Electronic Supplementary Information (ESI)

Brønsted acidic ionic liquids for cellulose hydrolysis in aqueous medium: Structural effects on acidity and glucose yield

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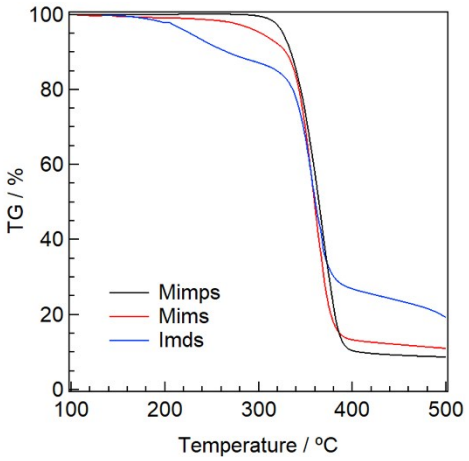
The file includes: Supporting Fig. S1–S3 and Table S1–S2



- Instrument: TG-DTA 7200 (Hitachi High-Technologies, Co. Ltd.)
- Apparatus: open-type aluminum pan
- Sample loading: 10 mg
- Heating rate: 10 °C min^{-1}
- N_2 flow: 200 mL min^{-1}

Fig. S1 TG curves of zwitterions.

Table S1 Thermal property of zwitterions

Zwitterion [a]	$T_{d\text{-}5\%}$ [b] / °C
Mimps	326
Mims	302
Imds	226

[a] Prior to TG measurement, each zwitterion was dried at 120°C for 1 h under N_2.
[b] $T_{d\text{-}5\%}$: 5% weight loss temperature.

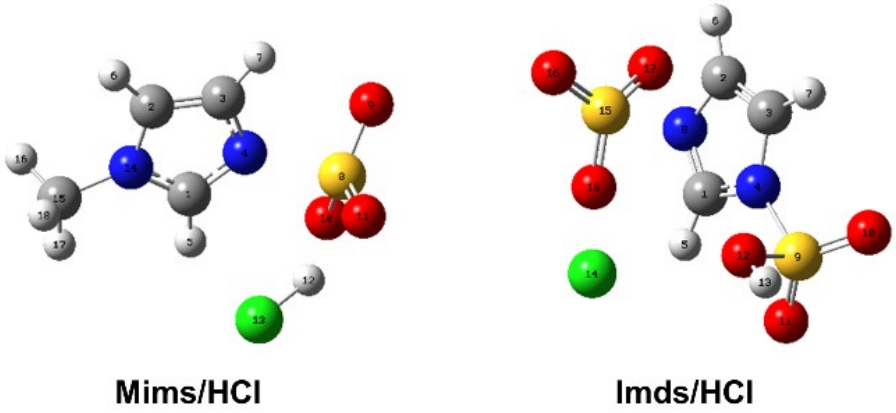
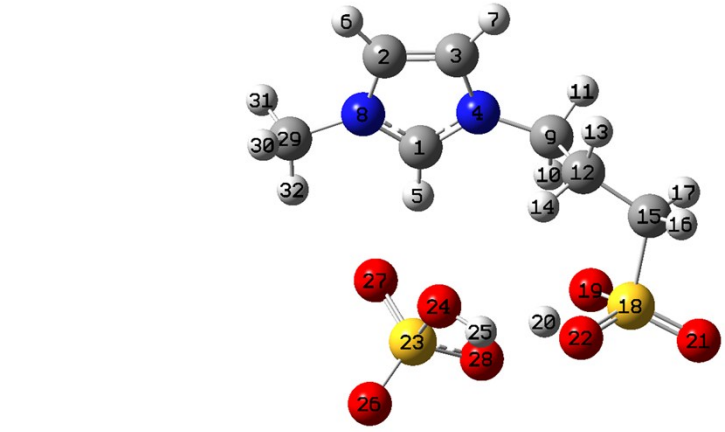


Fig. S2 Optimized molecular structures of BAILs with mono– or disulfuric acid groups using B3LYP/6-311G++(d, p).

