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Project :	Computational studies on carbon dioxide and amine interactions
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Introduction

Global warming is the biggest threat for world. Over emission of green house gases in the atmosphere, particularly carbon dioxide (CO_2), caused by fossil fuel combustion, is suggested to be mainly responsible for global warming. CO_2 emissions can be reduced by capturing and storing the CO_2 instead of releasing it into the atmosphere (CO_2 capture and storage; CCS). Chemical absorption using aqueous alkanolamines is an important industrial method for CO_2 capture. Monoethanolamine(MEA), 2-amino-2-methyl propanol(AMP) are some of the solvents which are mostly used in CO_2 capture technology. Reaction between CO_2 and alkanolamines end up with carbamate and bicarbonate as products.

Goal

The main goal of this project is to study interactions between carbon dioxide and substituted alkanolamines by using quantum chemical methods. CO_2 absorption capacity of alkanolamines depends on pK_a and carbamate stability of alkanolamines. We are mainly focusing on how electron withdrawing and donating groups alter CO_2 absorption capacity of alkanolamines.

Progress Achieved

We have successfully computed gas phase protonation, solvation energies (which are contributes to pK_a) and charge distribution on carbamates of substituted alkanolamines. From calculations we can conclude that substitution of fluorine on alkanolamines decreases gas phase protonation energy and charge on nitrogen atom(which is responsible for binding with CO_2) of alkanolamines.

Further Research

Currently we are concentrating on calculation of thermodynamic properties (enthalpy of formation, reaction energy) and optimization of transition state geometries.

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