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Theoretical Investigations of Reaction Mechanisms II

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Message from the Guest Editor

Molecular design, optimization of reaction conditions, and the planning of a chemical synthesis cannot be achieved without knowledge of reaction mechanisms and driving forces of chemical processes. Computational methods of quantum chemistry represent a powerful tool for the understanding of the reaction mechanisms and key factors governing chemical reactions. Such methods are indispensable for the interpretation and analysis of experimental results and provide invaluable information, complementary to the experimental data, about molecular systems and processes. Computational methods are extremely valuable for mechanistic studies of reactions proceeding via formation of short-lived intermediates that cannot be detected experimentally, being the only possibility to obtain information about intimate details of the chemical processes when experimental methods cannot help in the understanding of the reaction mechanisms. Manuscripts that report mechanistic studies of any organic, inorganic or organometallic reactions with help of computational methods or deal with understanding of the key factors and driving forces governing chemical processes are welcome for this Special Issue.

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Message from the Editor-in-Chief

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