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Improved United-Atom Force Field for 1-Alkyl-3-methylimidazolium Chloride

Page 4572. In the Supporting Information, in Table S1, the following charge values should be corrected as shown in bold:

TABLE S1: Force Field Parameters in this Work

atom	Lennard-Jones		charges/ e *	
	$\sigma/\text{\AA}$	$\epsilon/\text{kcal}\cdot\text{mol}^{-1}$	[C ₁ mim][Cl]	[C _n mim][Cl] ($n \geq 2$)
NA	3.250	0.170	0.0276	0.015
CR	3.400	0.086	0.0050	0.00
CW	3.400	0.086	-0.1734	-0.16
H5	1.247	0.030	0.1544	0.15
H4	1.604	0.030	0.2118	0.20
CN3	3.813	0.190	0.2543	0.26
CN2	3.822	0.142	0.2543	0.23
CT2	3.947	0.133		0.05*
CT3	3.902	0.185		0.00
Cl ⁻	3.742	0.150	-0.80	-0.80

* The value is for CT2 connected with CN2. For other CT2, the charges are set to zero.

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