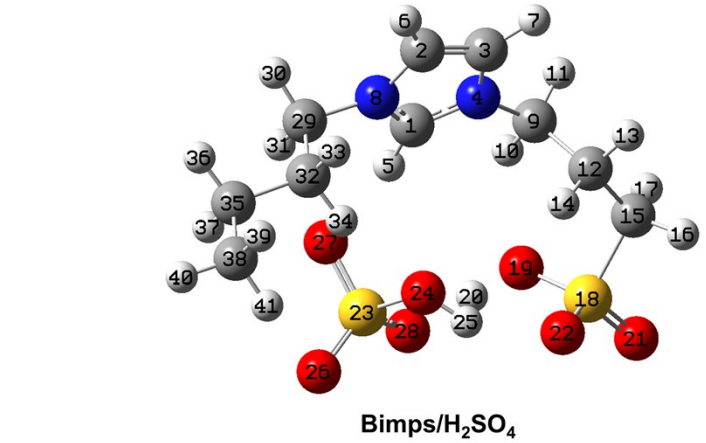
Table S2 Residual amount of residue after cellulose hydrolysis (160 °C, 15 min) in 1 M BAILs aqueous solution

Zw [a]	HX [b]	Glucose yield / %	Residue [c] / *wt*.%
Mimps	H_2SO_4	32.3±2.2	5.6
Bimps		30.7±2.2	19
Oimps		36.3±3.8	21
Mimps	HCl	23.7±0.3	24
Bimps		26.0±1.5	30
Oimps		27.7±1.2	26

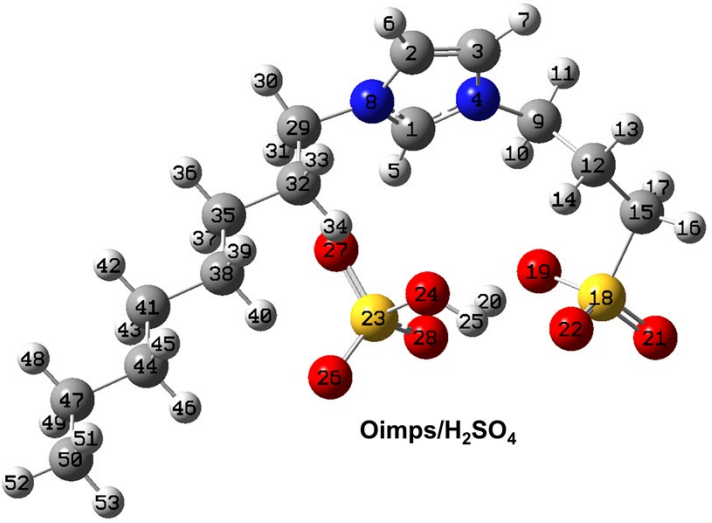
[a] Zw: zwitterion. [b] HX: kinds of acid used to prepare BAILs called as Zw/HX; X is corresponded to anion species. [c] Represented as *wt*.% to the starting weight of cellulose (10 mg).



Mimps/H_2SO_4



Bimps/H_2SO_4



Oimps/H_2SO_4

Fig. S3 (1) Optimized molecular structures of BAILs with HSO_4 anion using B3LYP/6-311G++(d, p).

