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Computer Modeling of Chemical Reactions in Enzymes and Solutions

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Описание: The book can be used in a one semester course for senior undergraduate and graduate students who are interested in understanding physical aspects of biochemistry and computer modeling of macromolecules. It can also be used as a self-study text and as a complement to other books. Although it follows a rigorous introductory outline, this book does not require significant prior knowledge, and many of the principles taught in the first three chapters can be adopted as working recipes even without a full understanding of their exact derivations. Several specific examples of enzymatic reactions are presented and analyzed to illustrate the approaches needed for simulating such reactions. These examples can be followed conveniently in studies of other systems. Many problems and computer exercises are provided to help readers test their understanding of actual modeling concepts and prepare them to handle larger molecular simulation packages in studies of biophysical problems.

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41 Lecture 11: Modelling Chemical Reactions in Solution: Theory and Applications 41. 42 How to trap (meaning find and optimize) a static transition state using an easily definable reaction coordinate: 1) Define chemically reasonable reaction coordinate (bond formation / breaking) 2) Perform a potential-energy surface (PES) scan along the defined reaction coordinate starting from a reactant (1D or 2D scans => maximum in 1D or saddle point in 2D a. 45 Lecture 12: Computer Modeling (Physical Chemistry) of Enzyme Catalysis, Metalloenzymes Leonor Michaelis () Maud Leonora Menten () 45. 46 HMM Equation defining 46. 47 adapted from Rokob, T. A.; Srnec, M.; Rulišek, L.: Dalton Trans. 2012, 41 COMPUTER MODELING OF CHEMICAL REACTION AND SOLUTIONS AliiEI ! WAII Sill/ University of Southern California Wiley Professional Paperback Edition Published 1997 A Wiley-Interscience Publication JOHN WILEY & SONS, INC. New York. Chichester Weinheim Brisbane Singapore Toronto. Los Angeles, California August 1991 ARIEH WARSHEL COMPUTER MODELING OF CHEMICAL REACTIONS IN ENZYMES AND SOLUTIONS. 1 BASIC CHEMICAL PRINCIPLES OF BONDING All molecules, small and large, are built from atoms which are connected to each other by chemical bonds. The chemistry of any molecule is determined by the type of bonds that exist between its atoms.