The Reaction Path in Chemistry: Current Approaches and Perspectives

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The reaction pathway (RP) technique is a powerful tool in theoretical chemistry and chemical reaction theory. The present book discusses the background of the concept, both mathematical and physical, and outlines new developments. Different approaches to the RP are described, with particular emphasis on gradient extremals and the treatment of zero eigenvalues of rotation in the Cartesian Hessian matrix along the RP. There is an excellent review of geometric optimization methods, together with an outline of density functional theory. Some contributions reveal the progress made in interface dynamics calculations based on RP potentials and tunnelling with electronic structure theory (`direct dynamics'). Includes the very latest results in excited-state RP calculations (H transfer) and a theoretical view of the RPs of photodissociation processes using time-resolved femtosecond spectroscopy. The passage from the RP to the reaction mechanism is described by means of fundamental groups and symmetry rules.

Audience: Researchers in theoretical chemistry, molecular modeling, physical chemistry, kinetics, and the biosciences.

Review(s): ` ... will be of use to any chemist with a desire to know about how chemical reactions are described in detail. It is especially useful for the computationally minded researcher who wants to go beyond the standard description of chemical reactions in terms of structures of reactant(s), transition state, and product(s).'
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Contents and Contributors: An introduction to the nomenclature and usage of the reaction path concept; *D. Heidrich.* From reaction path to reaction mechanism: Fundamental groups and symmetry rules; *P. G. Mezey.* Loose definitions of reaction path; *X. Chapuisat.* Role and treatment of zero eigenvalues of rotation in the Cartesian force constant matrix along the reaction path; *T. Iwai, A. Tachibana.* The invariance of the reaction path description in any coordinate system; *W. Quapp.* Second-order methods for the optimization of molecular potential energy surfaces; *T. Helgaker et al.* Gradient extremals and their relation to the minimum energy path; *W. Quapp et al.* Density functional theory - calculations of potential energy surfaces and reaction paths; *G. Seifert, K. Krüger.* Using the reaction path concept to obtain rate constants from *ab initio* calculations; *A. D. Isaacson.* Direct dynamics methods for the calculation of reaction rates; *D. G. Truhlar. Ab initio* studies of reaction paths in excited- state hydrogen transfer processes; *A. L. Sobolewski, W. Domcke.* Viewing the reaction path with the help of time-resolved femtosecond spectroscopy; *C. Meier, V. Engel.* Index.