Book Review

The Reaction Path in Chemistry: Current Approaches and Perspectives, *D. Heidrich, Editor, University of Leipzig, Germany; Kluwer, Dordrecht, Boston, London, 1995; 297 pp. Hardcover, U.S. $145.00. ISBN 0-792-33589-9*

The concept of reaction paths (RPs) is fundamental in chemistry and intertwines theory with experiment. It serves as a framework for qualitative modeling as well as for quantitative treatment.

Three important fields of research regarding reaction paths are identified by the editor of the present book: (i) analysis of potential energy surfaces and calculation of chemically interesting points on the RP, (ii) development of reaction theories which goes beyond transition-state theory and can be applied to chemical problems using the RP concept, and (ii) investigation of specific chemical reactions with RP concepts.

The book begins with a very useful ''Introduction to the Nomenclature and Usage of the RP Concept'' written by the editor, D. Heidrich. In the following section, some aspects of RP theory are discussed in several contributions: Mezey (From RP to Reaction Mechanism: Fundamental Groups and Symmetry Rules), Chapuisat (Loose Definitions of Reaction Paths), Tachibana and Iwai (Zero Eigenvalues of Rotation in the Cartesian Force Constant Matrix), and Quapp (The Invariance of the Reaction Path Description in any Coordinate System).

Different techniques of calculating points on the RP are covered in chapters by Helgaker, Ruud, and Taylor (Second-order Methods for the Optimization of Molecular Potential Energy Surfaces), Quapp, Imig, and Heidrich (Gradient Extremals and Their Relation to the Minimum Energy Path), and Seifert and Krüger (Density Functional Theory-Calculations of Potential Energy and Reaction Paths).

Two chapters inform about the calculation of reaction rates by current variational TS theory: Isaacson (Using the RP Concept to Obtain Rate Constants from *Ab Initio* calculations) and Truhlar (Direct Dynamics Method for the Calculation of Reaction Rates). Reaction paths for excited-state hydrogen-transfer processes are discussed by Sobolewski and Domcke and, finally, a chapter by Meier and Engel deals with the experimental efforts of viewing the RP by time-resolved femtosecond spectroscopy.

The book will be very useful for any chemist, whether experimentalist or theoretician, who wants an up-to-date account of modern reaction path theory. It should be included in the library of any physical organic, chemical physics or theoretical chemistry library and would be bought by many chemists were not the price so prohibitively high!

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