

The parameters of the [CMIM]Cl molecules in simulations are listed in **Table I**.

Table I New Atom Types and Parameters for [CMIM]Cl

atom types					
type	mass	element	comment		
o2h	15.9994	O	hydroxyl oxygen		
o1=	15.9994	O	oxygen in carbonyl		
c3'	12.01115	C	carbonyl carbon		
c4	12.01115	C	generic sp ³ carbon		
c4z	12.01115	C	carbon, sp ³ , bonded to -N ₃		
c3a	12.01115	C	aromatic carbon		
n2=	14.0067	N	nitrogen		
Equivalences					
type	nonB	bond	angle	torsion	oop
o2h	o2h	o2h	o2	o2	o2
o1=	o1=	o1=	o1=	o1=	o1=
c3'	c3'	c3'	c3'	c3'	c3'
c4	c4	c4	c4	c4	c4
c4z	c4z	c4	c4	c4	c4
c3a	c3a	c3a	c3a	c3a	c3a
n2=	n2=	n2=	n2=	n2=	n2=
Bond Increments					
c3a		n2=		0.199	0.199
n2=		c4z		0.345	0.345
c3a		c3a		0	0
n2=		c4		0.345	0.345
c4		c4z		0	0
c4		c3'		0	0
c3'		o1=		0.45	-0.45
Bond					
<i>I</i>	<i>J</i>	R0	K2	K3	K4
n2=	c3a	1.4	350	0	0
n2=	c4z	1.474	337.06	-147.37	213.633
c3a	c3a	1.417	470.8361	-627.6179	1327.6345
n2=	c4	1.474	337.06	-147.37	213.633
c4	c4z	1.53	299.67	-501.77	679.81
c4	c3'	1.514	312.3719	-465.829	473.83

c3'	o1=	1.216	823.7948	-1878.7939	2303.531	
Angle						
<i>I</i>	<i>J</i>	<i>K</i>	Theta0	K2	K3	K4
c3a	n2=	c3a	120	60	0	0
n2=	c3a	c3a	120	60	0	0
c3a	c3a	n2=	120	60	0	0
n2=	c4z	c4	117.317	55.242	0	0
c4	c3'	o1=	119.3	65.1016	-17.9766	0
c4	c3'	o2h	100.3182	88.8631	-3.8323	-7.9802
o1=	c3'	o2h	118.9855	98.6813	-22.2485	10.3673
Torsion						
<i>I</i>	<i>J</i>	<i>K</i>	<i>L</i>	V1	V2	V3
c3a	n2=	c3a	c3a	0	1	0
c4z	n2=	c3a	c3a	0	1	0
c3a	n2=	c3a	n2=	0	1	0
c4z	n2=	c3a	n2=	0	1	0
c3a	n2=	c4	c4	0	0	-0.02
n2=	c3a	c3a	n2=	0	4.5	0
c3a	c3a	n2=	c3a	0	0	0
n2=	c4z	c4	c3'	0	0	0
c4z	c4	c3'	o1=	0	0.78	0
c4z	c4	c3'	o2h	-2.5594	2.2013	0.0325
Non-bond (LI9-6)						
<i>I</i>		<i>r</i>		<i>E</i>		
c3'		3.9		0.064		
c4		3.854		0.062		
c4z		3.65		0.08		
c3a		3.915		0.068		
o1=		3.43		0.192		
o2h		3.58		0.096		
n2=		3.83		0.096		

The parameters of the [DMIM]PF₆ molecules in simulations are listed in **Table II**.

Table II New Atom Types and Parameters for [DMIM]PF₆

atom types			
type	mass	element	comment
c4	12.01115	C	generic sp ³ carbon
c4z	12.01115	C	carbon, sp ³ ,

c3a		12.01115		C	aromatic carbon	
n2=		14.0067		N	nitrogen	
Equivalences						
type	nonB	bond	angle	torsion	oop	
c4	c4	c4	c4	c4	c4	
c4z	c4z	c4	c4	c4	c4	
c3a	c3a	c3a	c3a	c3a	c3a	
n2=	n2=	n2=	n2=	n2=	n2=	
Bond Increments						
c3a		n2=		0.199	0.199	
n2=		c4z		0.345	0.345	
c3a		c3a		0	0	
n2=		c4		0.345	0.345	
c4		c4z		0	0	
Bond						
<i>I</i>	<i>J</i>	R0	K2	K3	K4	
n2=	c3a	1.4	350	0	0	
n2=	c4z	1.474	337.06	-147.37	213.633	
c3a	c3a	1.417	470.8361	-627.6179	1327.6345	
n2=	c4	1.474	337.06	-147.37	213.633	
c4	c4	1.53	299.67	-501.77	679.81	
Angle						
<i>I</i>	<i>J</i>	<i>K</i>	Theta0	K2	K3	K4
c3a	n2=	c3a	120	60	0	0
n2=	c3a	c3a	120	60	0	0
c3a	c3a	n2=	120	60	0	0
n2=	c4z	c4	117.317	55.242	0	0
c4z	c4	c4	112.67	39.516	-7.443	-9.5583
c4	c4	c4	112.67	39.516	-7.443	-9.5583
Torsion						
<i>I</i>	<i>J</i>	<i>K</i>	<i>L</i>	V1	V2	V3
c3a	n2=	c3a	c3a	0	1	0
c4z	n2=	c3a	c3a	0	1	0
c3a	n2=	c3a	n2=	0	1	0
c4z	n2=	c3a	n2=	0	1	0
c3a	n2=	c4	c4	0	0	-0.02
n2=	c3a	c3a	n2=	0	4.5	0
c3a	c3a	n2=	c3a	0	0	0
c4	c4	c4	c4	0	0.0514	-0.143

Non-bond (LI9-6)		
<i>I</i>	<i>r</i>	\mathcal{E}
c4	3.854	0.062
c4z	3.65	0.08
c3a	3.915	0.068
n2=	3.83	0.096
