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Modeling the Capture of CO₂ by Aminomethylpropanol Using Accelerated Quantum Chemical Molecular Dynamics calculation

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【Introduction】

In the gas absorption industry, carbon dioxide removal from gaseous mixtures with alkanolamine solutions is classified as adiabatic gas absorption. Recently, aminomethylpropanol (AMP) solution has been introduced as commercially attractive over conventional amines, because it has a loading capacity of up to 1 mol of CO₂ per mole of AMP, and it has excellent absorption characteristics, superior stripping qualities, higher degradation resistance, and a lower corrosion rate [1]. In this study, theoretical calculations were done to find out the probable mechanism of the reaction of CO₂ and AMP.

【Method】

Novel quantum chemical molecular dynamics approach was used to investigate the absorption of CO₂ by alkanolamines in aqueous solution. In the new developed method we combine molecular dynamics (MD) simulation implemented in New-Ryudo program with tight binding (TB) quantum chemical (QC) calculations implemented in New-Colors program. The purpose of such combination is to investigate the CO₂ absorption in real scale with accurate energy perturbation.

【Results and Discussion】

A model of (Amin-CO₂-H₂O) consists of 30 (wt%) of the amine was constructed. First the constructed model was simulated by MD for 2 ps to provide structural relaxation. The obtained structure was used for a new MD to investigate the formation of HCO₃⁻ anion and AmineH⁺ cation. Since those intermediates structures may be the key role of the rate of CO₂ absorption. Fig. 1 shows two snapshots for the formation of HCO₃⁻ and AMPH⁺. We found that the HCO₃⁻ anion was formed after 50 fs (Fig 1a). The small size of this formed intermediate is the main reason for its fast formation. The librated proton (H⁺) was bounded to the AMP giving AMPH⁺ cation (Fig. 1b). According to our results the H⁺ proton interacted with AMP after 750 fs. The reason for this slow interaction is the methyl groups in side chain of the N-adjacent atom. As a result of that the absorption of CO₂ is slow down.

Reference

[1] I. Baek *et al.*, *Int. J. Thermophys.*, **21**, 1175 (2000).

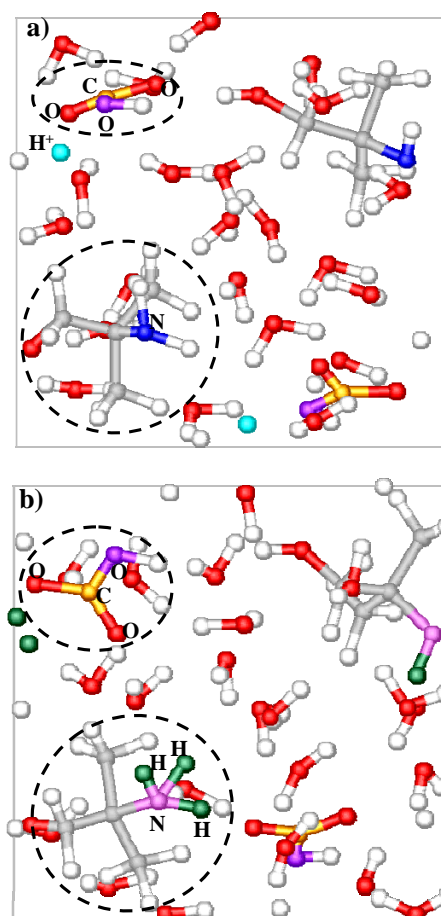


Fig.1 Snapshots of the MD simulation showing the formation of: a) HCO₃⁻ anion and b) AMPH⁺ cation.