Electronic Supplementary Material (ESI) for RSC Advances.

A Green Sorbent for CO_2 Capturing: α-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*

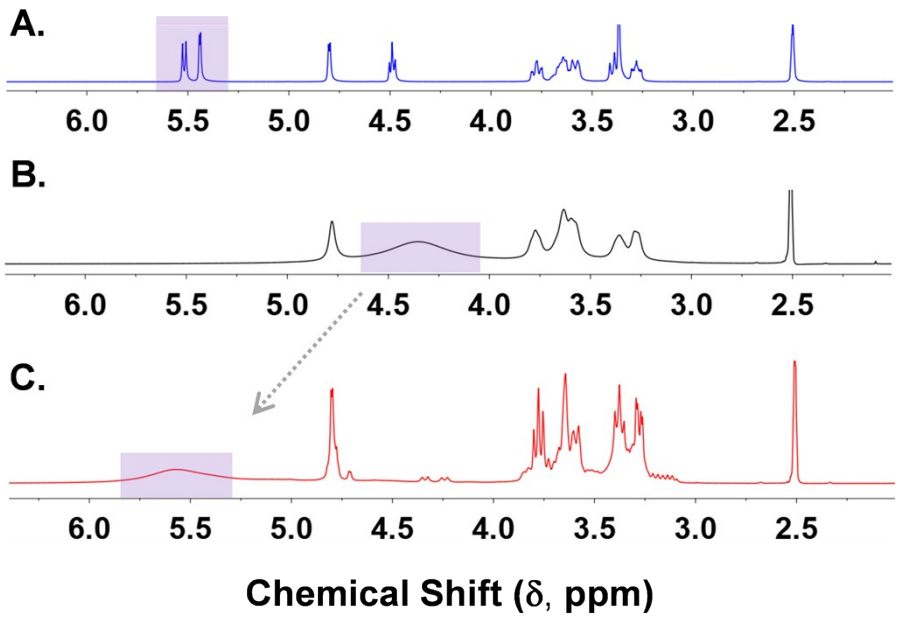

Figure S1. ^{1}H NMR spectra of: **(a)** α-CD/DMSO-d_6 (**blue**). **(b)** & **(c)** α-CD/KOH/DMSO-d_6 before (**black**) and after (**red**) bubbling CO_2, respectively.

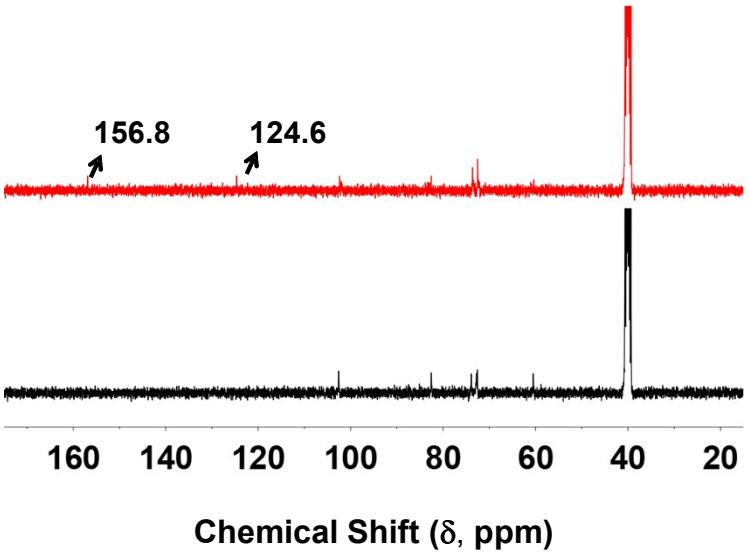

Figure S2. ^{13}C NMR spectra of α-CD/NaH/DMSO-d_6 before (**black**) and after (**red**) bubbling CO_2.

