

Media Reviews

A Fifty-Year Love Affair with Organic Chemistry. By William S. Johnson. *Profiles, Pathways, and Dreams: Autobiographies of Eminent Chemists*; American Chemical Society: Washington, DC, 1998. Illustrations. xxvii + 229 pp. 15.7 × 23.3 cm. \$34.95. ISBN 0-8412-1834-X.

This latest volume is the twentieth in Jeffrey I. Seeman's projected 22-volume series of autobiographies of 20th-century organic chemists that began publication in 1990. We are fortunate that Seeman began his series as soon as he did, for nine of his autobiographees - Derek H. R. Barton, Arthur J. Birch, Melvin Calvin, Egbert Havinga, Michael J. S. Dewar, Herman Mark, Tetsue Nozoe, Vladimir Prelog, and William S. Johnson - have already died during the publication of the series to date.

In 1985, when Seeman asked Johnson to write a *Profiles* volume, his response was initially negative: "I'm sorry to turn you down, but there is no way that I could tell the results of all my students. It would not be fair to leave any of them out," a reflection of his primary concern for the feelings of his former students and collaborators. In fact, according to Seeman, "No contributor to *Profiles* wrote to as many of his former students for updated information and sent his draft manuscript to so many individuals."

Unfortunately, Johnson's death at the age of 82 on August 19, 1995 prevented him from experiencing the satisfaction of being selected by his colleagues as one of *Chemical & Engineering News'* "Top 75 Distinguished Contributors to the Chemical Enterprise" or of seeing his *Profiles* volume in print. Fortunately, his former students, colleagues, and friends, Ted Bartlett and Ray Conrow, reviewed the final manuscript, galleys, and page proofs of this book, and Ted Bartlett, Paul Bartlett, John D. Roberts, and Gilbert Stork contributed an 8-page epilogue that complements Johnson's own words, adds a warm, personal final touch that he was unable to provide, and incorporates his final research, including unpublished results, into the volume. They summarize his two top priorities - people and chemistry: "For cationic cyclization processes... Johnson's name is synonymous with the field He was a truly enjoyable person. All who knew him will forever admire his chemical style and personal philosophies."

With great candor and flashes of humor, Johnson describes his travels, honors, and awards such as the Roger Adams (1977) and Arthur C. Cope Awards (1989), hobbies (tennis, gymnastics, and hiking), his research and that of his colleagues, controversies, and consulting, editorial, and writing activities. He also includes personal reminiscences, poems and limericks, anecdotes such as a remark by Stork that "brought the house down, and I laughed so hard as to cause conversion of an incipient hernia into a major rupture requiring surgery soon after I returned home," the state of his health (which was "quite good into his seventies"), and opinions on education, grantsmanship, scientific ethics, creativity, excessive governmental regulations, and future trends in chemistry. He confides to us many of his philosophical observations: "Most chemistry departments are hotbeds of idle gossip, which often spreads all over the world." "It is my feeling, from observing chemists, that people who have exalted opinions of themselves, are generally unhappy individuals." His list of 185 references includes

publications through 1994 as well as two left unpublished at the time of his death.

Born in New Rochelle, New York on February 24, 1913, William Summer Johnson had little interest in school as a youngster. His father, after being told by the principal of New Rochelle High School that his son "would never amount to anything," sent him to his own alma mater, the Governor Dummer Academy, a private boys' prep school for Harvard founded in 1763, where he earned top grades. Bill's father lost almost all his possessions in the Great Depression, but Bill was able to continue his schooling with a full scholarship. He attended Amherst College with the aid of a scholarship and various odd jobs such as tending furnace, washing dishes, and playing the saxophone in dance bands (he seriously considered becoming a professional musician). Here he became enamored with organic chemistry, which he taught as an instructor for a year after his graduation *magna cum laude* in 1936. He then worked with a fellowship under Louis Fieser, who sparked his interest in steroids, at Harvard University, from which he received his M.A. (1938) and Ph.D. (1940) degrees, the latter in record time (22 months in residence).

In 1940 Johnson joined the faculty at the University of Wisconsin, "one of the best places for organic chemistry at that time," where he rose through the ranks, eventually becoming Homer Adkins Professor of Chemistry (1954 - 1960), "the first research professorship in chemistry without any classroom teaching requirements". On December 27, 1940 he married Barbara Allen. Because the couple had no children, she was able to accompany him during his frequent foreign travels. That same year Johnson began to satisfy his predilection for organic synthesis by directing his attention to the total synthesis of steroids, "which soon proved to be the hottest synthetic target of the time." He describes the primitive conditions and the culmination of his early work in the stereoselective synthesis of equilenin. Because "grossly distorted versions have been circulating for years," he also relates a shocking tale of violence that occurred in his laboratory in September 1951 when one of his graduate students (who is not identified) shot and wounded a labmate, "an event which had a significant effect on me and a number of my students, drawing us together in a lasting way."

Although Johnson's main interest was research and teaching and though he had "an ideal setup at Wisconsin with superb facilities," in 1960 he accepted an invitation to become head of, and to upgrade, the Stanford University Chemistry Department. With faculty recruiting as his primary concern, he was able to add Carl Djerassi, Paul J. Flory, Harden M. McConnell, Henry Taube, and Eugene E. van Tamelen to the department, resulting in its spectacular rise from 15th to 5th place in the nation. He offers retrospective observations on how to improve a chemistry department. When asked for advice on attracting top students, Johnson replied, "Add some distinguished scholars to your faculty." He remained at Stanford for the rest of his career, serving as department head for nine years.

