Electronic Supplementary Information

CO₂ capture and activation by superbase/polyethylene glycol and its subsequent conversion

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Table of Contents

1. General experimental methods S2
2. Characterization of the absorption system, amidinium/guanidinium alkylcarbonate salts, aziridines, ureas and oxazolidinones S2
3. Reference S7
4. The ¹H NMR and ¹³C NMR Charts, IR spectra for the absorption system, amidinium/guanidinium alkylcarbonate salts, aziridines, ureas and oxazolidinones S8
1. General experimental methods:

Caution

Experiments using compressed gases CO₂ are potentially hazardous and must only be carried out by using the appropriate equipment and under rigorous safety precautions.

Materials

Superbases and PEG used in this work were purchased from Alfa Aesar-A Johnson Matthey Company and dried under vacuum at 70 °C for one week before use. CO₂ with a purity of 99.999% was commercially available. Amines was refluxed for 10 h with CaH₂ and distilled prior to use. NH₂PEG150NH₂¹ and aziridines² was synthesized according to the reported method.

Experimental methods

¹H NMR spectra was recorded at Bruck 400 spectrometer in CDCl₃ and CDCl₃ (7.26 ppm) was used as internal reference, ¹³C NMR was recorded at 100.6 MHz in CDCl₃ and CDCl₃ (77.0 ppm) was used as internal reference. GC analyses were performed on Shimadzu GC-2014, equipped with a capillary column (RTX-17, 30 m × 0.25 μm) using a flame ionization detector. In situ FTIR was collected on a Mettler Toledo React IR ic10, Diamond ATR probe, using ic IR analysis system. The probe is placed in the middle of the absorption mixture, which is constantly stirred by magnetic whisk, and the spectra are collected in situ during CO₂ absorption. Infrared (IR) spectra were recorded on a Bruker Tensor27 FT-IR spectrophotometer with KBr pellets.

General procedure for CO₂ absorption

In a typical procedure, CO₂ capture was carried out in a 10 mL Schlenk flask. The absorbents were charged into the reactor at room temperature. Then, the air in the flask was replaced by CO₂ and a needle was used for CO₂ bubbling, which was inserted in the bottom of the flask. The absorption reaction was conducted at 40 °C with a CO₂ bubbling rate of 0.1 L/min. The amount of CO₂ absorbed was determined by an Analytical Balance within an accuracy of ±0.0001 g every five minutes. Absorption/desorption was determined by several cycles of repeated experiments.

General procedure for synthesis of value-added chemicals using captured CO₂

Taking the synthesis of 1,3-dibutylurea as an example: Firstly, DBU (3 mmol, 0.4567 g) and PEG₁₅₀ (3 mmol, 0.45 g) were charged into a glass tube, in which CO₂ was bubbled through a needle. Then, 1-butylamine was added after CO₂ absorption reached equilibrium. The tube was placed into a 25 mL stainless steel autoclave and then the mixture was stirred at predetermined temperature for 5 min to reach the equilibration. When the reaction finished, the reactor was cooled in ice-water and CO₂ was ejected slowly. An aliquot of sample was taken from the resultant mixture and dissolved in dry CH₂Cl₂ for GC analysis.

2. Characterization of the absorption system, amidinium/guanidinium alkylcarboxylate salts, aziridines, ureas and oxazolidinones

**DBU (1,8-diazabicyclo[5.4.0]undec-7-ene):**

¹H NMR (400 MHz, CDCl₃) δ 3.23 (t, J = 5.6 Hz, 2 H), 3.13-3.18 (m, 4 H), 2.33-2.35 (m, 2 H), 1.72-1.77 (m, 2 H), 1.60 (s, 4 H), 1.52 (s, 2 H); ¹³C NMR (100.6 MHz, CDCl₃) δ 161.6, 52.8, 48.3, 44.0, 37.2, 29.7, 28.4, 25.9, 22.3. IR 3420, 2924, 2851, 1616, 1486, 1441, 1366, 1260, 1233, 1183, 1115, 1060, 991, 955 cm⁻¹.

**PEG₁₅₀ (triethylene glycol, MW = 150 Da):**

¹H NMR (400 MHz, CDCl₃) δ 3.71 (t, J = 4.8 Hz, 4 H), 3.65 (s, 4 H), 3.59 (t, J = 4.8 Hz, 4 H), 3.40 (s, 2 H); ¹³C NMR (100.6 MHz, CDCl₃) δ 72.6, 70.3, 61.5. IR 3446, 2865, 2360, 2341, 2136, 1954, 1653, 1457, 1351, 1082, 937, 889, 830, 571, 525 cm⁻¹.