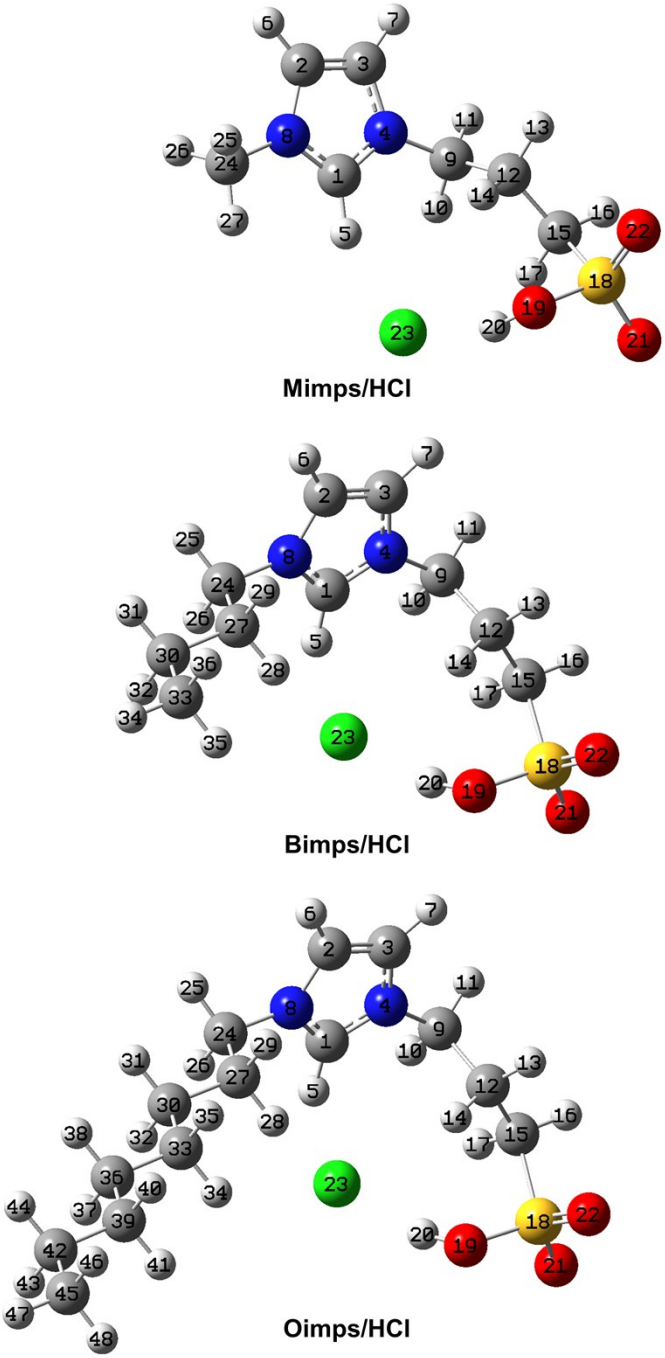


Fig. S3 (2) Optimized molecular structures of BAILs with Cl anion using B3LYP/6-311G++(d, p).

