Supporting Information

Alkali can accelerate the cellulose dissolution in aqueous 1-ethyl-3-methylimidazole acetate (EmimAc/10% water)

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Results and discussion Section

Supplementary NMR analysis

The induced or conjugated effect of electron donating group leads to the both increase of electron cloud density outside the nucleus and shielding effect, and the NMR absorption shift to upfield, δ value becomes lower. On the contrary, the induced effect or conjugate effect of electron withdrawing group leads to the higher δ value and the NMR absorption shift to downfield. Specifically, the enhancement of hydrogen bonding leads to the decrease of electron cloud density, resulting in downfield shift, and vice versa (Yu et al., 2014).

Water act as both strong hydrogen bond donor and hydrogen bond acceptor. Therefore, it can form a hydrogen bond either as a donor with oxygen in Ac^- or as an acceptor with hydrogen in $Emim^+$. Because the hydrogen bond forming ability of water is stronger than that of Ac^-, the hydrogen bond between Ac^- and hydrogen on imidazole

ring is replaced by water molecule after adding water, leading to the electron cloud density on imidazole ring increases, the shielding effect is enhanced then, and the H2, H4, H5 moves to upfield (Zhang et al., 2010). At the same time, the addition of water molecules also reduces the tightness of π-π stacking between the imidazole rings and weakens the deshielding effect, which also leads to the H2, H4, H5 shifting to the upfield. What's more, after the electrostatic interaction between acetate anion and imidazole cation is destroyed by water, the positive charge of imidazole ring increases rapidly, the deshielding effect of protons on imidazole ring increases, which is also one of the reasons for the ^{1}H-NMR shift to upfield (Chen et al., 2014).

Moreover, the Δδ on the H2 is much higher than that of other H, indicating that water or NaOH-a preferentially combine with hydrogen at C2-H of $Emim^{+}$ position to form hydrogen bonding, the results was consistent with the reported data (Cammarata et al., 2001; Ficke et al., 2010; Bogdan et al., 2015). The imidazole ring has certain positive electricity and has a strong interaction with water molecules, the amount of H2, H4 and H5 on the imidazole ring shift greatly; For alkanes, due to the polarity difference between alkanes and water molecules, the interaction between them is not very strong, so the range of H6, H7 and H8 moving to upfield is small (Chen et al., 2014).

Supplementary Figures

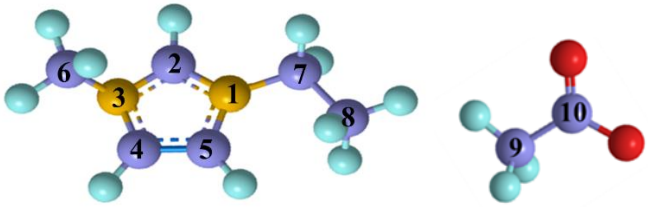

Fig. S1 Chemical structure of $Emim^+$ and Ac^- of EimAc with the proton resonances labeled, hydrogen atoms are displayed in light blue, carbon atoms are in purple, oxygen atoms are in red and nitrogen atoms are displayed in yellow.