**DBU/PEG₁₅₀ + CO₂:**

¹H NMR (400 MHz, CDCl₃) δ 3.56-3.70 (m, 12 H), 3.29-3.34 (m, 6 H), 2.61 (s, 2 H), 1.85-1.90 (m, 2 H), 1.66-1.67 (m, 4 H), 1.59 (s, 2 H); ¹³C NMR (100.6 MHz, CDCl₃) δ 164.1, 158.5, 72.6, 70.3, 64.1, 61.3, 53.5, 48.4, 40.6, 34.1, 29.3, 27.6, 24.8, 20.8.
Fig. S1 The $^1$H NMR of DBU, PEG$_{150}$ and DBU/PEG$_{150}$ + CO$_2$ (CDCl$_3$, 400 MHz).
Table S1 The comparison of $^1$H and $^{13}$C NMR chemical shifts of DBU, PEG$_{150}$ and DBU/PEG$_{150}$ + CO$_2$

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Figure S2. Results of *in situ* FT-IR spectroscopy monitoring CO₂ capture by DBU/PEG₁₅₀ system at various times starting from CO₂ bubbling; The spectrum of DBU and PEG₁₅₀ was subtracted; ◆: CO₂ began to be bubbled at 40 °C; ◇: Temperature was gradually increased from 40 °C to 120 °C.

Figure S3. The scanning thermogravimetric analysis (TGA) results for DBU/PEG₆₀₀+CO₂ with a 10 °C min⁻¹ temperature ramping rate to 700 °C.

**PEG₆₀₀ (polyethylene glycol, MW = 600 Da):**

¹H NMR (400 MHz, CDCl₃) δ 3.57-3.69 (m, 44H), 2.75 (s, 2H); ¹³C NMR (100.6 MHz, CDCl₃) δ 72.4, 70.4, 70.2, 61.6. IR 3375, 2870, 1636, 1457, 1350, 1297, 1249, 1107, 951, 845, 735, 559 cm⁻¹.

**DBU/PEG₆₀₀ + CO₂:**

¹H NMR (400 MHz, CDCl₃) δ 3.59-3.70 (m, 53H), 3.29 (t, ³J = 5.6 Hz, 2H), 2.46 (s, 2H), 1.78-1.84 (m, 2H), 1.65 (s, 4H), 1.57 (s, 2H); ¹³C NMR (100.6 MHz, CDCl₃) δ 164.6, 157.7, 157.7, 77.2, 72.0, 69.8, 69.6, 63.5, 60.6, 53.3, 47.9, 38.4, 32.1, 28.5, 26.5, 23.8, 19.4. IR 3350, 2867, 2361, 2343, 1647, 1613, 1456, 1351, 1315, 1291, 1250, 1110, 993, 953, 885, 837, 731, 694, 546, 526 cm⁻¹.

**TBD (1,5,7-triazabicyclo[4.4.0]dec-5-ene):**

¹H NMR (400 MHz, CDCl₃) δ 3.29 (t, ³J = 5.6 Hz, 4H), 3.24 (t, ³J = 6 Hz, 4H), 1.96 (m, 4H); ¹³C NMR (100.6 MHz, CDCl₃) δ 151.2, 46.6, 38.0, 20.7. IR 3477, 3418, 3234, 3157, 2967, 2943, 2875, 2797, 2749, 2361, 2343, 1662, 1573, 1477, 1445, 1421, 1378, 1321, 1295, 1202, 1069, 884, 711, 671, 590 cm⁻¹.

**TBD/PEG₆₀₀ + CO₂:**
1H NMR (400 MHz, CDCl₃) δ 3.56-3.68 (m, 62H), 3.21-3.27 (m, 8H), 1.91-1.97 (m, 4H); 13C NMR (100.6 MHz, CDCl₃) δ 158.8, 150.7, 77.2, 72.0, 69.9, 69.7, 64.0, 60.7, 46.2, 37.0, 20.3. IR 3308, 3160, 2869, 2362, 1943, 1667, 1574, 1456, 1377, 1350, 1323, 1291, 1252, 1203, 1107, 951, 844, 745, 730, 714 cm⁻¹.

DBN ([1,5-diaza bicyclo[4.3.0]non-5-ene]):
1H NMR (400 MHz, CDCl₃) δ 3.28 (t, 3J = 4.8 Hz, 2H), 3.21 (t, 3J = 6.8 Hz, 2H), 3.13 (t, 3J = 6 Hz, 2H), 2.38 (t, 3J = 7.6 Hz, 2H), 1.83-1.91 (m, 2H), 1.70-1.76 (m, 2H); 13C NMR (100.6 MHz, CDCl₃) δ 160.5, 51.2, 43.8, 42.8, 31.3, 20.6, 19.4. IR 3409, 2929, 2845, 1651, 1496, 1422, 1363, 1288, 1232, 1195, 1133, 1051, 961, 903, 737, 677, 574 cm⁻¹.

