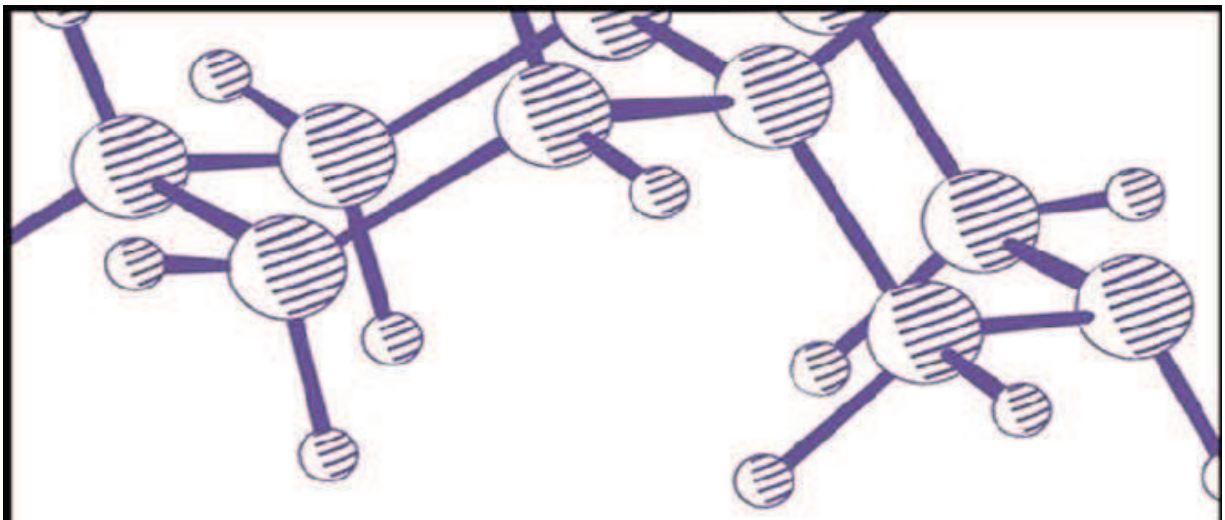
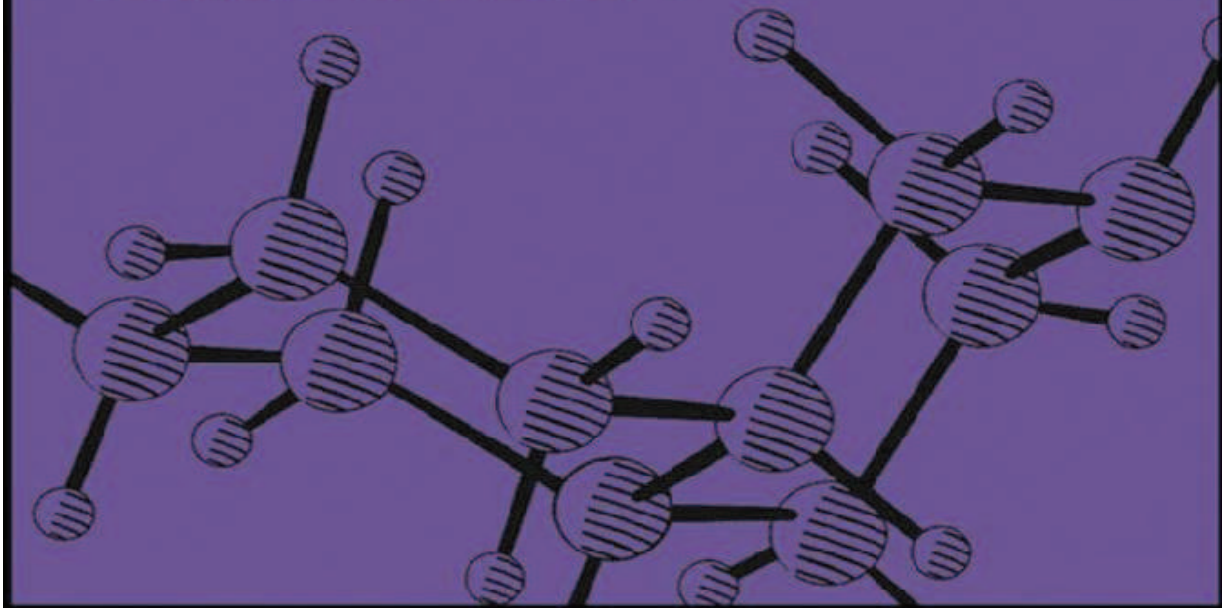


COMPUTATIONAL CHEMISTRY USING THE PC

Third Edition

DONALD W. ROGERS



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Live joyfully with the wife whom thou lovest all the days of the life of thy vanity, which He hath given thee under the sun, all the days of thy vanity: for that is thy portion in this life, and in thy labor which thou takest under the sun.

Ecclesiastes 9:9

THIS BOOK IS DEDICATED TO KAY

Contents

Preface to the Third Edition

It is a truism (cliche?) that microcomputers have become more powerful on an almost exponential curve since their advent more than 30 years ago. Molecular orbital calculations that I ran on a supercomputer a decade ago now run on a fast desktop microcomputer available at a modest price in any popular electronics store or by mail order catalog. With this has come a comparable increase in software sophistication.

