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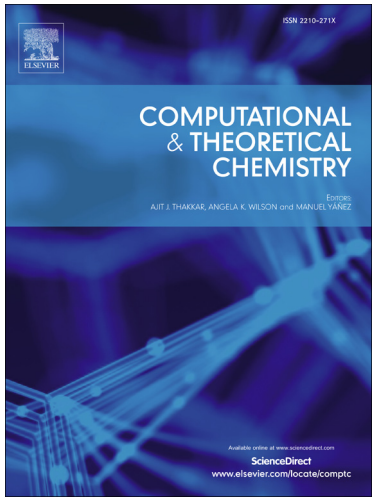

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Comparative analysis of linear and non-linear transition state of hydrogen transfer reaction between benzoyl type radicals with skipped alkadienes

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Abstract

Traditional linear transition states have been extensively investigated, and many models have been used to study them. However, few studies have described the detailed mechanism of nonlinear transition states. This paper describes a system to analyze nonlinear transition states. The hydrogen abstraction reaction is the simplest atom transfer reaction, and this reaction was used to generate the nonlinear transition state. We used a distortion/interaction model and the bond-energy–bond-order method to probe the differences between the nonlinear and the linear transition states. We also investigated whether flexible and rigid structures have an effect on the reaction energies. Based on the quantum chemical study, we obtained relevant energies and factors for the four reactions studied. The results showed that the distortion energy and activation barrier of nonlinear transition state reactions are much higher than those of the corresponding linear transition state reactions. It is concluded that the reaction of a rigid structure and a nonlinear transition state has a late transition state, while the reaction of a flexible structure and a linear transition state has an early transition state. We believe that the nonlinear transition state is different from the traditional linear transition state.

Keywords: Hydrogen abstraction, deformation/interaction model, nonlinear transition state,

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