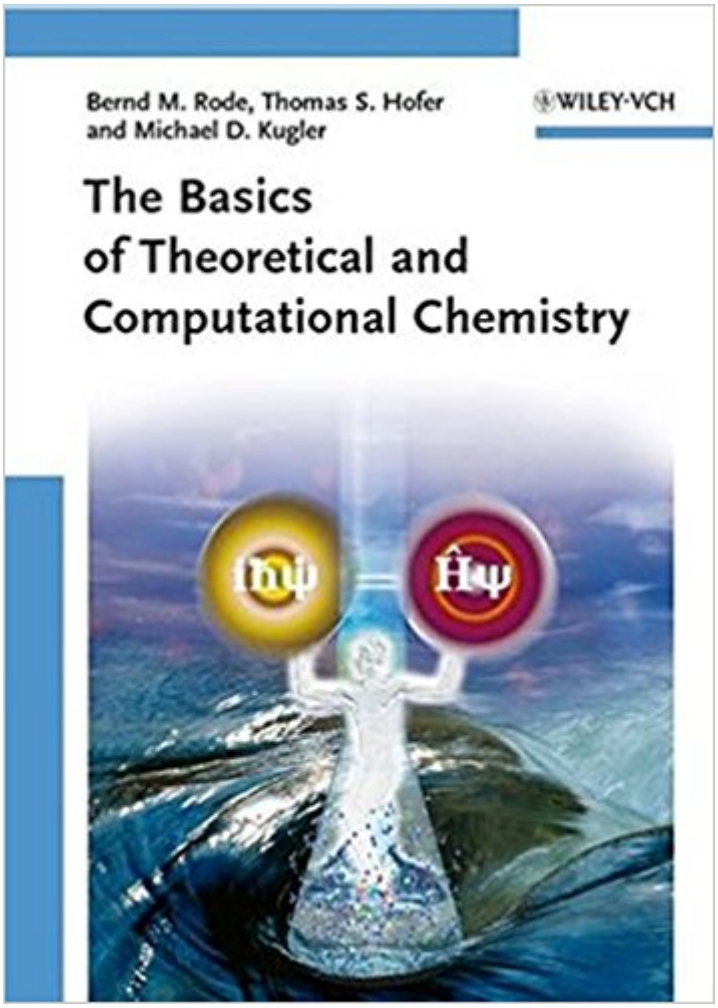
The Basics Of Theoretical And Computational Chemistry



Synopsis

This textbook does away with the classic, unimaginative approach and comes straight to the point with a bare minimum of mathematics -- emphasizing the understanding of concepts rather than presenting endless strings of formulae. It nonetheless covers all important aspects of computational chemistry, such as - vector space theory - quantum mechanics - approximation methods - theoretical models - and computational methods. Throughout the chapters, mathematics are differentiated by necessity for understanding - fundamental formulae, and all the others. All formulae are explained step by step without omission, but the non-vital ones are marked and can be skipped by those who do not relish complex mathematics. The reader will find the text a lucid and innovative introduction to theoretical and computational chemistry, with food for thought given at the end of each chapter in the shape of several questions that help develop understanding of the concepts. What the reader will not find in this book are condescending sentences such as, 'From (formula A) and (formula M) it is obvious that (formula Z).'

Book Information

Hardcover: 195 pages

Publisher: Wiley-VCH; 1 edition (March 12, 2007)

Language: English

ISBN-10: 3527317732

ISBN-13: 978-3527317738

Product Dimensions: 6.9 x 0.6 x 9.7 inches

Shipping Weight: 1.2 pounds (View shipping rates and policies)

Average Customer Review: 2.0 out of 5 stars 1 customer review

Best Sellers Rank: #1,888,188 in Books (See Top 100 in Books) #88 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #1713 inÂ Books > Medical Books > Medicine > Internal Medicine > Pathology > Clinical Chemistry #4671 inÂ Books > Science & Math > Chemistry > General & Reference