There is a splendid democratization implied by mass-market computers. One does not have to work at one of the world's select universities or research institutes to do world class research. Your research equipment now consists of an off-the-shelf microcomputer and your imagination.

At the first edition of this book, in 1990, I made the extravigant claim that ''a quite respectable academic program in chemical microcomputing can be started for about $1000 per student''. The degree of difficulty of the problems we solve has increased immeasurably since then but the price of starting a good teaching lab is probably about half of what it was. To equip a workstation for two students, one needs a microcomputer connected to the internet, a BASIC interpreter and a beginner's bundle of freeware which should include the utility programs suggested with this book, a Huckel Molecular Orbital program, TINKER, MOPAC, and GAMESS.

There are 42 Computer Projects included in this text. Several of the Computer Projects connect with the research literature and lead to extensions suitable for undergraduate or MS thesis projects. All of the computer projects in this book have been successfully run by the author. Unfortunately, we still live in an era of system incompatibility. The instructor using these projects in a teaching laboratory is urged

to run them first to sort out any system specific difficulties. In this, the projects here are no different from any undergraduate experiment; it is a foolish instructor indeed who tries to teach from untested material.

The author wishes to acknowledge the unfailing help and constructive criticism of Frank Mc Lafferty, the computer tips of Nikita Matsunaga and Xeru Li. Some of the research which gave rise to Computer Projects in the latter half of the book were carried out under a grant of computer time from the National Science Foundation through the National Center for Supercomputing Applications both of which are gratefully acknowledged.

Donald W. Rogers
Greenwich Village, NY
July 2003

Preface to the Second Edition

A second edition always needs an excuse, particularly if it follows hard upon the first. I take the obvious one: a lot has happened in microcomputational chemistry in the last five years. Faster machines and better software have brought more than convenience; there are projects in this book that we simply could not do at the time of the first edition.

Along with the obligatory correction of errors in the first edition, this one has five new computer projects (two in high-level *ab initio* calculations), and 49 new problems, mostly advanced. Large parts of Chapters 9 and 10 have been rewritten, more detailed instructions are given in many of the computer projects, and several new illustrations have been added, or old ones have been redrawn for clarity. The BASIC programs on the diskette included here have been translated into ASCII code to improve portability, and each is written out at the end of the chapter in which it is introduced. Several illustrative input and output files for Huckel, self-consistent field, molecular mechanics, *ab initio*, and semiempirical procedures are also on the disk, along with an answer section for problems and computer projects.

One thing has not changed. By shopping among the software sources at the end of this book, and clipping popular computer magazine advertisements, the prudent instructor can still equip his or her lab at a starting investment of about $2000 per workstation of two students each.

Preface to the First Edition

This book is an introduction to computational chemistry, molecular mechanics, and molecular orbital calculations, using a personal microcomputer. No special computational skills are assumed of the reader aside from the ability to read and write a simple program in BASIC. No mathematical training beyond calculus is assumed. A few elements of matrix algebra are introduced in Chapter 3 and used throughout.

The treatment is at the upperclass undergraduate or beginning graduate level. Considerable introductory material and material on computational methods are given so as to make the book suitable for self-study by professionals outside the classroom. An effort has been made to avoid logical gaps so that the presentation can be understood without the aid of an instructor. Forty-six self-contained computer projects are included.

The book divides itself quite naturally into two parts: The first six chapters are on general scientific computing applications and the last seven chapters are devoted to molecular orbital calculations, molecular mechanics, and molecular graphics. The reader who wishes only a tool box of computational methods will find it in the first part. Those skilled in numerical methods might read only the second. The book is intended, however, as an entity, with many connections between the two parts, showing how chapters on molecular orbital theory depend on computational techniques developed earlier.

Use of special or expensive microcomputers has been avoided. All programs presented have been run on a 8086-based machine with 640 K memory and a math coprocessor. A quite respectable academic program in chemical microcomputing can be started for about $1000 per student. The individual or school with more expensive hardware will find that the programs described here run faster and that

more visually pleasing graphics can be produced, but that the results and principles involved are the same. Gains in computing speed and convenience will be made as the technology advances. Even now, run times on an 80386-based machine approach those of a heavily used, time-shared mainframe.

Sources for all program packages used in the book are given in an appendix. All of the early programs (Chapters 1 through 7) were written by the author and are available on a single diskette included with the book. Programs HMO and SCF were adapted and modified by the author from programs in FORTRAN II by Greenwood (*Computational Methods for Quantum Organic Chemistry*, Wiley Interscience, New York, 1972). The more elaborate programs in Chapters 10 through 13 are available at moderate price from Quantum Chemistry Program Exchange, Serena Software, Cambridge Analytical Laboratories and other software sources [see Appendix].

I wish to thank Dr. A. Greenberg of Rutgers University, Dr. S. Topiol of Burlex Industries, and Dr. A. Zavitsas of Long Island University for reading the entire manuscript and offering many helpful comments and criticisms. I wish to acknowledge Long Island University for support of this work through a grant of released time and the National Science Foundation for microcomputers bought under grant #CSI 870827.

Several chapters in this book are based on articles that appeared in *American Laboratory* from 1981 to 1988. I wish to acknowledge my coauthors of these papers, F. J. McLafferty, W. Gratzer, and B. P. Angelis. I wish to thank the editors of *American Laboratory*, especially Brian Howard, for permission to quote extensively from those articles.