Ester Group–Induced Formation of Alkylcarbonate Species from CO_2 and Tetramethylammonium Salts with a β -Amino Acid Anion

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Tetramethylammonium salts bearing a β -amino acid anion (TMAA) were synthesized via Michael addition reaction of amines with methyl acrylate followed by the hydrolysis and neutralization with tetramethylammonium hydroxide, and their CO₂ capture performances were evaluated in water or alcohol. Thus prepared TMAAs were found to interact with CO₂ in a 1:1 mode in both water and an alcohol. FT-IR and ¹³C NMR spectroscopy studies on the interactions of TMAA with CO₂ indicate that the type CO₂ adduct varies with the solvent employed. In water solvent, bicarbonate species is produced, whereas hydroxyethylcarbonate and methylcarbonate species are generated in EG and methanol, respectively. Computational calculations show that the carboxylate groups of TMAAs contribute to the formation and stabilization of 1:1 CO₂ adducts through the hydrogen bonding interactions with the hydrogen atom of amino groups.