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A new approach to the study of amine-CO_2 system based on the absolute reaction rate theory

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Abstract (less than 300 words)

Aiming for a carbon-free society, CO_2 capturing technologies are gathering attention. Amine solutions are well-known CO_2 adsorbents. Quantum mechanical reaction analyses can identify transition states to clarify adsorption mechanisms of amine solutions with obtaining free energies of reactions.

So far, we have been developing a reaction kinetics simulator; Kinerator [1]. This program simulates the rate of reaction progress using those free energies. However, in case of solving a complicated system in which the reaction rates are significantly different and some reactions sharing same substrates exist, there is a problem that the computational time to carry on numerical integration becomes huge.

In this study, we made a second visit to the reaction kinetics and devised simultaneous ordinary differential equations to efficiently solve these complicated systems using numerical solutions. We also implemented them into our Kinerator. For applications, we applied this to some amine solutions represented by AMP(2-amino-2-methyl-1-propanol) and PZ(piperazine) due to clarify detailed reaction profiles in a short time range depending on CO_2 concentration and temperatures. Especially for AMP, we were able to reproduce actual measurement values [2] with extremely high accuracy using free energies obtained by SMD/B3LYP/6-311++G(d,p)//SMD/B3LYP/6-31G(d) level of theory based on the mechanism of Yamada *et al.* [3].

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