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Project	Computational Studies on CO_2 and Amine Interactions
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Introduction

The emission of greenhouse gases in the atmosphere, particularly carbon dioxide, caused by fossil fuel combustion, has been claimed to be responsible for global warming. Capturing of carbon dioxide from exhaust gases by using aqueous amine solutions is an important process for the reduction of the emission of these gases from power plants. Monoethanolamine (MEA) is used as an industrial solvent for carbon dioxide capture from exhaust gases. However, MEA has certain disadvantages like high heat of carbamate formation, high energy demand for regeneration and high degradation rates which makes MEA not an optimum solvent for CO_2 capture from power plants.

Goal

The reaction between primary and secondary amines leads to the formation of carbamate. Tertiary and sterically hindered amines do not form carbamate, instead they form ammonium compounds and bicarbonate.

$$2\,RNH_2 + CO_2 \rightleftharpoons RNHCO_2^- + RNH_3^+$$

$$CO_2 + H_2O + R_3N \rightleftharpoons HCO_3^- + R_3NH^+$$

CO_2 absorption by aqueous amines is a reversible process and the degree of reversibility depends on the properties of the amine, e.g. its pK_a. Amines that forms stable carbamates exhibit fast reaction rates and high energy demand for solvent regeneration. Amines that form more bicarbonate than carbamate exhibit slow reaction rates and require less energy for solvent regeneration.Our goal is to develop new absorbents for CO_2 capture, which still bind strongly to CO_2 and would release CO_2 in the regeneration step at a much reduced cost i.e. less heat of formation of carbamate than MEA.

Progress achieved

We studied the effect of electronic and steric groups on the basicity and reaction energy of MEA with CO_2 by using quantum chemical methods. It was found that β-fluoro substituted MEA has required less energy for regeneration step, which is most important for CO_2 capture.

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References

1. S.Gangarapu, *ChemPhysChem* **2012**, *13*, 3973-3980