Supplementary Material (ESI) for Energy & Environmental Science

Supplementary Information

Ether-functionalized ionic liquids as highly efficient SO_2 absorbents

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Fig. S-1. A photograph of a high pressure FT-IR cell

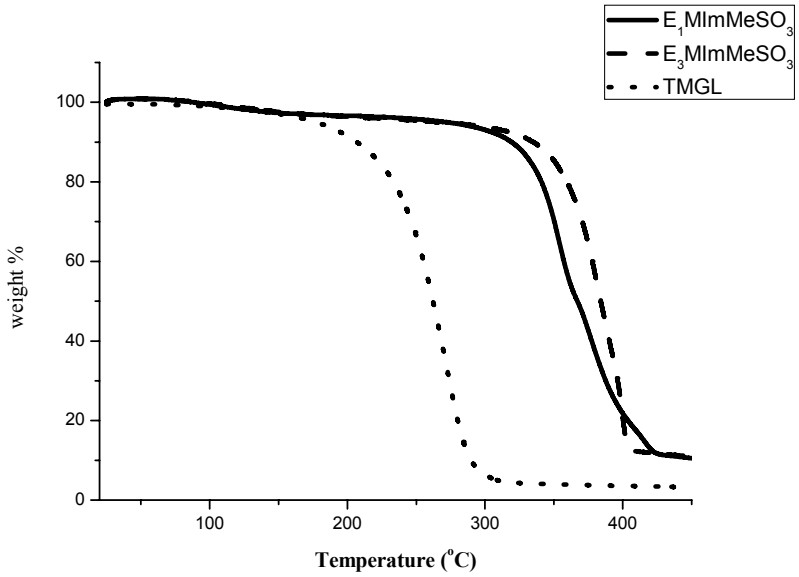

Fig. S-2TGA curves of RTILs

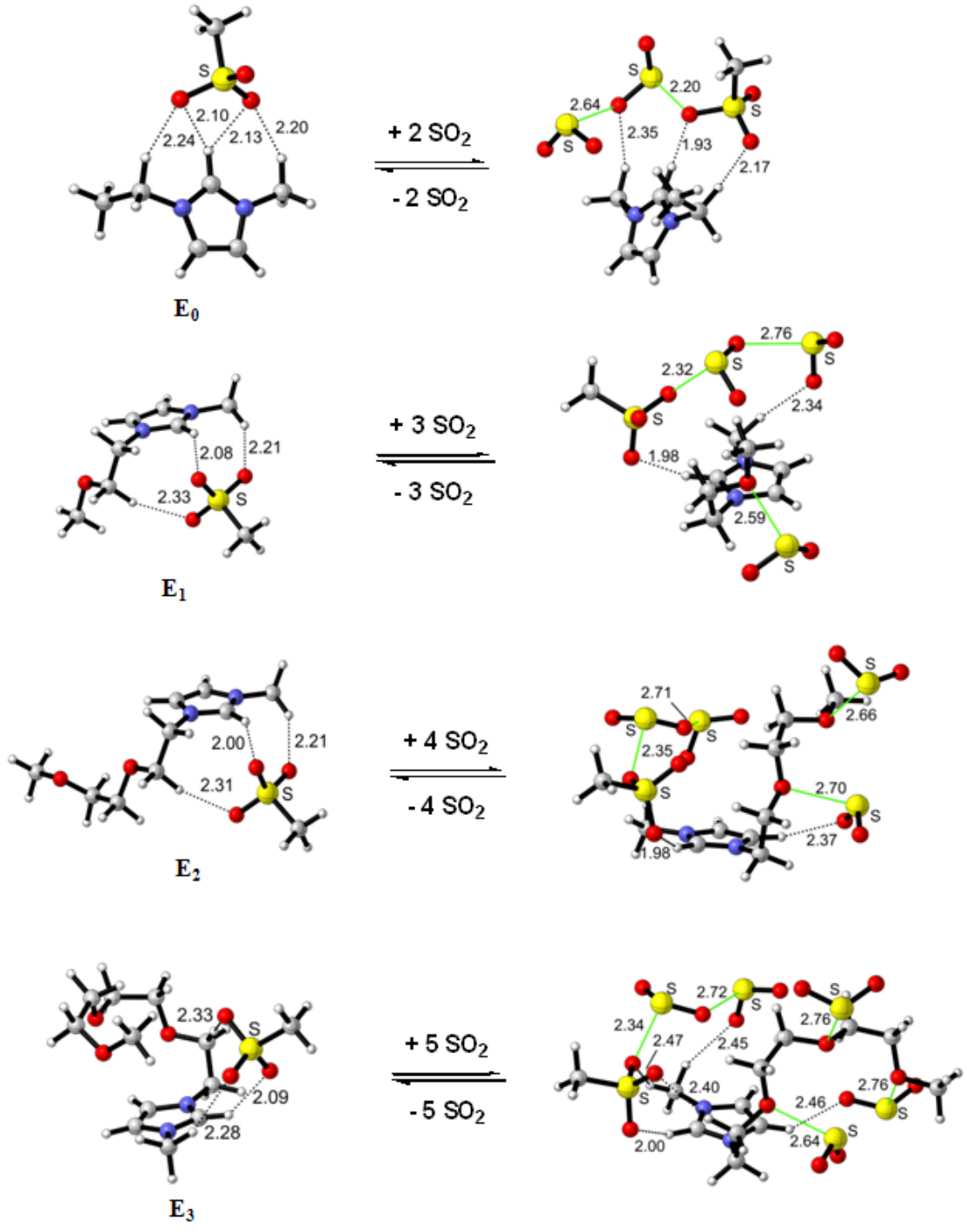

Fig. S-3 Optimized structures of $\mathbf{E_0}$, $\mathbf{E_1}$, $\mathbf{E_2}$, and $\mathbf{E_3}$ are and their interactions with SO_2.

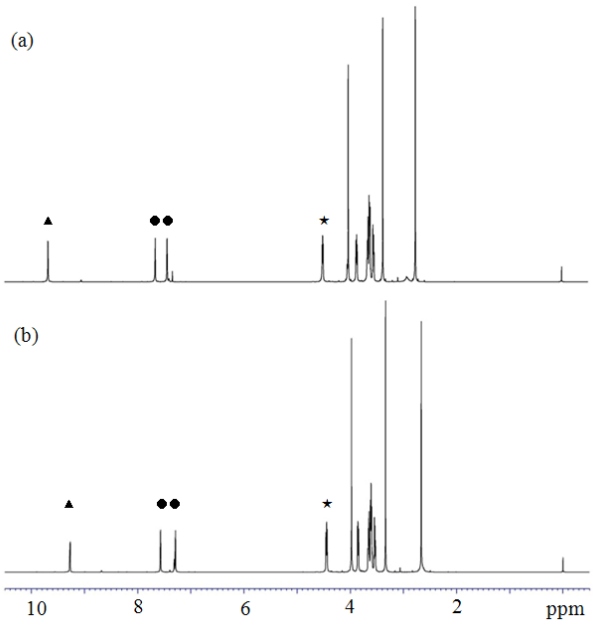

Fig. S-4. ^{1}H NMR spectra of $\mathbf{E_3}$ showing the interactionswith SO_2: (a) $\mathbf{E_3}$, (b) $\mathbf{E_3}$ under pressure of 2 bar of SO_2: (▲) C(2)-H, (●) C(4)-H and C(5)-H, and (★) N-CH_2.

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 $\mathbf{E_3}$ using a high pressure NMR tube. Fig. S-4-(a) and (b)are the ^{1}H NMR spectra of $\mathbf{E_3}$ and $\mathbf{E_3}$ under pressure of 2 bar of SO_2, respectively. When a NMR tube containing a $CDCl_3$ solution of $\mathbf{E_3}$ 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. Thisis 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_2interacts weakly with the ether oxygen atoms in $\mathbf{E_3}$ through physical interactions.