

Supporting information

Efficient CO₂ absorption by azolide-based deep eutectic solvents

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Experimental section

Materials and characterizations: Tetraethylammonium hydroxide (35% w/w) water solution and the exchange resin (OH⁻ type) were purchased from Alfa Aesar. Imiazole (99%) and Ethylene glycol (99.5%, Super dry) were obtained from J&K scientific. Ethylene glycol was dried by 4Å molecular sieve prior to use. 1,2,4-Triazole was provide by Beijing Ouhe Technology Co., LTD. Tetraethylphosphonium bromide ([P₂₂₂₂]⁺Br⁻) was purchased from TCI. The infrared spectra were recorded on a PerkinElmer Frontier FTIR spectrometer on a KBr disk. The ¹H NMR spectra were taken on a Bruker spectrometer (400 MHz) and the ¹³C NMR spectra were recorded at 100.6 MHz, using the d₆-DMSO as the internal reference.

Synthesis of azolide ILs. All the azolide ILs were prepared based on the reported procedure.^[1] Typically, for the synthesis of [P₂₂₂₂][Triz], a solution of [P₂₂₂₂][OH] in water was prepared from [P₂₂₂₂][Br] using the anion-exchange resin method. The concentration of [P₂₂₂₂][OH] in water solution was titrated with potassium hydrogen phthalate. Equimolar 1,2,4-triazole was added to the water solution of [P₂₂₂₂][OH]. After the mixture was stirred for 2 hours at room temperature, the water in the solution was removed by using rotary evaporation at 70 °C. The obtained product was dried under vacuum at 80 °C.

Synthesis of DESs: The azolide IL and ethylene glycol were simply mixed at the molar ratio of 1:2. Then, the mixture was stirred at 80 °C until a liquid was formed, which was cooled down to room temperature prior to use.

Absorption and Desorption of CO₂: A DESs (~2g) was added into a glass tube with an inner diameter of 10 mm. The glass tube was partially immersed into the water bath at 25 °C. Carbon dioxide was bubbled through the needle into the DESs at a flow rate of 50 ml / min. The weight of the absorbent was weighed at regular intervals using an electronic analytical balance with an accuracy of ±0.1 mg.

In the desorption of CO₂, N₂ of atmospheric pressure (50 mL /min) was bubbled through the solutions at required temperature. The weight of the solution was

determined at regular intervals during the desorption process by the electronic balance.

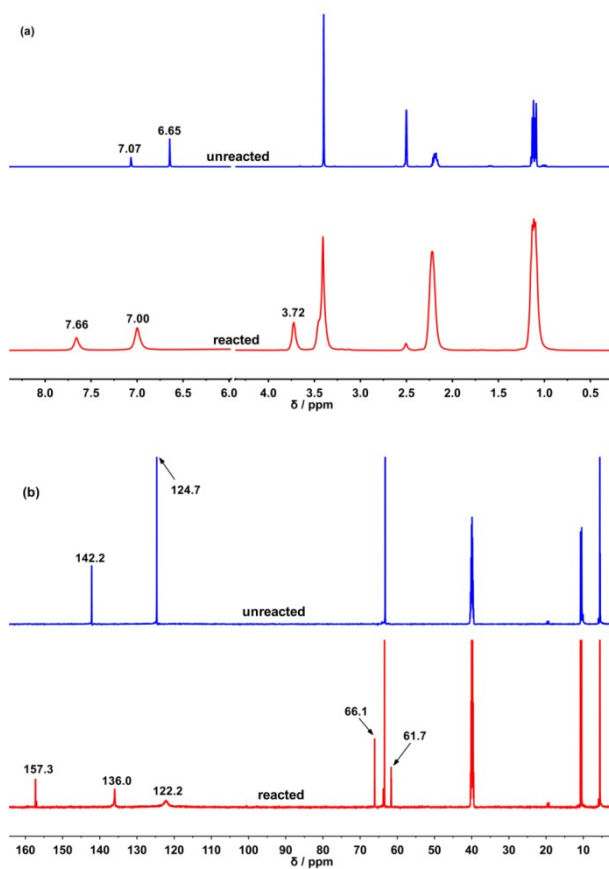
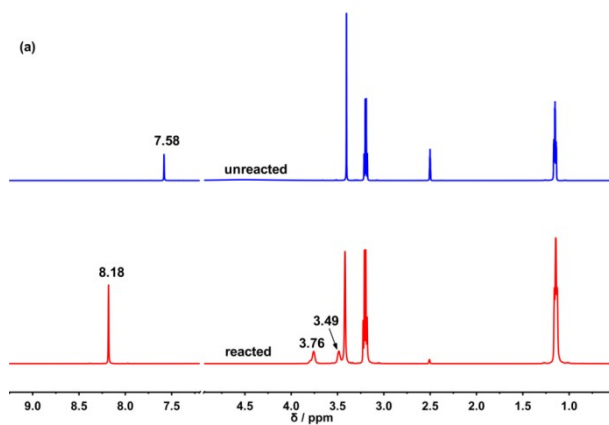


Fig. S1. The ^1H (a) and ^{13}C NMR (b) spectra of $[\text{P}_{2222}][\text{Im}]\text{-EG}$ (1:2) before and after CO_2 uptake.



