Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

In Silico Insights into the Solvation Characteristics of the Ionic Liquid 1-Methyltriethoxy-3-Ethylimidazolium Acetate for Cellulosic Biomass

SUPPLEMENTAL INFORMATION

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Supplemental Information

Table 1. List of charges calculated for the cation from OPLS-AA method (Sambasivarao, S. V.; Allen, C.; Acevedo, O., Development of OPLS-AA force field parameters for ionic liquid simulations and their applications in elimination reactions. *Abstracts of Papers of the American Chemical Society* 2013, *245*.) and tail using corresponding MP2/ccVTZ RESP method.

Atom Number	Atom Name	Atom Type	Charge
1	C6	c3	-0.24
2	H8	hc	0.08
3	H9	hc	0.08
4	H10	hc	0.08
5	C5	c3	-0.17
6	H6	h1	0.18
7	H7	h1	0.18
8	N2	na	0.22
9	C4	cd	-0.09
10	C3	cc	-0.24
11	H4	h4	0.27
12	H5	h4	0.27
13	C2	cc	-0.24
14	H3	h5	0.27
15	N1	na	0.22
16	C1	c3	-0.27
17	H1	h1	0.14
18	H2	h1	0.14
19	C7	c3	0.40
20	H11	h1	0.02
21	H12	h1	0.02
22	O1	os	-0.50
23	C8	c3	0.15
24	H13	h1	0.03
25	H14	h1	0.03
26	C9	c3	0.33
27	H15	h1	-0.02
28	H16	h1	-0.02
29	O2	os	-0.58
30	C10	c3	0.33
31	H17	h1	-0.02
32	H18	h1	-0.02
33	C11	c3	0.18
34	H19	h1	0.01
35	H20	h1	0.01
36	O3	os	-0.43
37	C12	c3	0.08
38	H21	h1	0.04
39	H22	h1	0.04
40	H23	h1	0.04

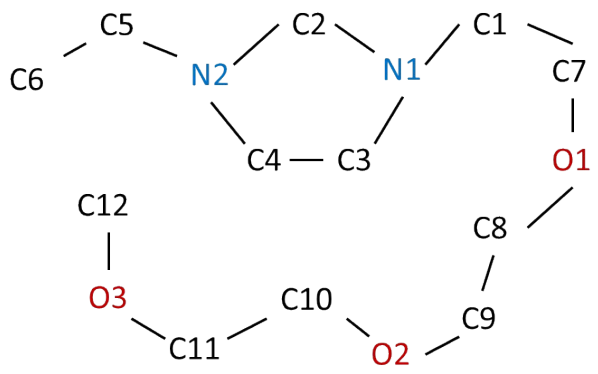

Figure 1. Map of cation showing atom names for use with table of charges.