DNM/[1,3-dimethylimidazolidin-2-ylidene)cyclohexanamine):
1H NMR (400 MHz, CDCl₃) δ 3.38-3.43 (m, 1H), 3.11 (s, 4H), 2.76 (s, 6H), 1.15-1.72 (m, 10H); 13C NMR (100.6 MHz, CDCl₃) δ 155.4, 54.0, 44.9, 36.5, 31.3, 25.8, 25.2.

NH₂PEG₃₀NH₂:
1H NMR (400 MHz, CDCl₃) δ 3.47 (s, 4 H), 3.35 (t, 3J = 5.2 Hz, 4 H), 2.71 (t, 3J = 5.2 Hz, 4 H), 1.17 (s, 1 H); 13C NMR (100.6 MHz, CDCl₃) δ 73.2, 70.0, 41.5. IR 3393, 2869, 1576, 1473, 1375, 1352, 1307, 1114, 817 cm⁻¹.

NH₂PEG₃₀NH₂/PEG150(molar ratio: 1: 2) + CO₂:
1H NMR (400 MHz, CDCl₃) δ 3.72 (t, 3J = 4 Hz, 12H), 3.66 (s, 8H), 3.59-3.62 (m, 12H), 3.54 (t, 3J = 4.8 Hz, 2H), 1.17 (s, 1 H); 13C NMR (100.6 MHz, CDCl₃) δ 62.8, 72.3, 69.8, 68.2, 60.7, 40.9, 39.3. IR 3365, 2870, 2361, 2342, 1576, 1558, 1473, 1457, 1350, 1279, 1256, 1109, 1035, 952, 890, 847, 763, 729, 698 cm⁻¹.

1.3-Dipropyl urea:
1H NMR (300 MHz, CDCl₃) δ 4.90 (bd, N-H), 3.08 (t, 3J = 6.45 Hz, 4H); 13C NMR (75.5 MHz, CDCl₃) δ 158.8, 42.1, 23.4, 11.3.

1.3-Diisopropyl urea:
1H NMR (300 MHz, CDCl₃) δ 3.80-3.87 (m, 4H), 1.14 (d, 3J = 6.4 Hz, 12H); 13C NMR (75.5 MHz, CDCl₃) δ 157.0, 42.2, 23.5.

1.3-Dibutyl urea:
1H NMR (400 MHz, CDCl₃) δ 4.77 (s, 2 H), 3.12-3.13 (m, 4H), 1.42-1.49 (m, 4H), 1.28-1.37 (m, 4H), 0.91 (t, 3J = 7.2 Hz, 6H); 13C NMR (100.6 MHz, CDCl₃) δ 158.7, 40.2, 32.3, 20.0, 13.7.

1.1,3,3-Tetraethyl urea:
1H NMR (300 MHz, CDCl₃) δ 2.56 (t, 3J = 7.2 Hz, 8H), 1.36-1.49 (m, 8H), 1.24-1.33 (m, 8H), 0.87 (t, 3J = 7.2 Hz, 12H); 13C NMR (75.5 MHz, CDCl₃) δ 164.3, 49.7, 32.2, 20.5, 13.9.
Octahydro-benzoimidazol-2-one:
$^1$H NMR (300 MHz, D$_2$O) $\delta$ 3.12-3.32 (m, 2H), 1.53-1.60 (m, 4H), 1.15-1.35 (m, 4H); $^{13}$C NMR (75.5 MHz, D$_2$O) $\delta$ 164.1, 53.3, 32.2, 24.2.

1-Ethyl-2-phenylaziridine:
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.18-7.31 (m, 5H), 2.44 (q, $^3$J = 9.6 Hz, 2H), 2.30 (dd, $^3$J = 4.4 Hz, $^4$J = 4.8 Hz, 1H), 1.89 (d, $^2$J = 4.4 Hz, 1H). 1.65 (d, $^2$J = 8.8 Hz, 1H), 1.17 (t, $^3$J = 9.6 Hz, 3H); ESI-MS calcd for C$_{10}$H$_{13}$N 147.10, found 148.31 [M + H]$^+$. 