Customer Reviews

This textbook does away with the classic, unimaginative approach and comes straight to the point with a bare minimum of mathematics -- emphasizing the understanding of concepts rather than presenting endless strings of formulae. It nonetheless covers all important aspects of computational chemistry, such as vector space theory - quantum mechanics - approximation methods - theoretical models - and computational methods. Throughout the chapters, mathematics are differentiated by

necessity for understanding - fundamental formulae, and all the others. The former are explained step by step without omission, while the latter are given in the appendix for those readers who wish to delve into more complex mathematics. The reader will find the text a lucid and innovative introduction to theoretical and computational chemistry, with food for thought given at the end of each chapter in the shape of several questions that help develop understanding of the concepts. What the reader will not find in this book are condescending sentences such as, 'From (formula A) and (formula M) it is obvious that (formula Z)...' Bernd M. Rode is professor of theoretical and inorganic chemistry at the University of Innsbruck, Austria. He has taught theoretical chemistry at numerous universities in Asia, where he has also built up new computational chemistry institutions. He has authored nearly 400 scientific publications and obtained numerous honours and awards, among them three honorary doctoral degrees. His present research is focused on theory of liquids and solutions, but he also maintains an experimental group studying chemical evolution towards the origin of life. Thomas S. Hofer has graduated from a college of technology and obtained his PhD degree in chemistry at the University of Innsbruck in 2006. Since 2005, he has been working as assistant professor in theoretical chemistry at the University of Innsbruck. He has published 16 scientific articles, including two review articles. He has been awarded the Austrian nation-wide prize for outstanding studies. Michael Kugler obtained his secondary education in Tyrol and Upper Austria and is at present a graduate student of physics and chemistry at the University of Innsbruck.

Bernd Michael Rode is professor of theoretical and inorganic chemistry at the University of Innsbruck, Austria. He has taught theoretical chemistry at numerous universities in Asia, where he has also built up new computational chemistry institutions. He has authored nearly 400 scientific publications and obtained numerous honours and awards, among them three honorary doctoral degrees. His present research is focused on theory of liquids and solutions, but he also maintains an experimental group studying chemical evolution towards the origin of life. Thomas S. Hofer has graduated from a college of technology and obtained his M.Sc. degree in chemistry at the University of Innsbruck. Since 2005, he has been working as assistant professor in theoretical chemistry at the University of Innsbruck and will obtain his Ph.D. degree in this field in 2006. He has published 16 scientific articles, including two review articles. He has been awarded the Austrian nation-wide prize for outstanding studies. Michael Kugler obtained his secondary education in Tyrol and Upper Austria and is at present a graduate student of physics and chemistry at the University of Innsbruck.

While the stated goal of a treatment of theoretical and computational chemistry without irrelevant

mathematical details is admirable, this book falls far short of its ambitious goals.The thinness of the book, rather than evidence of concise exposition, leaves much to be desired in its selection of what mathematical details are omitted and what is left in. It is far too simplistic to the point of misleading, Even many of the pictures, while certainly colorful, are often banal and unproductive (Figure 4.1 is a prime example of a complete waste of ink).The book is unfortunately also rife with glaring mistakes. One particular egregious example is the use of the term ’molecular dynamics’ wherever ’molecular mechanics’ is meant, resulting in incorrect conflation of these concepts. Poor notation which fails to distinguish between states as kets vs. their position-space representations gets the authors into trouble, especially when writing expressions involving gradients, or worse, using kets in their exposition of molecular mechanics! Another fundamental error is the explicit use of a time operator when discussing energy-time uncertainty, which is wrong since energy-time uncertainty does *not* follow from the usual operator commutator relationships such as the one used to demonstrate position-momentum uncertainty (as explained in A. Peres’s book and many others).In conclusion, save your money and get another book. It is too full of errors, frivolous details and misleading ’derivations’ to be worth serious attention.

Theoretical Physics 6: Quantum Mechanics - Basics Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics Computational Chemistry: Reviews of Current Trends Computational Organic Chemistry Computational Chemistry: Reviews of Current Trends, Vol. 1 Modern Chemistry Florida: Holt Chemistry and Modern Chemistry FCAT Standardized Test Preparation What is Organic Chemistry? Chemistry Book 4th Grade | Children's Chemistry Books Surviving Chemistry Review Book: High School Chemistry: 2015 Revision - with NYS Chemistry Regents Exams: The Physical Setting