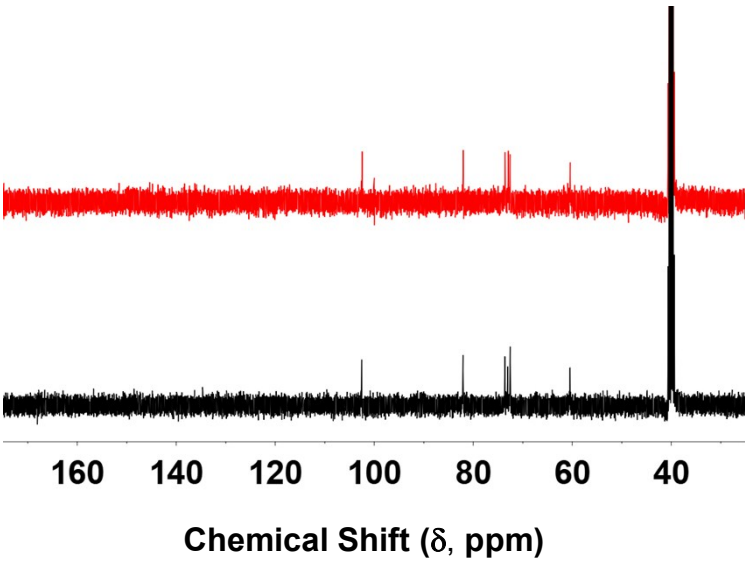

Figure S3. ^{13}C NMR spectra of permethylated α-CD/KOH/DMSO-d_6 before (**black**) and after (**red**) bubbling CO_2.

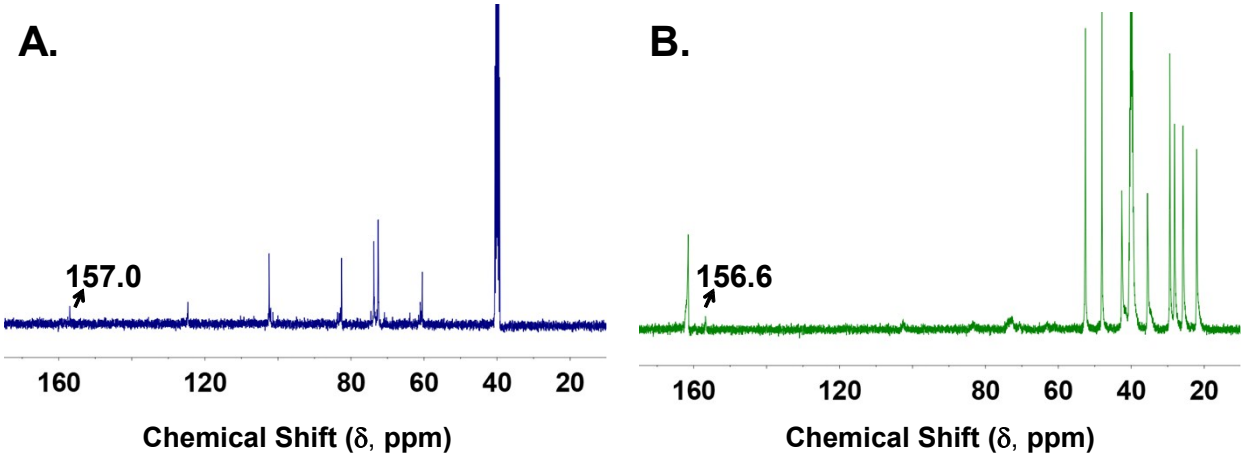

Figure S4. ^{13}C NMR spectra of: **(a)** α-CD/NaOH/DMSO-d_6 (**navy**). **(b)** α-CD/DBU/DMSO-d_6 (**green**) after bubbling CO_2.

Table S1. pK_a values in DMSO and gas phase proton affinity values of the hydroxyl group at the **C2** and **C6** positions.

Carbinol Position	**pK_a** [a]	**PA/ kcal mol^{-1}** [a]
C2	23.2	332.3
C6	29.2	349.6

[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.