1-Propyl-2-phenylaziridine:
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.95 (t, $^3$J = 10.0 Hz, 3H), 1.60-1.67 (m, 3H), 1.89 (d, $^2$J = 4.0 Hz, 1H), 2.24-2.33 (m, 2H), 2.43-2.51 (m, 1H), 7.18-7.31 (m, 5H); ESI-MS calcd for C$_{11}$H$_{15}$N 161.12, found 162.28 [M + H]$^+$. 

2-(4-Chlorophenyl)-1-ethylaziridine:
$^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 1.18 (t, $^3$J = 6.9 Hz, 3H), 1.65 (d, $^2$J = 6.6 Hz, 1H), 1.83 (d, $^2$J = 3.3 Hz, 1H), 2.25-2.46 (m, 3H), 7.15-7.23 (m, 4H); ESI-MS calcd for C$_{10}$H$_{12}$NCl 181.66, found 182.13 [M + H]$^+$. 

2-(4-Methylphenyl)-1-ethylaziridine:
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 1.19 (t, $^3$J = 7.2 Hz, 3H), 1.62 (d, $^2$J = 6.4 Hz, 1H), 1.86 (d, $^2$J = 3.2 Hz, 1H), 2.26 (dd, $^3$J = 3.6 Hz, $^3$J = 3.2 Hz, 1H), 2.31 (s, 3H), 2.37-2.48 (m, 2H), 7.09-7.15 (m, 4H); ESI-MS calcd for C$_{11}$H$_{15}$N 161.24, found 162.20 [M + H]$^+$. 

3-Ethyl-5-phenyloxazolidin-2-one:
Colorless liquid; $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 1.17 (t, $^3$J = 7.2 Hz, 3H), 3.29-3.45 (m, 3H), 3.92 (t, $^3$J = 8.7 Hz, 1H), 5.48 (t, $^3$J = 7.8 Hz, 1H), 7.34-7.42 (m, 5H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 12.4, 38.8, 51.5, 74.2, 125.4, 128.6, 128.8, 138.8, 157.5; ESI-MS calcd for C$_{11}$H$_{13}$NO$_2$ 191.09, found 192.29 (M + H)$^+$, 214.38 (M + Na)$^+$, 405.01 (2M + Na)$^+$. 

3-Ethyl-4-phenyloxazolidin-2-one:
Colorless liquid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 1.05 (t, $^3$J = 7.2 Hz, 3H), 2.79-2.88 (m, 1H), 3.48-3.57 (m, 1H), 4.10 (t, $^3$J = 8.0 Hz, 1H), 4.62 (t, $^3$J = 8.8 Hz, 1H), 4.81 (t, $^3$J = 7.2 Hz, 1H), 7.30-7.44 (m, 5H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 12.1, 36.8, 59.3, 69.7, 126.9, 129.0, 129.2, 137.8, 158.1; ESI-MS calcd for C$_{11}$H$_{13}$NO$_2$ 191.09, found 192.29 (M + H)$^+$, 214.38 (M + Na)$^+$, 405.01 (2M + Na)$^+$. 

3-Propyl-5-phenyloxazolidin-2-one:
Colorless liquid; $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 0.91 (t, $^3$J = 7.2 Hz, 3H), 1.52-1.61 (m, 2H), 3.18-3.31 (m, 2H) 3.40 (t, $^3$J = 8.0 Hz, 1H), 3.90 (t, $^3$J = 8.8 Hz, 1H), 5.46 (t, $^3$J = 8.0 Hz, 1H), 7.31-7.37 (m, 5H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 10.7, 20.3, 45.5, 51.8, 74.0, 125.2, 128.4, 128.5, 137.8, 157.6; ESI-MS calcd for C$_{12}$H$_{15}$NO$_2$ 205.11, found 206.30 (M + H)$^+$, 228.30 (M + Na)$^+$, 433.04 (2M + Na)$^+$. 

3-Ethyl-5-(4-chlorophenyl)oxazolidin-2-one:
White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 1.17 (t, $^3$J = 7.3 Hz, 3H), 3.30-3.43 (m, 2H), 3.69-3.76 (m, 1H), 3.92 (t, $^3$J = 8.7 Hz, 1H), 5.44 (t, $^3$J = 8.0 Hz, 1H), 7.27-7.38 (m, 4H); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 12.6, 45.5, 51.8, 74.0, 125.1, 125.4, 126.9, 129.1, 134.7, 137.4, 157.4; ESI-MS calcd for C$_{11}$H$_{12}$ClNO$_2$ 225.67, found 451.64 (2M + H)$^+$. 

