Book Review

# Quinoxalines, Supplement II. The Chemistry of Heterocyclic Compounds, Volume 61 Series edited by Edward C. Taylor and Peter Wipf. By D. J. Brown (Australian National University, Canberra). John Wiley & Sons, Inc.: Hoboken. 2004. xvi + 510 pp. $425.00. ISBN: 0-471-26495-4.

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BOOK REVIEWS

**The Quantum Classical Theory**. By Gert D. Billing (University of Copenhagen). Oxford University Press: New York. 2003. xii + 236 pp. $85.00. ISBN 0-19-514619-0.

In this book, Billing reviews the quantum classical theory, also known as semiclassical mechanics, from first-principles to the numerical treatment of molecular reaction dynamics. His approach provides students with a means of entry into this rare genre of science. While highlighting his own contributions, Billing surveys the area and achieves an up-to-date snapshot of semiclassical approximation.

A quantum treatment of molecular reaction dynamics quickly becomes unwieldy as one considers more complex reactions. A full quantum treatment is still only really possible for up to four-atom systems. This is because the number of basis functions scales exponentially with the number of degrees of freedom. Semiclassical mechanics offers a way around this problem. The idea is to approximate quantum dynamics in terms of classical trajectories and take advantage of the gentle scaling of classical mechanics.

Billing opens a discussion of the quantum classical theory by describing the path integral formulation of the quantum propagator and its classical limit. A description of Gaussian-evolving wave packets, as pioneered by Heller and co-workers, quickly follows. It is through this approach that Billing obtains equations of motion for the classical trajectory, rather than via steepest descent approximation of the path integral. The method is made rigorous, at least in principle, by attaching a Gauss−Hermite basis to the evolving trajectory; that is, the method must converge to exact quantum mechanics in the limit of many basis functions. The corresponding discrete variable representation is presented as a convenient numerical implementation of the approach. Although thorough with regard to the details of implementation, the treatment leaves open questions regarding the efficacy of the approach when classical trajectories bifurcate, a common circumstance for other than the simplest processes. It is not clear that a time-dependent basis set, referenced to only one orbit, is well suited in cases where many trajectories, and associated interference effects, are indicated. However, in an appendix, Billing does show how to split an evolving Gaussian into reflected and transmitted components upon collision with a barrier in one dimension.

Subsequent chapters introduce various levels of approximation to make viable the simulation of molecular collisions with various degrees of complexity. For example, divide and conquer strategies are introduced wherein some degrees of freedom are treated as classical, and others are treated via the quantum classical theory. It is shown that such a division works best when the associated classical and quantum degrees of freedom are weakly coupled. This section of the book highlights applications to diatom−diatom inelastic and reactive collisions. Later, polyatomic systems and scattering at surfaces are considered with the aid of a second quantization methodology based on a harmonic treatment of "bath" degrees of freedom. Reaction path and volume methods follow, which are also treated within the second quantization framework.

The Pechukas and Tully semiclassical treatments of nonadiabatic transitions, time-dependent Hartree methods, and centroid molecular dynamics also receive some attention in this book. With these and the other topics covered, the scope of the book is broad enough for the novice to get a fair idea of the field of semiclassical mechanics. At the same time, the novice is led all the way to numerical implementation of state-to-state rate computations.

Some of the figures are hard to follow, and a little more discussion of the physical significance of numerical results would have been nice. Nevertheless, the numerical studies, which are the primary focus of the figures, add great value to the book. In addition to being a valuable summary of many of Billing's contributions, this work is a useful reference on the quantum theory of molecular collisions.

Overall, the book is a welcome addition to the library of the scientist of semiclassical mechanics. Beyond the other works of Billing and the works of Child, there are very few books on the semiclassical treatment of molecular dynamics. Most other books in the area of semiclassics do not focus on molecular systems, and certainly not on the details of their simulation. This work is a fitting tribute to the late Gert Billing. His abundant energy, evident on each page of this book, will surely be greatly missed.

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JA033600H

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**Catalysis from A to Z: A Concise Encyclopedia. Second, Completely Revised, and Enlarged Edition**. Edited by Boy Cornils (Hofheim, Germany), Wolfgang A. Herrmann (Technical University of Munich), R. Schlögl (Fritz-Haber-Institute of the Max-Planck Society, Berlin), and Chi-Huey Wong (The Scripps Research Institute, La Jolla, CA). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2003. xxii + 840 pp. $145.00. ISBN: 3-527-30373-1.

In this book, approximately 4600 catalytic or catalysis-related terms are defined by 190 authors and coauthors who are all experts in their respective areas. Most of the entries contain references to "illustrate developments or important aspects of the keyword" and cross-references, where appropriate. Keywords are also given in German and French.

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**Quinoxalines, Supplement II. The Chemistry of Heterocyclic Compounds, Volume 61**. Series edited by Edward C. Taylor and Peter Wipf. By D. J. Brown (Australian National University, Canberra). John Wiley & Sons, Inc.: Hoboken. 2004. xvi + 510 pp. $425.00. ISBN: 0-471-26495-4.

Unsigned book reviews are by the Book Review Editor.

This book updates Volumes 5 and 35 of this series on quinoxalines and covers the literature on quinoxalines from approximately 1976−2002, with some references to 2003. Information about the "synthesis, reactions, spectroscopic, and physical properties for each class of compounds" is provided, and an alphabetical table of all simple quinoxalines reported through 2002 is included.

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**Analytical Method Validation and Instrument Performance Verification**. Edited by Chung Chow Chan (Eli Lilly Canada, Inc.), Herman Lam (GlaxoSmithKline Canada, Inc.), Y. C. Lee (Pantheon YM, Inc.), and Xue-Ming Zhang (Novex Pharma). John Wiley & Sons, Inc.: Hoboken, NJ. 2004. x + 304 pp. $89.95. 0-471-25953-5.

Given the need for generating reliable analytical data, this book provides practical guidance for validating common and not-so-common analytical methods and for verifying the performance of instruments in compliance with current Good Manufacturing Practices. The first half of the book covers such methods and includes topics such as the validation of potency and dissolution as well as the validation of methods for pharmaceutical excipients, heavy metals, and bioanalysis. The second half encompasses the performance of instruments, ranging from common analytical instruments, such as HPLC, UV−vis spectrometers, and pH meters, to computer systems and software. Each chapter follows the same general format, beginning with, to paraphrase part of the preface, a discussion of general requirements, followed by strategies and steps to fulfill those requirements, and ending with a description of common problems and solutions. A subject index completes the book.

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**Basic Principles in Applied Catalysis**. Edited by Manfred Baerns (Institut für Angewandte Chemistry, Berlin). Springer-Verlag: Berlin, Heidelberg, New York. 2004. x + 558 pp. $189.00. ISBN: 3-540-40261-6.

This book, written by an international group of experts in the field, covers the basic principles and the application of important catalytic reactions and catalysts currently used in industry. Its 16 chapters are organized into the following sections: Introduction; Selected Reactions in Heterogeneous Catalysis; Preparation, Functionality and Characterization of Heterogeneous Catalysts; Homogeneous Catalysis, Polymerization Catalysis and Biocatalysis; and Catalytic Reaction Engineering. A subject index completes the book.

JA040918G

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