

## Preface

Congratulations! The fact that you are reading these words suggests that you are a chemistry educator who is anxious to expand your knowledge of chemistry and the tools used to study chemistry! Or, perhaps you are a chemistry student, also looking to broaden your horizons, explore new areas of chemistry not typically taught at the high school (or even undergraduate) level, or investigate a possible area for further study or even a career. Regardless, the area of chemistry being discussed in this book – molecular modeling – is rapidly becoming one of the most important of all chemical disciplines. As you will see, molecular modeling, also often referred to as computational chemistry, is easily becoming as important to chemistry and the study of chemistry as a lab full of test tubes and beakers. Regardless of your purposes in studying computational chemistry, its usefulness as a research tool, as a teaching tool, and as a learning tool is quickly becoming indisputable.

This book is designed primarily to support teachers and students who wish to use the computational chemistry laboratory resources provided by the North Carolina High School Computational Chemistry server. This computing resource is located in the offices of the Shodor Center for Computational Science Education, in Durham, North Carolina. This resource, provided by funding from the Burroughs Wellcome Fund and the North Carolina Center for Science, Mathematics, and Technology, provides North Carolina high school students and teachers with round-the-clock access to four of the most powerful computational chemistry software programs, all accessible with a simple to use Web-based user interface. The server can be used just as the competent chemistry educator uses his or her “wet lab” facilities – as a place to explore basic chemistry concepts, validate lessons learned in the classroom, and introduce chemistry students to the tools and techniques that chemists use to study chemistry. Individual students or small groups of students can also use the server to explore topics in more detail, or to develop projects for submission to local, regional, state, or national science competitions. Access to the server is available to all North Carolina pre-college students and their teachers free of charge.

This book is not, however, a Users Guide (a very good Users Guide is available online). The purpose of this book is to explain what molecular modeling can do for you, how you do it, and why you are doing it. For example, one of the menu choices when you are performing a computation is a 3-21G basis set. What is a basis set? What does it do? What is the meaning of 3-21G? Why is that important? These are the types of questions that this book looks to answer. The book is divided into four sections. Section I talks about the different technologies of molecular modeling, such as *ab initio*, semi-empirical, and density functional theory (DFT). Section II talks about the techniques of molecular modeling, such as how one performs a vibrational frequency analysis of a molecule. Section III describes the tools of molecular modeling. What is the difference between Gaussian and MOPAC software? How does one choose which of those software packages to use for a specific calculation? Does it matter (it does!)? How does your choice affect the accuracy of your answer? In Section IV, we present information of interest to the educational community. For the chemistry educator, we present some of the “lessons learned” from 20+ years of teaching basic chemistry concepts using computational methods. We also discuss how a chemistry teacher might teach computational chemistry as a course, or perhaps as an enrichment unit during the three or four weeks following

the completion of AP Chemistry exams. For both the chemistry educator and the chemistry research student, Section IV also presents ideas, tips, and guidelines on how to do a computational chemistry research project, with a focus on using the NC High School Computational Chemistry server.

The book is organized as a study guide, and uses the format found in the “Instant Notes” series by Garland Press. Each chapter starts with a series of several Key Notes. Following each Key Note, there is a very short discussion – typically one paragraph – describing that particular note. The purpose of this section is to provide the chemistry educator or student with the minimal knowledge needed to perform a computational chemistry calculation. From reading these notes, you will have a minimal idea of what a basis set is, but will not be able to differentiate between a 3-21G basis set and a 6-311+G(p,d) basis set. To be able to do that, the remainder of each chapter provides a more detailed description of each of the five or six keynotes.

The target audience for this book is the high school chemistry educator. The goal of the book is to take the topic of molecular modeling and make it simple, without making it simplistic. Understanding molecular modeling is not horrendously difficult, but it does require effort! You may have to read a chapter several times, try out a number of labs, and give yourself time for some of the jargon and concepts to become familiar. We encourage chemistry educators to think about teaching the materials they currently cover in their courses in a new way, utilizing this book and the server as a resource. Research shows that students who discover concepts and make connections *on their own* have a deeper and longer lasting grasp of the material. In this book, we try to use lots of analogies and examples, include graphics to help with various concepts, and use a writing style that is one step above conversational. We try to limit, but not eliminate, the inclusion of complicated mathematical equations and formulas. Molecular modeling is, as we shall state again later, a mathematical science. We are also assuming a reasonable knowledge level of general chemistry.

At the end of the book there are a series of computational labs, designed for both classroom use and use by individual research students. The reader can use the book as a “just in time” resource, consulting the appropriate chapter at the appropriate time to make sense of what the lab is trying to achieve. Classroom educators might also use this book as the textbook for an elective course in computational chemistry, as is being done with high school students and student researchers at the North Carolina School of Science and Mathematics (NCSSM).

Writing this book would not have been possible without the support and friendship of the wonderful folks at the Burroughs Wellcome Fund and the North Carolina Center for Science, Mathematics, and Technology, to whom this book is dedicated. Gratitude is also expressed to the staff at Shodor, especially Simon Karpen and his team of cracker-jack system administrators, who are working relentlessly to keep the server running and available to do the work of computation. Jonathan Stuart-Moore and his group of graphic designers and layout artists also contributed to the graphics and layout for the book. Jon Collins, a chemistry teacher and North Carolina Kenan Fellow in Computational Chemistry, contributed his insights and expertise as a classroom chemistry teacher, and also provided content support. Wonderful support (development of labs and editorial reviews) was provided by a very talented team of undergraduate and high school interns at Shodor, including Jenna Ingersoll (Sewanee College),

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We certainly welcome comments from teachers and students who use this book. Suggestions for improvement would be particularly useful. Also, we note that any errors present are solely our responsibility.

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