CO_2 Capture by Amine Solvents: Structure-Property-Efficiency Relationship from Density Functional Theory

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Possible reaction pathways for CO2 capture by several amine solvents in water are investigated with the density functional theory at the B3LYP/6-311++G** level in combination with the Poisson-Boltzmann continuum-solvation model for water. Since the experimental acidity constants (pKa values) of the reactants are reproduced very well (within 1 pKa unit) from the calculation, we assume that our calculation method should be appropriate to describe the acid-base chemistry involved in the CO2 capture process. A few common key quantities (properties) are identified to correlate well with the CO2 capture characteristics of different types of amine solvents (primary and secondary amines and alkanolamines) including monoethanolamine (MEA), 2-amino-2-methyl-1-propanol (AMP), ammonia, hydrazine, piperidine, and piperazine. This information is used as a principle to design a new compound (or mixture of compounds) which would exhibit the optimum properties required to maximize the CO2 loading capacity and rate.