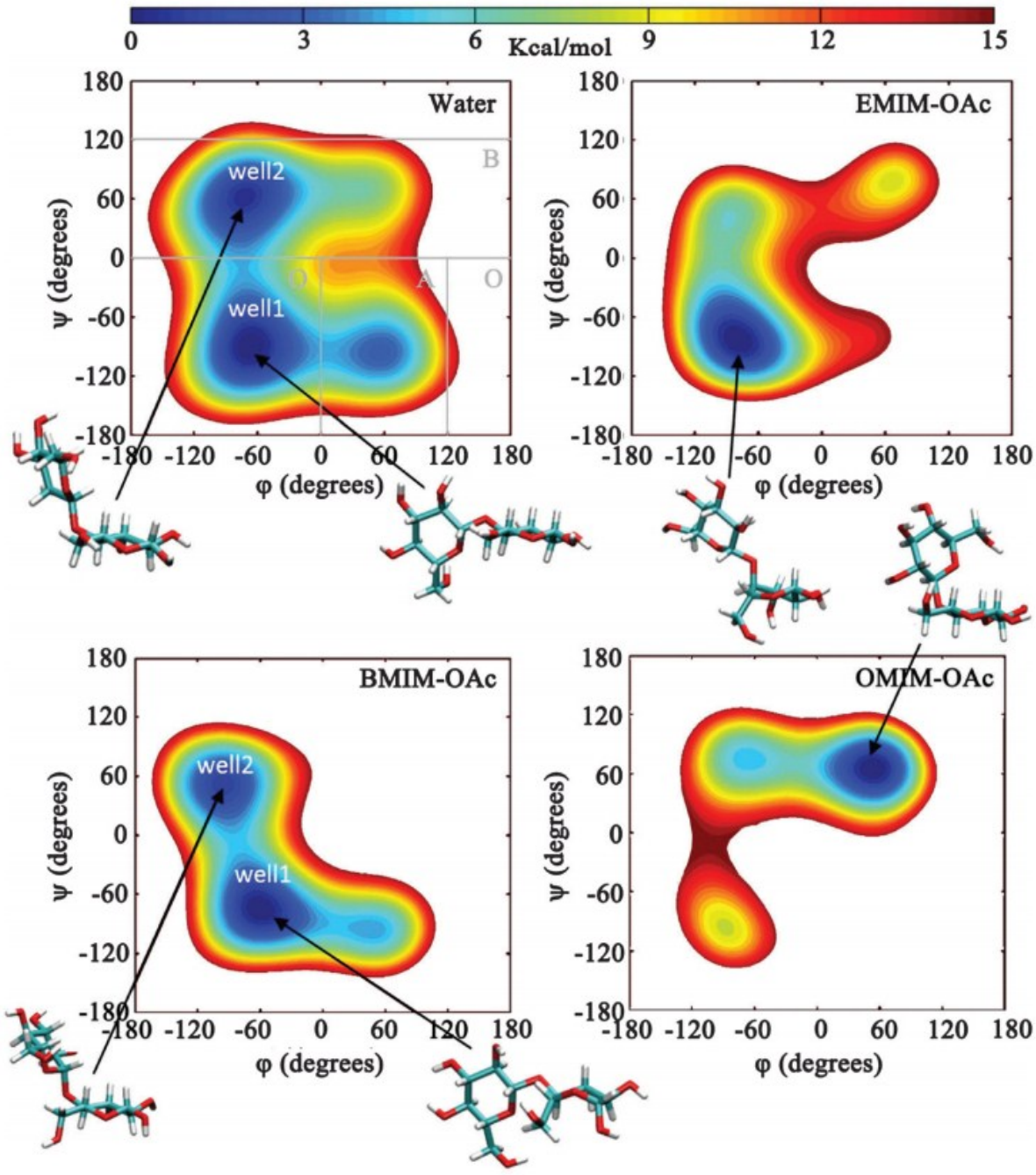

Figure 2. Free energy surfaces for cellobiose in water and dialkyl-imidazolium acetate ionic liquids from Bharadwaj, V. S.; Schutt, T. C.; Ashurst, T. C.; Maupin, C. M., Elucidating the conformational energetics of glucose and cellobiose in ionic liquids. *Physical Chemistry Chemical Physics* 2015, *17* (16), 10668-10678. Intended for comparison with free energy surface of the glycosidic bond of glucose in the oilgo(ethoxy) IL.

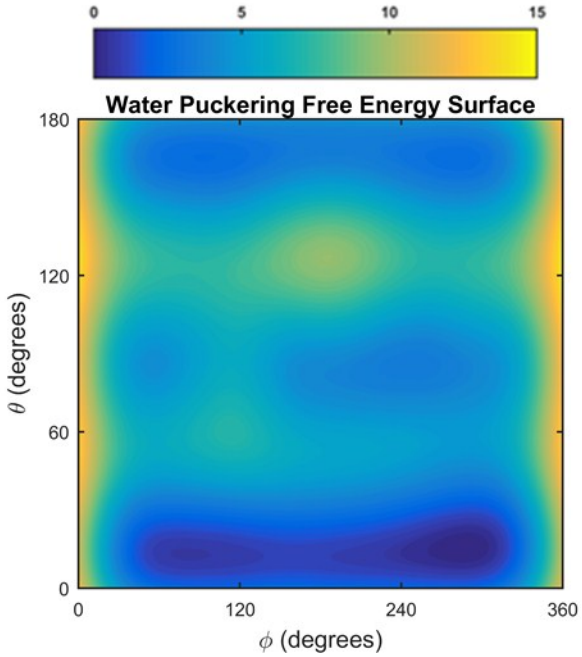

Figure 3. Free energy surface of the puckering coordinates for glucose in water showing strong energetic preference towards the $^4C_1$ conformation (low θ values).

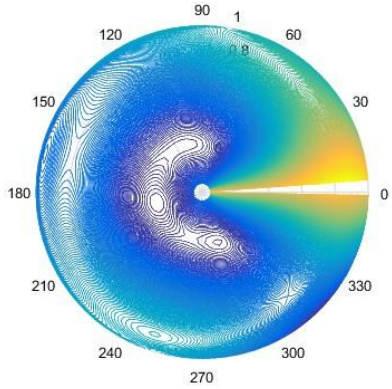

Figure 4. The free energy of ring puckering of glucose in [Me-$(OEt)_3$-Et-IM^+] [OAc^-] IL plotted as a top-down view of the northern hemisphere of the cremer-pople coordinates.