An experimental/computational study of steric hindrance effects on CO2 absorption mechanism using nonaqueous/aqueous AMP

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Abstract

The reaction kinetics and molecular mechanisms of CO2 absorption using nonaqueous and aqueous amine solutions were analyzed by the stopped-flow technique and ab initio molecular dynamics (AIMD) simulations. Pseudo first-order rate constants (k0) of reactions between CO2 and amines were measured. A kinetic model was proposed to correlate the k0 to the amine concentration, and was proved to perform well for predicting the relationship between k0 and the amine concentration. The experimental results showed that AMP/MDEA only took part in the deprotonation of MEA-zwitterion in nonaqueous MEA+AMP/MEA+MDEA. In aqueous solutions, AMP can also react with CO2 through base-catalyzed hydration mechanism beside the zwitterion mechanism. The molecular mechanisms of CO2 absorption were also explored by AIMD simulations coupled with metadynamics sampling. The predicted free-energy barriers of key elementary reactions verified the kinetic model and demonstrated the different molecular mechanisms for the reaction between CO2 and AMP in nonaqueous and aqueous systems.

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