

## Supporting Information for

# Equimolar CO<sub>2</sub> capture by imidazolium-based ionic liquids and superbase systems

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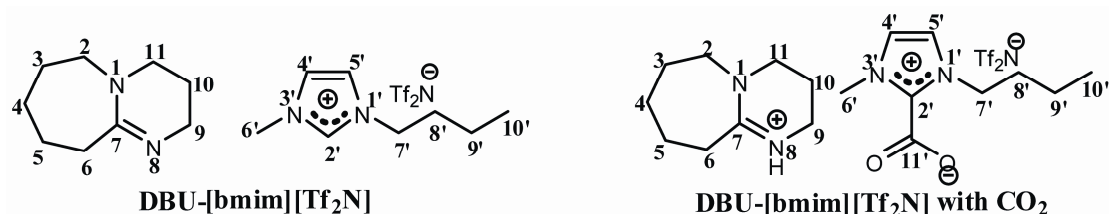
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### 1. $^1\text{H}$ and $^{13}\text{C}$ NMR in DBU-[bmim][Tf<sub>2</sub>N] with and without CO<sub>2</sub> system

**DBU-[bmim][Tf<sub>2</sub>N]**  $^1\text{H}$  NMR (CDCl<sub>3</sub>) 0.97 (m, 3H, bmim C10'), 1.37 (t, 2H, bmim C9'), 1.60 (t, 2H, DBU C3), 1.67(t, 4H, DBU C4 and C5), 1.89 (t, 4H, DBU C10 and bmin C8'), 2.40 (s, 2H, DBU C11), 3.24 (t, 6H, DBU C2, C6 and C9), 3.95 (s, 3H, bmim C6'), 4,17 (t, 2H, bmim C7'), 7.40 (d, 2H, bmin C4' and C5');  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>) 12.9 (bmim C10'), 19.0 (bmim C9'), 20.8 (DBU C10), 24.8 (DBU C4), 27.4 (DBU C5), 29.0 (DBU C6), 31.6 (DBU C3), 34.6 (bmim C6'), 35.2 (bmim C8'), 41.0 (DBU C11), 48.4 (DBU C9), 49.1 (bmim C7'), 53.1 (DBU C1), 117.8 (bmim C4'), 121.1 (bmim C5'), 122.0 (Tf<sub>2</sub>N C1), 122.7 (Tf<sub>2</sub>N C2), 136.0 (bmim C2'), 163.2 (DBU C7) ppm.

After the absorption of CO<sub>2</sub>, **DBU-[bmim][Tf<sub>2</sub>N] with CO<sub>2</sub>**  $^1\text{H}$  NMR (CDCl<sub>3</sub>) 0.93 (m, 3H, bmim C10'), 1.35 (t, 2H, bmim C9'), 1.72 (t, 6H, DBU C3, C4 and C5), 1.67(t, 4H, DBU C5 and bmim C8'), 1.87 (t, 4H, DBU C10 and bmim C8'), 2.60 (s, 2H, DBU C11), 3.42 (t, 6H, DBU C2, C6 and C9), 4.11 (s, 3H, bmim C6'), 4,56 (t, 2H, bmim C7'), 7.22 (s, 2H, bmin C4' and C5'), 11.66 (s, 1H, DBU N8);  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>) 12.9 (bmim C10'), 19.2 (bmim C9'), 20.1 (DBU C10), 24.3 (DBU C4), 26.9 (DBU C5), 28.9 (DBU C6), 32.4 (DBU C3), 33.5 (bmim C6'), 37.1 (bmim C8'), 39.6 (DBU C11), 48.1 (DBU C9), 49.4 (bmim C7'), 53.5 (DBU C1), 118.0 (bmim C4'), 121.2 (bmim C5'), 122.1 (Tf<sub>2</sub>N C1), 123.4 (Tf<sub>2</sub>N C2), 141.3 (bmim C2'), 155.6 (bmim C11'), 164.3 (DBU C7) ppm.



**Scheme S1.** Numbering scheme for positions in DBU-[bmim][Tf<sub>2</sub>N] system with and without CO<sub>2</sub>.

## 2. IR data with assignment in MTBD-[bmim][Tf<sub>2</sub>N] with CO<sub>2</sub> system

According to the literature,<sup>1-4</sup> the key bands for MTBD-[bmim][Tf<sub>2</sub>N] with CO<sub>2</sub> in Fig 2 can be assigned as follows:  $\nu_{\max}/\text{cm}^{-1}$ , 2965 and 2878 (CH stretch), 1669 (C=O stretch), 1600 (CN stretch), 1507 (NH stretch), 1443 (C=C stretch), 1349 (CH stretch), 1322 (SO<sub>2</sub> stretch) 1226 (CF stretch), 1175 (CH stretch), 1051 (SNS stretch).

### References:

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