Supplementary Information

Ether-functionalized ionic liquids as highly efficient SO₂ absorbents

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Fig. S-1. A photograph of a high pressure FT-IR cell
Fig. S-2 TGA curves of RTILs
Fig. S-3 Optimized structures of $E_0$, $E_1$, $E_2$, and $E_3$ are and their interactions with SO$_2$. 
Fig. S-4. $^1$H NMR spectra of $E_3$ showing the interactions with SO$_2$: (a) $E_3$, (b) $E_3$ under pressure of 2 bar of SO$_2$: (▲) C(2)-H, (●) C(4)-H and C(5)-H, and (★) N-CH$_2$.

To support the computational results on the nature of SO$_2$ absorption in ether-functionalized ILs, $^1$H NMR experiment was conducted in CDCl$_3$ with $E_3$ using a high pressure NMR tube. Fig. S-4-(a) and (b) are the $^1$H NMR spectra of $E_3$ and $E_3$ under pressure of 2 bar of SO$_2$, respectively. When a NMR tube containing a CDCl$_3$ solution of $E_3$ was pressurized with SO$_2$, the peak associated with the C(2)-H of the imidazolium ring is up-field shifted by 0.406 ppm from 9.678 to 9.272 ppm, indicating that the interaction between C(2)-H and methane sulfonate anion is reduced upon interaction with SO$_2$. This is reasonable because both SO$_2$ and C(2)-H possess acidic character and thus compete with each other toward the interaction with the basic methane sulfonate anion, resulting in the reduction of positive character on the imidazolium ring. Similarly to C(2)-H, the peaks corresponding to C(4)-H, C(5)-H, and N-CH$_2$ also up-field shifted. However, contrary to our expectation, there are no distinct changes in chemical shifts for the peaks associated with CH$_2$ and CH$_3$ connected to ether groups, suggesting that SO$_2$ interacts weakly with the ether oxygen atoms in $E_3$ through physical interactions.