Computational and Experimental Study of the Interactions Between Ionic Liquids and Volatile Organic Compounds

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Supplementary Information

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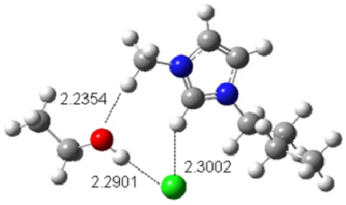
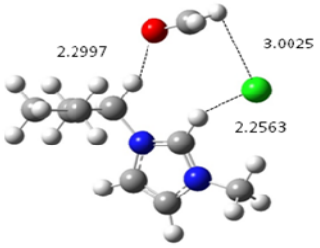
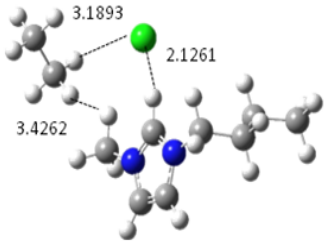
(a)



(b)



(c)



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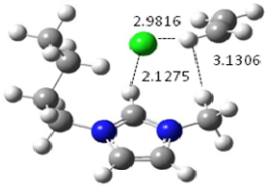

(e)

Figure S-1 Optimized geometries, including interaction lengths (in Å) of C_4mimCl and different types of VOCs. (a) Optimized geometry of C_4mimCl and methanol. (b) Optimized geometry of C_4mimCl and ethanol. (c) Optimized geometry of C_4mimCl and formaldehyde. (d) Optimized geometry of C_4mimCl and ethane. (e) Optimized geometry of C_4mimCl and ethylene. The numbers represent the interaction lengths in units of Angstroms.

Table S-1 Interaction lengths between C_4mimCl and different VOCs using the HF calculations.

Interacting compounds	Interaction lengths at different positions, Å			
	H•••Cl[a]	O•••H[a]	H•••H[a]	C•••H[a]
methanol + C_4mimCl	2.2869	2.2157	b	b
ethanol + C_4mimCl	2.2901	2.2354	b	b
isopropanol + C_4mimCl	2.3186	2.2166	b	b
2-methyl-1-propanol + C_4mimCl	2.2847	2.2153	b	b
3-methyl-1-butanol + C_4mimCl	2.2950	2.2184	b	b
formaldehyde + C_4mimCl	3.0025	2.2997	b	b
acetaldehyde + C_4mimCl	2.6316	2.3003	b	b
butanal + C_4mimCl	3.0078	2.2428	b	b
acetone + C_4mimCl	2.9246	2.2930	b	b
ethane + C_4mimCl	3.1893	NA[c]	3.4262 [b]	b
propane + C_4mimCl	3.2544	NA[c]	3.2426 [b]	b
ethylene + C_4mimCl	2.9816	NA[c]	3.1306 [b]	b
cis-2-butene + C_4mimCl	3.2179	NA[c]	3.2270 [b]	b
acetylene + C_4mimCl	2.5978	NA[c]	2.7916 [b]	b
toluene + C_4mimCl	3.0425	NA[c]	b	2.9234

[a] The first atom represents the atom in the VOC while the second atom represents the atom in C_4mimCl.

[b] These calculated interactions are not significant (since they are larger) as compared to the other interaction lengths listed in the Table. The numbers presented are the shortest interaction lengths. However, these lengths are still quite large as compared to those of the oxygenated compounds..

[c] Not available since there is no oxygen atom in alkanes, alkenes, alkynes, or aromatic hydrocarbon.

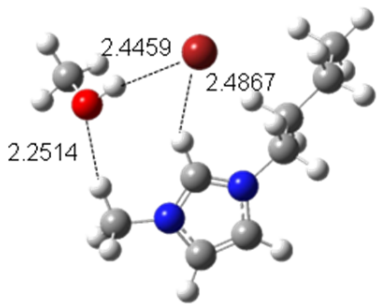

Figure S-2 Optimized geometry of C_4mimBr and methanol. The numbers represent the interaction lengths in units of Angstroms.

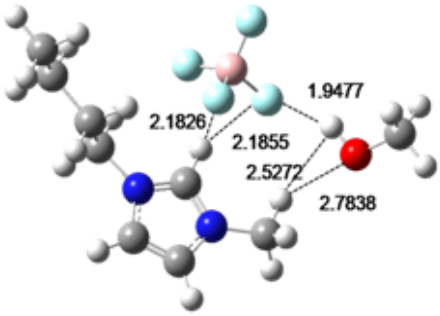

Figure S-3 Optimized geometry of C_4mimBF_4 and methanol. The numbers represent the interaction lengths in units of Angstroms.

Table S-2 Interaction atoms and lengths for methanol with different types of ionic liquids

Interaction compounds	Interaction lengths	
	H••• Halogen atom [a,b]	O•••H[b]
methanol + C_4mimCl	2.2869	2.2157
methanol + C_4mimBr	2.4459	2.2514
methanol + C_4mimBF_4	1.9477	2.7838

a. Halogen atom represents Cl, Br and F in C_4mimCl, C_4mimBr and C_4mimBF_4, respectively.

b. The first atom represents the atom in methanol while the second atom represents the atom in the ionic liquid.

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