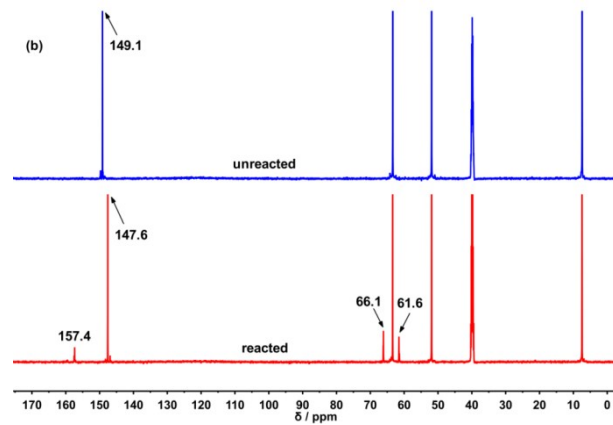
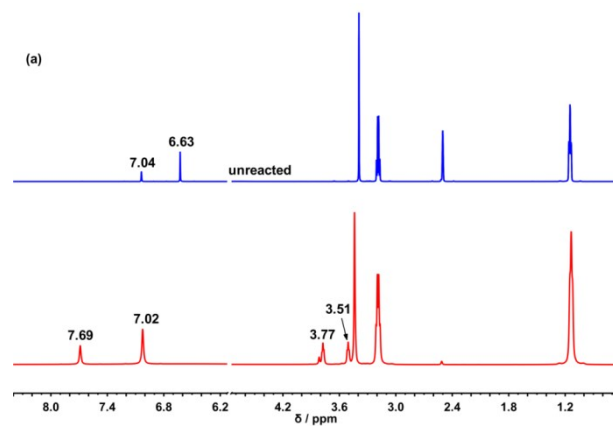


Fig. S2. The ¹H (a) and ¹³C NMR (b) spectra of [N₂₂₂₂][Triz]-EG (1:2) before and after CO₂ uptake.



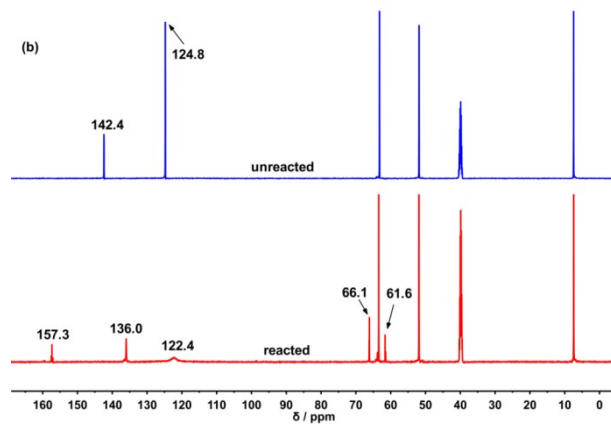


Fig. S3. The ^1H (a) and ^{13}C NMR (b) spectra of $[\text{N}_{2222}][\text{Im}]\text{-EG}$ (1:2) before and after CO_2 uptake.

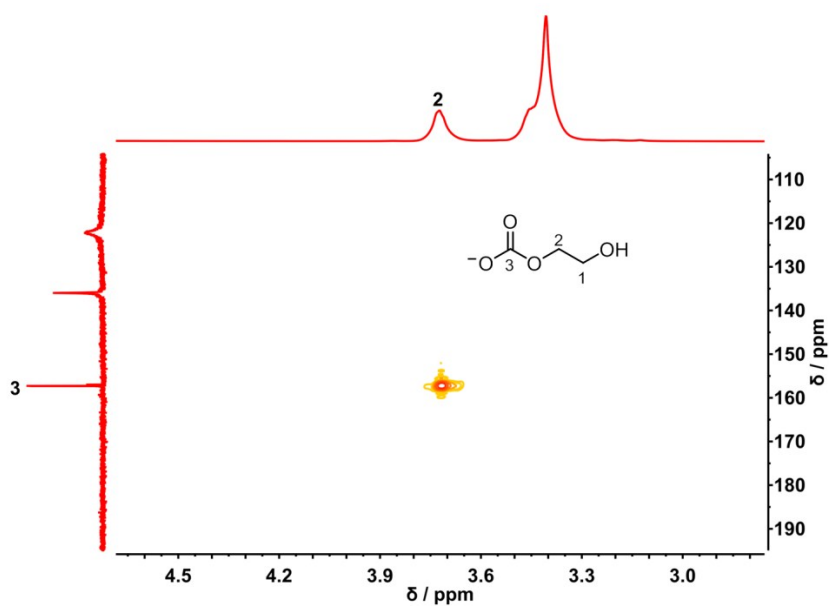


Fig. S4. The ^1H - ^{13}C HMBC spectra of $[\text{P}_{2222}][\text{Im}]\text{-EG}$ (1:2) after CO_2 uptake.

