A Green Sorbent for CO$_2$ Capturing: $\alpha$-Cyclodextrin based Carbonate in DMSO Solution

Ala’a F. Eftaiha,*a Abdussalam K. Qaroush,*b Fatima Alsoubani,a Thomas M. Pehl,c Carsten Troll,c Bernhard Rieger,c Bassem A. Al-Maythalony,d and Khaleel I. Assaf*e

a. Department of Chemistry, The Hashemite University, P.O. Box 150459, Zarqa 13115, Jordan. E-mail: alaa.eftaiha@hu.edu.jo
b. Department of Chemistry, Faculty of Science, The University of Jordan, Amman 11942, Jordan. E-mail: a.qaroush@ju.edu.jo
c. WACKER-Lehrstuhl für Makromolekulare Chemie, Technische Universität München, Lichtenbergstraße 4, Garching bei München, Germany.
d. King Abdulaziz City for Science and Technology-Technology Innovation Center on Carbon Capture and Sequestration (KACST-TIC on CCS), King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia.
e. Department of Chemistry, Faculty of Science, Al-Balqa Applied University, P.O. Box 19117, Al-Salt, Jordan. E-mail: k.assaf@jacobs-university.de

Figure S1. $^1$H NMR spectra of: (a) $\alpha$-CD/DMSO-$d_6$ (blue). (b) & (c) $\alpha$-CD/KOH/DMSO-$d_6$ before (black) and after (red) bubbling CO$_2$, respectively.
Figure S2. $^{13}$C NMR spectra of $\alpha$-CD/NaH/DMSO-$d_6$ before (black) and after (red) bubbling CO$_2$.

Figure S3. $^{13}$C NMR spectra of permethylated $\alpha$-CD/KOH/DMSO-$d_6$ before (black) and after (red) bubbling CO$_2$. 
Table S1. $pK_a$ values in DMSO and gas phase proton affinity values of the hydroxyl group at the C2 and C6 positions.

<table>
<thead>
<tr>
<th>Carbinol Position</th>
<th>$pK_a$</th>
<th>PA/ kcal mol$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2</td>
<td>23.2</td>
<td>332.3</td>
</tr>
<tr>
<td>C6</td>
<td>29.2</td>
<td>349.6</td>
</tr>
</tbody>
</table>

$^a$ Calculations were carried out using the B3LYP density functional with the 6-31G* basis set; see the computational method section in the main text.