 \pm 15.89$	$318.87 \pm 17.02$	$334.86 \pm 16.88$	$348.41 \pm 17.29$	$353.47 \pm 17.21$	$343.26 \pm 17.06$
anion-OH	$508.86 \pm 8.44$	$481.01 \pm 10.87$	$466.38 \pm 11.97$	$455.16 \pm 11.86$	$457.49 \pm 11.74$	$456.75 \pm 11.56$
head-OH	$30.43 \pm 5.20$	$36.14 \pm 5.76$	$37.43 \pm 5.84$	$37.55 \pm 5.84$	$38.59 \pm 5.85$	$37.91 \pm 5.85$
OH-OH	$8.27 \pm 2.74$	$20.03 \pm 4.22$	$24.92 \pm 4.84$	$28.35 \pm 4.91$	$27.10 \pm 4.72$	$26.53 \pm 4.64$
Total	$847.44 \pm$	$856.05 \pm$	$863.59 \pm$	$869.47 \pm$	$876.65 \pm$	$864.45 \pm$

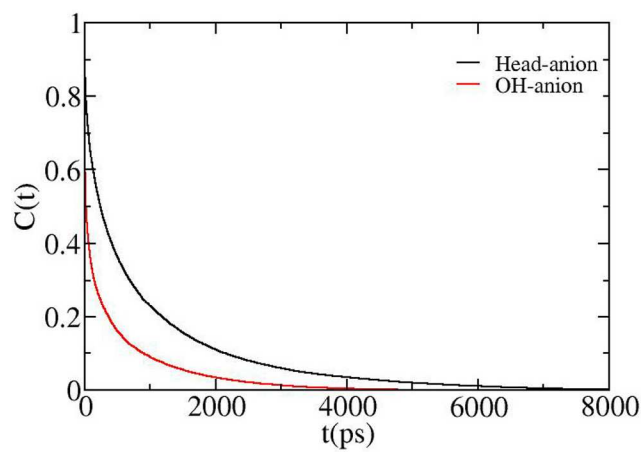
17.90      18.99      19.51      19.95      20.32      19.47



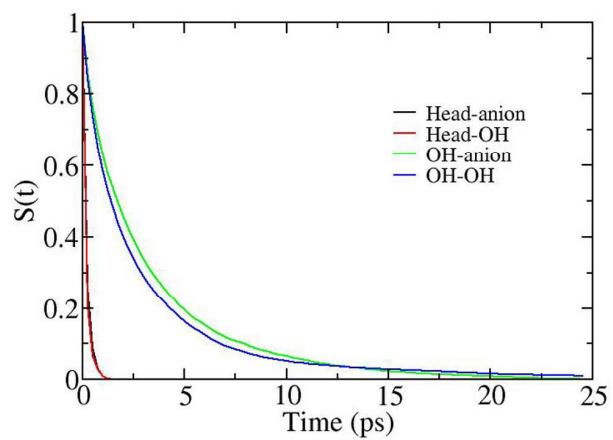
**Figure S2.** Instantaneous HOPs for anions, cationic head groups, hydroxyl groups, tail groups, and middle carbon groups (denoted as CT6) in the P<sub>8</sub> system.



**Figure S3.** MSDs of cationic head groups and anions in the P<sub>8</sub> system.



**Figure S4.** Time correlation functions of head-anion and OH-anion in the  $P_8$  system.



**Figure S5.** Time correlation functions of hydrogen bonds in the  $P_8$  system.