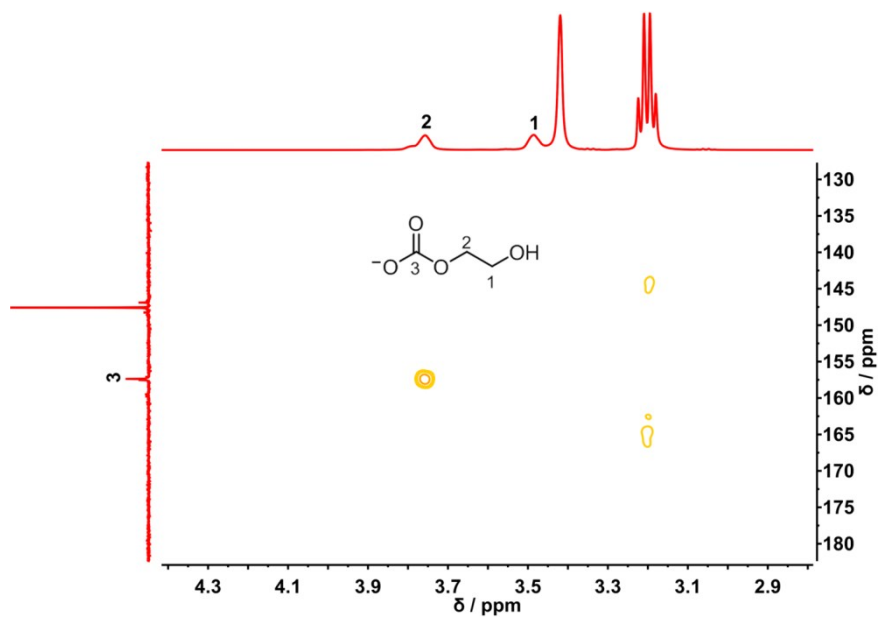


Fig. S5. The ^1H - ^{13}C HMBC spectra of $[\text{N}_{2222}][\text{Triz}]\text{-EG}$ (1:2) after CO_2 uptake.

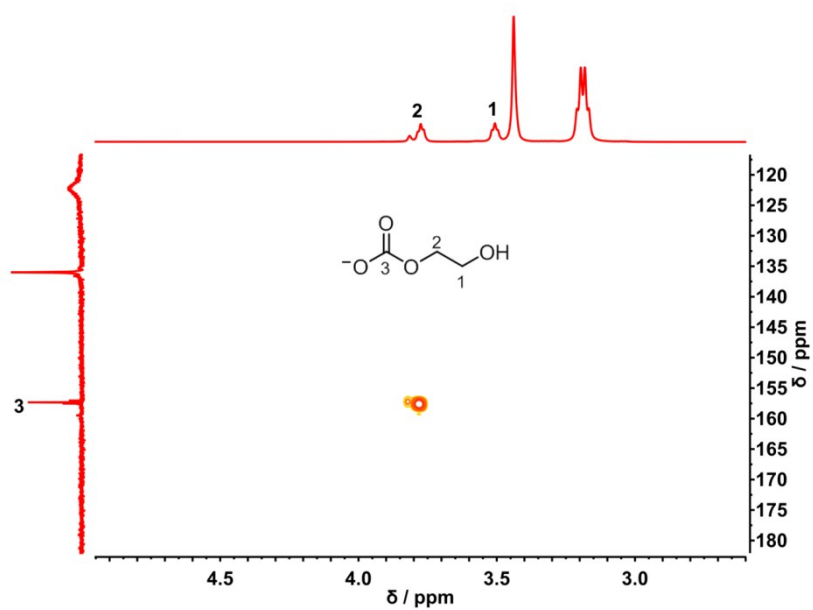


Fig. S6. The ^1H - ^{13}C HMBC spectra of $[\text{N}_{2222}][\text{Im}]\text{-EG}$ (1:2) after CO_2 uptake.

References:

- [1] C. Wang, X. Luo, H. Luo, D.-e. Jiang, H. Li, S. Dai, *Angew. Chem. Int. Ed.*, **2011**, *50*, 4918-4922.