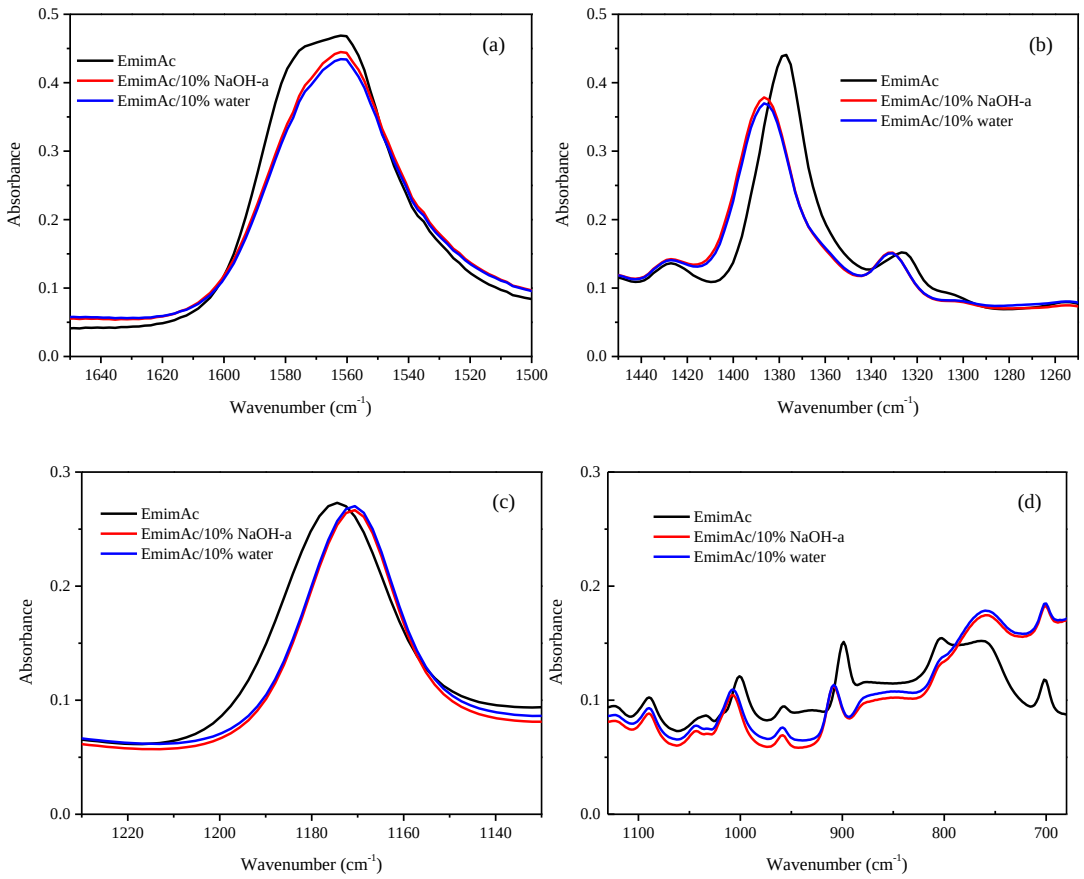

Fig. S2 ATR-IR spectra amplified at 1650cm^{-1}-1500cm^{-1} (a); amplified at 1450cm^{-1}-1250cm^{-1} (b); amplified at 1230cm^{-1}-1130cm^{-1} (c); amplified at 1130cm^{-1}-680cm^{-1} (d).

Supplementary Tables

Table S1 Vibrational frequencies of EmimAc, EmimAc/water and EmimAc/NaOH-a

Wavenumber (cm^{-1})			$\Delta\upsilon$ (cm^{-1}) EmimAc /10% NaOH-a	$\Delta\upsilon$ (cm^{-1}) EmimAc /10% water	Absorbance change	Assignment
EmimAc	EmimAc /10% NaOH-a	EmimAc /10% water				
702	700	700	-2	-2	↑	Asymmetric waging of the ring HC^4-C^5H
761	759	759	-2	-2	↑	Asymmetric waging of the ring HC^4-C^5H
898	908	908	+10	+10	↓	bending vibration of (C^9-C^{10}) of acetate
957	958	958	+1	+1	↓	Symmetric C^2-N-C^4 stretch
1001	1007	1007	+6	+6	↓	A ring out of plane asymmetric stretching, with contributions from the (N)$C^{4,5}H_2$(N) , C^6H_3(N)C^2N,
1033	1043	1043	+10	+10	↓	CCH scissors
1089	1089	1089	-	-	↓	C^6H_3 waggig
1174	1170	1170	-4	-4	↓	A ring in-plane asymmetric stretching, with contributions from the (N)CH_2 , CH_3(N)CN, and CC stretchings, results in a strong peak ($C^{2,4,5}$-H)
1254	1254	1254	-	-	↓	C^7-C^8H_3 twist vibration
1327	1331	1331	+4	+4	-	-CH_2-curl vibration
1378	1386	1386	+8	+8	↓	$C^{9,10}$ symmetric stretching band
1427	1427	1427	-	-	↑	C^9H_3 connected with Ac^- group
1567	1567	1567	-	-	-	C^9-C^{10}=O asymmetric stretching band
2976	2981	2981	+5	+5	↑	Alkyl-C-H stretching vibrations, C^6H_3 and C^9H_3
3039	3076	3076	+37	+37	↑	C^2-H asymmetry stretching vibrations
3139	3145	3145	+6	+6	↑	$C^{4,5}$-H symmetry stretching vibrations

Table S2 DFT calculation of interaction energy for complexes

Complexes	E (complex) (au)	E ($Emim^+$) (au)	E (Ac^-) (au)	E (OH^-) (au)	E (Cell) (au)	E (water) (au)	Be(ha)	Be(ev)
$Emim^+$-Ac^-	-573.3102629	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.1369896	-3.72803497
$Emim^+$-OH^-	-420.6107486	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.1570478	-4.27389883
$Emim^+$-water	-421.1882203	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.0333555	-0.90773658
Ac^--water	-304.9130288	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.0149989	-0.40818007
OH^--water	-152.1999829	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.0215255	-0.58579496
OH^--OH-Cell	-763.1082131	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.0775437	-2.11027425
Ac^--OH-Cell	-915.8033519	-344.7150541	-228.4582192	-75.7386467	-687.304455	-76.4398107	-0.0494366	-1.34536763

Reference

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