Supporting Information

Hydrogen-Bond Rich Ionic Liquids with Hydroxyl Cationic Tails

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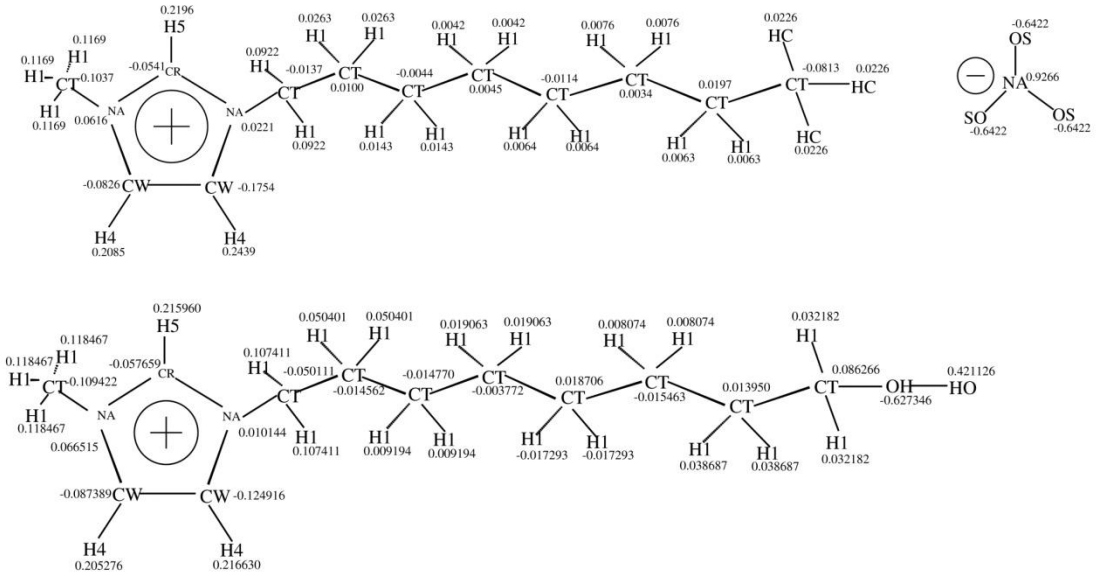
a) Partial charges



The partial charges were calculated by using the scheme associated with the AMBER force filed[1] as follows. We first optimized the molecular structures by *ab initio* calculation at the theoretical level of MP2/6-31g*, and then calculated the

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electric potential of the IL molecules. Finally the RESP method[2] was used to obtain the best fit of the partial charges. The above figure shows the partial charges for the C_8 and C_{OH} molecules.

b) Force Field Parameters

The parameters for the bonded and van der Waals interactions of C_8 and C_{OH} molecules were all taken from the standard AMBER 2 force field.[1]

1) Valence bond parameters [k_r in kcal/(mol·Å) and r_{eq} in Å].

bond	k_r	r_{eq}	bond	k_r	r_{eq}
CR-NA	954.0	1.343	CW-NA	854.0	1.381
CT-NA	674.0	1.475	CT-CT	620.0	1.526
CW-H4	734.0	1.080	CT-H1	680.0	1.090
CW-CW	1040.0	1.370	CR-H5	734.0	1.080
CT-HC	680.0	1.090	NA-OS	600.0	1.260
CT-OH	639.6	1.410	OH-HO	1105.3	0.960

2) Valence angle parameters [k_θ in kcal/(mol radian^2) and θ_{eq} in degree].

angle	k_θ	θ_{eq}	angle	k_θ	θ_{eq}
CR-NA-CW	140.0	120.0	CW-NA-CT	140.0	125.8
NA-CR-NA	140.0	120.0	NA-CR-H5	70.0	120.0
NA-CW-H4	70.0	120.0	CW-CW-H4	70.0	128.2

NA-CT-H1	70.0	109.5	CT-CT-H1	100.0	109.5
H1-CT-H1	70.0	109.5	HC-CT-HC	70.0	109.5
CR-NA-CT	140.0	125.8	NA-CW-CW	140.0	120.0
NA-CT-CT	160.0	111.2	CT-CT-HC	100.0	109.5
CT-CT-CT	80.0	109.5	OS-NA-OS	300.0	120.0
CT-CT-OH	100.0	109.5	H1-CT-OH	100.0	109.5
CT-OH-HO	110.0	108.5			

3) Dihedral angle parameters [V_n in kcal/mol and γ in degree].

