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甲醇对 1-丁基-3-甲基咪唑四氟硼酸离子液体结构与性质影响的模拟研究

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Simulation Study of the Effect ofMethanol on the Structure and Properties of 1-Butyl-3-methylimidazolium Tetrafluoroborate Ionic Liquid

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S1 键拉伸参数

S1 Bond Stretching Potential Parameters

Bonds	r_0 /Å	K_r /kJ·mol^{-1}·Å^{-2}	Bonds	r_0 /Å	K_r /kJ·mol^{-1}·Å^{-2}
(a) $[BMIM]^+$			C2-C1	1.529	1121
CR-HA	1.080	1536	NA-C1	1.466	1410
CW-HA	1.080	1536	CT-CS	1.529	1121
C1-H1	1.090	1423	CS-C2	1.529	1121
CT-HC	1.090	1423	(b) BF_4^-		
CS-HC	1.090	1423	B-F	1.393	1213.36
C2-HC	1.090	1423	(c) methanol		
CW-NA	1.378	1787	C-H	1.090	1423.60
CR-NA	1.315	1996	C-O	1.410	1339.80
CW-CW	1.341	2176	O-HO	0.960	2315.40

S2 键角弯曲参数

S2 Bond Angle Potential Parameters

Angles	θ_0/ degree	K_θ/kJ·mol^{-1}·rad^{-2}	Angles	θ_0/ degree	K_θ/kJ·mol^{-1}·rad^{-2}
(a) $[BMIM]^+$			HC-CS-CT	110.7	156.6
CW-NA-CR	108.0	292.6	HC-CS-C2	110.7	156.6
CW-NA-C1	125.6	292.6	HC-C2-C1	110.7	156.6
CR-NA-C1	126.4	292.6	HC-C2-CS	110.7	156.6
NA-CR-HA	125.1	146.3	HC-CT-HC	107.8	138.1
NA-CR-NA	109.8	292.6	HC-CS-HC	107.8	138.1
NA-CW-CW	107.1	292.6	HC-C2-HC	107.8	138.1
NA-CW-HA	122.0	146.3	H1-C1-H1	107.8	138.1
CW-CW-HA	130.9	146.3	(b) BF_4^-		
CS-C2-C1	112.7	418.4	F-B-F	109.5	209.2
CT-CS-C2	112.7	418.4	(c) methanol		
C2-C1-NA	112.7	418.4	H-C-H	109.5	146.5
H1-C1-C2	110.7	156.6	H-C-O	109.5	209.3
H1-C1-NA	110.7	156.6	C-O-HO	108.5	230.3
HC-CT-CS	110.7	156.6			

S3 二面角扭曲参数

S3 Dihedral Torsion Potential Parameters

Dihedrals	V_1/ kJ·mol^{-1}	V_2/ kJ·mol^{-1}	V_3/ kJ·mol^{-1}
(a) [BMIM]$^+$			
X-NA-CR-X	0	19.46	0
X-CW-CW-X	0	44.98	0
X-CW-NA-X	0	12.55	0
CW-NA-C1-H1	0	0	0.519
CR-NA-C1-H1	0	0	0
CW-NA-C1-C2	-7.154	6.106	0.794
CR-NA-C1-C2	-5.269	0	0
NA-C1-C2-CS	-7.480	3.164	-1.203
NA-C1-C2-HC	0	0	0
C1-C2-CS-HC	0	0	1.531
CT-CS-C2-HC	0	0	1.531
CS-C2-C1-H1	0	0	1.531
C2-CS-CT-HC	0	0	1.531
H1-C1-C2-HC	0	0	1.331
HC-C2-CS-HC	0	0	1.331
HC-CS-CT-HC	0	0	1.331
CT-CS-C2-C1	7.28	-0.657	1.167
Dihedrals	V_n(kJ·mol^{-1})	γ/degree	n
(c) methanol			
H-C-O-HO	0	0.7	3

S4 非键参数

S4 Nonbonded Potential Parameters

Atoms	σ /Å	ε /kJ·mol^{-1}	Atoms	σ /Å	ε /kJ·mol^{-1}
(a) [BMIM]$^+$			NA	3.25	0.71128
CR	3.55	0.29288	(b) BF_4^-		
CW	3.55	0.29288	B	3.5814	0.39784
C1	3.50	0.27614	F	3.1181	0.25522
C2	3.50	0.27614	(c) methanol		
CS	3.50	0.27614	C	3.4001	0.4581
CT	3.50	0.27614	H	2.6498	0.0657
H1	2.50	0.12552	O	3.0668	0.8809
HC	2.50	0.12552	OH	1.0692	0.0000
HA	2.42	0.12552			