

### Analysis of CO<sub>2</sub>-NH<sub>3</sub>-H<sub>2</sub>O System by PCA and 2D IR COS

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Herein, the influence of reaction temperature on the CO<sub>2</sub> and NH<sub>3</sub> reaction in an aqueous solution is demonstrated by a principal component analysis (PCA) and the two dimensional correlation analysis (2D IR COS) obtained from FT-IR, dependent on the reaction time. In contrast to the reaction at 298 K, conversion of the dominant reaction from carbamation to bicarbonation and respective conformational changes were observed at 278 K by PCA and 2D IR COS. The PCA results elucidate that the turnover of two major reactions with the reduction of pH values was tracked in region II, where precipitation of ammonium bicarbonate occurred due to the limitation of solubility at this turning point. The interrelation of and the sequential variation of conformations in regions I and II were investigated by synchronous and asynchronous 2D correlation analyses. The combination of PCA and 2D IR COS provides a powerful and useful analytic method to capture and monitor the dynamics of complex chemical reactions.