Additions and Corrections

Physical Organic Chemistry of Transition Metal Carbene Complexes. 17.[1] Kinetics of the Reactions of (Arylthio-alkoxycarbene)pentacarbonyl Complexes of Chromium(0) and Tungsten(0) with Thiolate Ions in Aqueous Acetonitrile: pK_a Values of the Metal-Protonated Tetrahedral Adducts Formed between Carbene Complexes and Thiolate Ion [*J. Am. Chem. Soc.* **1999**, *121*, 11384−11394]. CLAUDE F. BERNASCONI* AND MAHAMMAD ALI

Page 11391, subsection **B. k_1^{RS} and k_{-1}**: The second sentence should be replaced by the following. This reversal indicates that the *intrinsic* rate constants, k_o,[11] for the MeS complexes are substantially smaller than for the MeO complexes.

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Book Reviews

Computational Molecular Biology. Theoretical and Computational Chemistry Series. Vol. 8. Edited by Jerzy Leszczynski (Jackson State University, Jackson, MS). Elsevier: Amsterdam and New York. 1999. xvi + 646 pp. $327.50. ISBN 0-444-50030-8.

This book provides very good coverage of the computational techniques used in the study and modeling of biomolecules. The book consists of 16 chapters covering such topics as the application of hybrid quantum mechanical/molecular mechanical potentials for the description of enzyme systems, *ab initio* studies on nucleic acid bases and the radiation damage to DNA, protein structure prediction, and drug design strategies. The book presents an excellent blend of theoretical studies of biomolecules. It is well-organized, with distinctive sections describing studies of DNA and protein, interspersed with studies of the calculation of binding free energies and electrostatic properties.

Chapter 1 (P. Amara and M. J. Field) introduces quantum mechanical (QM) and molecular mechanical (MM) Hamiltonians and presents an overview of the hybrid QM/MM potentials. Section 4 of this chapter describes the use of hybrid potentials in the treatment of several enzyme systems. Chapter 2 (S. Scheiner) presents an excellent overview of proton transfer in model biomolecules. Using results from *ab initio* studies, the author details proton-transfer properties by way of single-well and double-well potentials and discusses hydrogen bond flexibility and different types of hydrogen bonds (LBHB, SSHB, etc.).

With this foundation, the next six chapters focus on computational studies of nucleic acid bases. In Chapter 3, Šponer, Hobza, and Leszczynski present a detailed overview of *ab initio* studies on nucleic acid bases, covering the choice of basis sets and the importance of basis set superposition error (BSSE) and describing the geometric features of the base pairs. Chapters 4 (M. Orozco et al.) and 5 (L. Gorb and J. Leszczynski) offer insights into the effects of solvation on the geometries of nucleic acid base pairs and various theoretical treatments for the inclusion of solvation effects. In Chapter 6 (M. Aida, M. Kaneko, and M. Dupuis), pyrimidine dimers are studied using *ab initio* methods to obtain a detailed understanding of the radiation-induced damage to DNA. Radiation-induced damage to DNA is also investigated in Chapter 7 (A.-O. Colson and M. D. Sevilla) through molecular orbital studies on DNA base radicals. Using molecular dynamics simulation studies, Bansal, Ravikiran, and Chowdhury present a detailed description of the geometric features in guanine-rich helical structures (Chapter 8).

Using the example of HIV-1 protease, Tawa, Topol, and Burt present the calculation of the relative binding free energies of some inhibitors in Chapter 9. Chapter 10 (W. A. Sokalski et al.) outlines the methodology to model the electrostatic effects in biomolecules.

Chapters 11−14 discuss the use of various computational approaches for protein structure prediction, for modeling DNA−protein interactions, and for studies on small-molecule and peptide interactions with membranes. Chapter 11 (J. Skolnick, A. Kolinski, and A. R. Ortiz) discusses the use of simplified models for the prediction of protein folding and presents the current approaches to this problem such as threading, restraint models, and evolutionary-based methods. It is a challenging task to model protein−DNA interactions even with state-of-the-art computational power and tools. The authors of Chapter 12 (K. Zakrzewska and R. Lavery) are of similar opinion and point out some of the areas that need to be addressed in order to gain a better understanding of these biomolecular interactions. Continuing on this subject, Chapter 13 (A. Pohorille et al.) describes simulation studies of small molecules and peptides interacting with membrane proteins. Using an explicit water model and a continuum solvent model, Chapter 14 (J. D. Madura and A. Wierzbicki) presents simulation studies on the modeling of antifreeze proteins.

Chapter 15 (N. Bodor, P. Buchwald, and M.-J. Huang) describes some of the QSAR-based approaches to retrometabolic drug design studies. Using a model based on quantum mechanics, Chapter 16 (R. Wallace) presents an overview of the complexity of treating neural aspects of membrane biophysics computationally.

My only criticism of this book is that more careful editing is needed. This book does manage to cover a wide range of theoretical applications for biomolecular problems. Overall, it should be very useful to researchers in a wide range of specialties.

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