Systematic Generation and Analysis of Reaction Path Networks by the Artificial Force Induced Reaction Method

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Paths of chemical reactions are studied theoretically by exploring the potential energy surface (PES) while performing quantum chemical calculations. Equilibrium (EQ) structures of molecules and transition state (TS) structures of chemical reactions are computed as local minima and first-order saddle points on the PES. Therefore, development of a method for finding EQs and TSs systematically is an important subject.

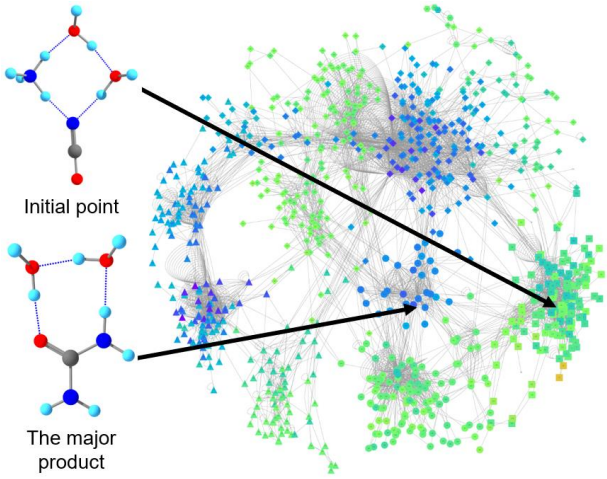

Figure 1. A reaction path network for Wöhler's urea synthesis [5].

We have developed an automated reaction path search method called an artificial force induced reaction (AFIR) method [1]. It has been used to elucidate mechanisms of various organic reactions [2]. The AFIR method has been implemented in the global reaction route mapping (GRRM) program, where the AFIR method for molecular systems is available in GRRM17 [3].

The AFIR method can generate a network of reaction paths. The resultant reaction path networks contain hundreds or more EQs. We have developed a kinetic theory called a rate constant matrix contraction (RCMC) method which is applicable to huge reaction path networks [4]. Furthermore, by combining the AFIR method with the RCMC method, we have established an approach by which, starting from a set of reactants and catalysts, the product and all byproducts, their generation ratio, as well as their generation mechanisms can be elucidated automatically [5]. This approach enabled systematic prediction of chemical reactions. In the presentation, its applicability and limitation will be discussed.

The AFIR method itself is applicable to chemical reactions of various types such as photoreactions, enzyme reactions, reactions on metal surfaces, phase transitions, and so on. Application examples to these reactions will also be presented.

References

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