Crystalline Products of CO_2 Capture by Amines

Victoria Sena, Sofia Antal, Omar Cano, Boris Averkiev, Tatiana Timofeeva

Department of Chemistry, New Mexico Highlands University, Las Vegas, NM

Department of Chemistry and Biochemistry, University of Colorado Boulder, Boulder, CO

Due to their unique ability to react directly and reversibly with CO_2 to form carbamates, primary and secondary amines are widely acknowledged as a prospective means of CO_2 capture and solid storage. Piperazine has become a prime focus of amine-based research for post-combustion capture. The kinetics of piperazine's reversible reactivity with CO_2 have been vastly described in literature. A series of experiments was carried out to determine the effectiveness of certain amines in CO_2 capture.

Different conditions of reactions of amines with CO_2 were utilized to obtain crystalline products. The following amines were used: anhydrous piperazine and its hexahydrate, 2,6 dimethylpiperazine, 4-piperidone monohydrate hydrochloride, piperidine and 4methylpiperidine. Saturated aqueous amine solutions were prepared, as well as a 1:1 water:ethanol solutions. CO_2 was added to these solutions sourcing from both solid (dry ice) and gas. Time intervals and rates of CO_2 distribution were varied to discover if it affected the structure of final products. In addition to saturated solutions, pure piperidine, dimethylpiperizine, anhydrous piperazine, and its hexahydrate were allowed to react with atmospheric CO_2. Crystalline products obtained from this spontaneous reactions were analyzed.

Single crystal X-Ray analysis revealed the formation of mono- and dicarbamate derivatives that have been previously observed, with the exception of a monohydrate product. Cation-anion interactions and hydrogen bonding patterns in the resulting carbamates are discussed.