Supporting Information

Cation-assisted interactions between N-heterocycles and CO$_2$

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**Table 1.** The binding energies (kJ/mol) calculated with the B3LYP, MP2, and M06-2X methods.

<table>
<thead>
<tr>
<th>Complex</th>
<th>B3LYP</th>
<th>MP2</th>
<th>M06-2X</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Without Li$^+$</td>
<td>With Li$^+$</td>
<td>∆E</td>
</tr>
<tr>
<td>1</td>
<td>-11.8</td>
<td>-25.7</td>
<td>-13.8</td>
</tr>
<tr>
<td>10</td>
<td>-106.8</td>
<td>-129.4</td>
<td>-22.6</td>
</tr>
<tr>
<td>12</td>
<td>-32.9</td>
<td>-122.1</td>
<td>-89.2</td>
</tr>
</tbody>
</table>

Calculations were carried out using the functionals of B3LYP,$^{[1]}$ MP2$^{[2]}$ and M06-2X $^{[3]}$ with the 6-31++(d,p) basis set, respectively.
Figure 1. NBO and NRT analyses of pyrr-CO$_2$-Li$^+$ complexes (10).
**SFigure 2.** Binding energy of neutral six-membered NHCs and CO$_2$ with Li$^+$ versus the NBO charge of the reacting N atom.

**SFigure 3.** Binding energy of five-membered NHCs and CO$_2$ with Li$^+$ versus the NBO lone pair energy of the reacting N atom.
Reference

