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Computational Modeling and Mathematical Optimization of Organic Reaction Mechanisms

Communication Info

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Abstract

Understanding organic reaction mechanisms is fundamental to the rational design of chemical synthesis. This paper presents a computational framework that integrates mathematical modeling and optimization techniques to analyze organic reaction pathways. Differential equations and potential energy surface analysis are employed to describe reaction kinetics and transition states, while optimization algorithms are used to identify energetically favorable reaction routes. By combining chemical theory with numerical methods, the study demonstrates how computational tools can reduce experimental trial-and-error, improve yield prediction, and enhance mechanistic understanding. The approach highlights the growing importance of applied mathematics and computer science in modern organic chemistry research.

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