dihedral	V_n	γ	n	dihedral	V_n	γ	n
HC-CT-CT-NA	0.156	0.0	3	HC-CT-CT-H1	0.156	0.0	3
CT-NA-CR-H5	2.325	180.0	2	CT-NA-CR-NA	2.325	180.0	2
CT-NA-CW-CW	1.500	180.0	2	CT-NA-CW-H4	1.500	180.0	2
NA-CR-NA-CW	2.325	180.0	2	CR-NA-CW-H4	1.500	180.0	2
CW-NA-CR-H5	2.325	180.0	2	CR-NA-CW-CW	1.500	180.0	2
NA-CW-CW-NA	5.375	180.0	2	NA-CW-CW-H4	5.375	180.0	2
CT-CT-CT-H1	0.156	0.0	3	CT-CT-CT-CT	0.156	0.0	3
H1-CT-CT-H1	0.156	0.0	3	NA-CT-CT-CT	0.156	0.0	3
NA-CT-CT-H1	0.156	0.0	3	HC-CT-CT-CT	0.156	0.0	3
H1-CT-NA-CW	0.0	0.0	2	H1-CT-NA-CR	0.0	0.0	2
CW-NA-CT-CT	0.0	0.0	2	CR-NA-CT-CT	0.0	0.0	2
H4-CW-CW-H4	5.375	180.0	2	H5-CR-NA-NA[a]	1.100	180.0	2

CR-CW-NA-CT[a]	1.100	180.0	2	H4-CW-CW-NA[a]	1.100	180.0	2
OS-OS-NA-OS[a]	50.000	180.0	2	CT-CT-OH-HO	0.167	0.0	3
H1-CT-OH-HO	0.167	0.0	3	CT-CT-CT-OH	0.156	0.0	3
H1-CT-CT-OH	0.156	0.0	3				

[a]Improper torsions

4) Van der Waals parameters [ε in kcal/mol and σ in Å].

pair	ε	σ	pair	ε	σ
CW-CW[b]	0.0860	3.400	CW-NA	0.121	3.325
CW-H5	0.0359	2.911	CW-HC	0.0371	3.025
CT-CT	0.109	3.400	CT-H1	0.0418	2.936
CT-HC	0.0418	3.025	CT-H4	0.0404	2.955
CT-CW	0.0968	3.400	H1-H1	0.0160	2.471
H1-HC	0.0160	2.560	H1-H4	0.0155	2.491
H5-H5	0.0150	2.422	H5-HC	0.0155	2.536
H5-NA	0.0505	2.836	HC-HC	0.0160	2.650
HC-NA	0.0522	2.950	H4-H4	0.0150	2.511
CW-H1	0.0371	2.936	CW-H4	0.0359	2.955
CT-H5	0.0404	2.911	CT-NA	0.136	3.325
H1-H5	0.0155	2.446	H1-NA	0.0522	2.861
H5-H4	0.0150	2.466	HC-H4	0.0155	2.580
H4-NA	0.0505	2.880	OS-OS	0.170	3.001
NA-NA	0.170	3.250	NA-OS	0.170	3.125
H1-OS	0.0522	2.736	H4-OS	0.0505	2.756
CW-OS	0.121	3.200	CT-OS	0.136	3.200
H5-OS	0.0505	2.711	HC-OS	0.0522	2.825
OH-HO	0.0	1.533	HO-HO	0.0	0.0
OH-CW	0.135	3.233	HO-CW	0.0	1.700
OH-CT	0.152	3.233	HO-CT	0.0	1.700
OH-H5	0.0560	2.743	HO-H5	0.0	1.210
OH-H4	0.0560	2.788	HO-H4	0.0	1.255
OH-NA	0.190	3.158	HO-NA	0.0	1.625
OH-H1	0.0580	2.768	HO-H1	0.0	1.235
OH-OS	0.190	3.033	HO-OS	0.0	1.500
OH-OH	0.211	3.066			

[b]CR type atom has the same van der Waals parameters as CW atom.

References

1. W. D. Cornell, P. Cieplak, C. I. Bayly, I. R. Gould, K. M. Merz, D. M. Ferguson, D. C. Spellmeyer, T. Fox, J. W. Caldwell and P. A. Kollman, *J. Am. Chem. Soc.*, 1995, **117**, 5179-5197.

2. C. I. Bayly, P. Cieplak, W. D. Cornell and P. A. Kollman, *J Phys Chem-Us*, 1993, **97**, 10269-10280.