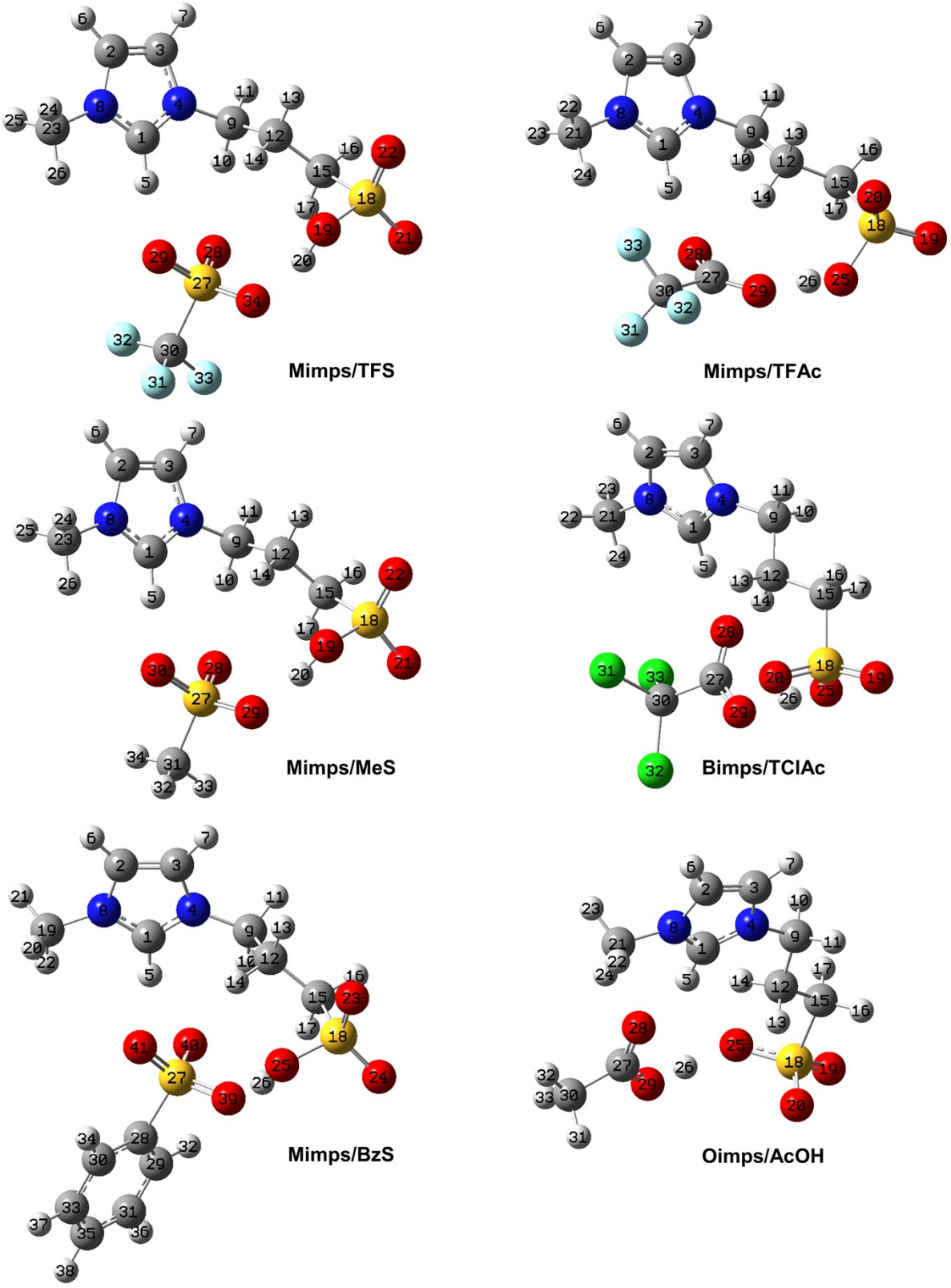
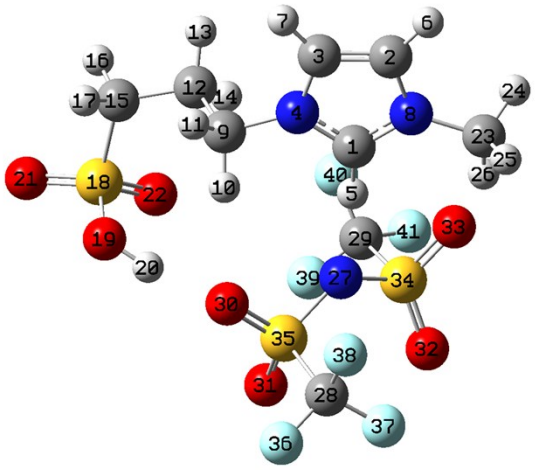
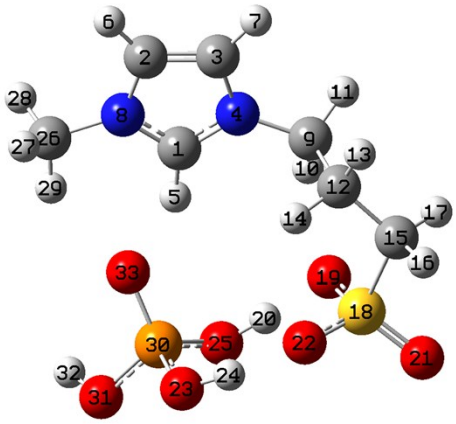


Fig. S3 (3) Optimized molecular structures of BAILs with sulfonic acid anon or carboxylic acid anion using B3LYP/6-311G++(d, p).



Mimps/HTFSI



Mimps/H_3PO_4

Fig. S3 (4) Optimized molecular structures of BAILs with TFSI anon or phosphoric acid anion using B3LYP/6-311G++(d, p).