3-Ethyl-5-p-tolyloxazolidin-2-one:
White solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 1.18 (t, $^3$J = 7.3 Hz, 3H), 1.62 (d, $^3$J = 6.4 Hz, 1H), 1.87 (d, $^3$J = 3.2 Hz, 1H), 2.27 (dd, $^3$J = 6.6 Hz, $^3$J = 3.2 Hz, 1H), 2.31 (s, 3H), 2.36-2.48 (m, 2H), 7.09-7.15 (m, 4H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 12.6, 21.2, 38.9, 51.6, 74.3, 125.6, 129.5, 135.8, 138.7, 157.7; ESI-MS calcd for C$_{12}$H$_{15}$NO$_2$ 205.25, found 206.45 (M + H)$^+$, 411.15 (2M + H)$^+$. 

3. Reference
4. The $^1$H NMR and $^{13}$C NMR Charts, IR spectra for the absorption system, amidinium/guanidinium alkylcarbonate salts, urea and oxazolidinones
IR spectrum of DBU:

![IR spectrum of DBU](image)

Wavenumber cm⁻¹

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1H NMR (CDCl₃, 400 MHz)

![1H NMR spectrum](image)
IR spectrum of PEG$_{150}$: 

13C NMR (CDCl$_3$, 100.6 MHz)
1H NMR (400 MHz, CDCl₃)

13C NMR (100.6 MHz, CDCl₃)
IR spectrum of PEG_{600}.
IR spectrum of DBU/PEG$_{600}$ + CO$_2$:

![IR spectrum of DBU/PEG$_{600}$ + CO$_2$](image)

Electronic Supplementary Material (ESI) for Energy & Environmental Science
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1H NMR (CDCl₃, 400 MHz)

13C NMR (CDCl₃, 100.6 MHz)

IR spectrum of TBD:
IR spectrum of TBD/PEG_{600} + CO_{2}:

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3308.71  3160.58  2869.84  2362.10  1943.54  1667.96  1574.37  1456.69  1377.38  1350.41  1323.51  1291.81  1252.14  1203.74  1107.97  951.43  844.62  745.85  730.32  714.07  500
1000  1500  2000  2500  3000  3500
Wavenumber cm^{-1}

5 10 15 20 25 30 35 40
Transmittance [%]
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**13C NMR** (CDCl\textsubscript{3}, 100.6 MHz)

TBD/PEG\textsubscript{600} + CO\textsubscript{2}
1H NMR (CDCl₃, 400 MHz)

13C NMR (CDCl₃, 100.6 MHz)

IR spectrum of DBN:
1H NMR  \(\text{CDCl}_3, 400 \text{ MHz}\)
IR spectrum of DBN/PEG<sub>600</sub> + CO<sub>2</sub>:

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1H NMR  (CDCl₃, 400 MHz)

13C NMR  (CDCl₃, 100.6 MHz)

IR spectrum of TMG:
13C NMR (CDCl₃, 100.6 MHz)

IR spectrum of TMG/PEG₆₀₀ + CO₂:

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IR spectrum of DMICH/PEG\textsubscript{600} + CO\textsubscript{2}:

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IR spectrum of NH$_2$PEG$_{150}$NH$_2$: 

H$_2$N $\overset{\text{C}}{\text{O}}$ $\overset{\text{C}}{\text{O}}$ $\overset{\text{C}}{\text{O}}$ NH$_2$

$^{13}$C NMR (CDCl$_3$, 100.6 MHz)
IR spectrum of NH$_2$PEG$_{150}$NH$_2$/PEG$_{150}$ (molar ratio: 1:2) + CO$_2$: 
1,3-Dipropyl urea:

\[
\begin{array}{c}
\text{H} \\
\text{O} \\
\text{N} \\
\text{N}
\end{array}
\]

\[^{1}H\text{ NMR (CDCl}_3\text{, 300 MHz)}\]
$^{13}$C NMR (CDCl$_3$, 75.5 MHz)

1,3-Diisopropyl-urea:

$^1$H NMR (CDCl$_3$, 300 MHz)
$^{13}$C NMR (CDCl$_3$, 75.5 MHz)
1H NMR (CDCl₃, 400 MHz)

13C NMR (100.6 MHz, CDCl₃)

1,1,3,3-Tetrabutyl urea:

¹H NMR (CDCl₃, 300 MHz)
Octahydro-benzoimidazol-2-one:

$^1$C NMR (CDCl$_3$, 75.5 MHz)

$^1$H NMR (D$_2$O, 300 MHz)
$^{13}$C NMR (D$_2$O, 75.5 MHz)
1H NMR (400MHz, CDCl3)

1H NMR (300MHz, CDCl3)
1H NMR (300 MHz, CDCl3)

13C NMR (75 MHz, CDCl3)
1H NMR (300 MHz, CDCl₃)

13C NMR (75 MHz, CDCl₃)

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