## Analysis on the Reaction between CO<sub>2</sub> and NH<sub>3</sub> in Aqueous System for CO<sub>2</sub> Capture

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We analyzed the reaction between  $\mathrm{CO}_2$  and  $\mathrm{NH}_3$  in aqueous system by calculation and experiment. The quatitative profile of six species could be obtained by calculation, while the experimental methods used to investigate the reaction qualitatively were 13C Solid State NMR and FT-IR at the initial concentration range of 5 to 25 wt%  $\mathrm{NH}_3$  under the condition of 25°C and 1 atm. As its loading of  $\mathrm{CO}_2$  increased above 0.5 in the process of reacting to  $\mathrm{CO}_2$ , the content of bicarbonate increased relatively by means of the formation reaction of or conversion into bicarbonate, demonstrating that solid precipitates were produced by ammonium bicarbonate due to the limitation of solubility. Depending on the concentration of NH3 and reaction time under the same experimental condition, pH of reaction products could be determined. When three species of products, which were ammonium carbamate, ammonium carbonate, and ammonium bicarbonate, approached to pHs which make themselves exist stably, the formation reaction of them occurs favorably. The qualitative behavior of reaction derived by FT-IR and pH measurement confirms the validity of simulation by comparing to the profiles of bicarbonate and carbamate by calculation.