Johnson's book reads like a "Who's Who in Organic Chemistry" with descriptions, impressions, and thumbnail sketches of such luminaries as Sir Robert Robinson ("Compulsively competitive, and had paranoid delusions that

others were trying to steal his ideas What a pity that this man could not relax and enjoy his own great talents.”), Robert B. Woodward, Gilbert Stork (“the funniest person I have ever known”), Carl Djerassi, Derek Barton, John D. (“Jack”) Roberts, and authors of other *Profiles* volumes.

During his long and productive career, Johnson made many contributions to contemporary organic chemistry, the genesis and course of which he describes lucidly with extensive use of 110 structural formulas, 75 reaction schemes, and occasional laboratory notebook pages. More than 350 graduate and undergraduate students, postdocs, and visiting professors (many of whom are shown in the 63 formal and informal photographs in the book) worked with him through five and a half decades on problems such as angular methylation; intramolecular Friedel-Crafts acylation reactions; conformational analysis; hydrochrysen approach to the total synthesis of steroids such as aldosterone, testosterone, cholesterol, conessine, progesterone, veratramine, and veratrum alkaloids (“a factor in a major change in attitude regarding steroid synthesis from the two- to the three-dimensional approach”); NMR spectroscopy; biomimetic polyene cyclization studies (“still ... one of our major efforts after 35 years”); solvolysis of sulfonate esters; tricyclization and tetracyclization reactions; corticoid synthesis via polyene cyclization methodology; stereoselective olefin syntheses; ortho ester Claisen condensation (“probably the most useful chemistry to emanate from our laboratories”); olefinic and chloro ketal Claisen reactions; enantiocontrolled generation of chiral centers during C-C bond formation mediated by homochiral acetals; and the fluorine atom as a C-S auxiliary in biomimetic cyclizations. In a 3-page chapter, “Some Concluding Remarks About Our Research,” Johnson states, “The reviewed research did not evolve from a master plan; indeed it was largely a matter of following one’s nose and trying to look at things that related to areas that were regarded as important issues of the time.”

Johnson’s entertaining, informative, and modestly priced volume is a gold mine of information and insights for synthetic organic chemists. A first-person saga of an individual committed both to the practice of scientific research and to his profession, it will also be of interest to both present and future generations of students and instructors of chemistry courses and the history of science as well as to all persons concerned with the human aspects of science.

George B. Kauffman and Laurie M. Kauffman,
[California State University Fresno](http://www.csufresno.edu/~george.kauffman)
george_kauffman@csufresno.edu

S1430-4171(99)03302-0

Molecular Thermodynamics. By Donald A. McQuarrie and John D. Simon. (1999) University Science Books, 55D Gate Five Road, Sausalito CA 94965, USA. 672 pp \$78.00, ISBN 1-891389-05-X.

This book is back-to-front - or so it might appear. The harmonic oscillator model of molecular vibration is introduced early in chapter one, molecular partition functions are discussed in chapter three, and symmetry numbers and normal coordinates shortly thereafter. In contrast, such apparently elementary concepts as enthalpy, work, and the First Law make an initial appearance two hundred pages into the book.

To many readers this will seem a very unconventional approach. In chemistry courses, classical thermodynamics is generally studied well before statistical thermodynamics. The latter is mathematically more challenging, and its links to experiment are more difficult to appreciate. Thus, students are often taken first through experimental thermochemical data, and then on to the interpretation of easily recognized observables such as heat and temperature changes; classical thermodynamics is presented as a rationalization of such data. To start with quantum mechanics would be madness, faculty might argue. And yet, it works. There are, of course, solid reasons why this is so. Quantum theory and statistical thermodynamics can indeed form a productive route into classical thermodynamics. Statistical thermodynamics is the more “fundamental” branch of the subject, allowing one to derive the values of macroscopic parameters from the motion and energetics of individual molecules. Indeed, one might argue that one can only really understand thermodynamics as a whole through an appreciation of how changes at the molecular level are responsible for changes in state functions.

The style of *Molecular Thermodynamics* recalls the authors’ successful text *Physical Chemistry: A Molecular Approach*; indeed, there appears to be significant overlap between the two books. As one delves into *Molecular Thermodynamics*, the authors’ decision to use quantum mechanics as a platform on which to build thermodynamics becomes progressively more understandable and persuasive. The authors address themselves firmly to honours chemists. Only the best students majoring in other subjects will find the book straightforward, even with the help of the inserts that introduce relevant mathematics. However, to the target market of the committed chemist the book has much to offer. The writing is exceptionally clear, and explanations are lucid and sound. Plenty of examples are used to illustrate the arguments, and figures are pertinent. I was a little concerned, however, that a few of the figures might be misleading. For example, in the figures showing the phase diagrams of water and carbon dioxide, the line separating solid and liquid phases is exactly vertical, (though students are warned obliquely in the legend that this is a consequence only of the scales used). Similarly, in the same figures, the lines separating gas from liquid, and gas from solid, are drawn as curves with continuous smooth first derivatives, which is incorrect for these substances. Nevertheless, most diagrams are simple, correct and relevant.

A welcome feature is the use of informative subsection headings. For example:

- 1.1 The Electronic Energy of Atomic Hydrogen is Quantized
- 2.1 All Gases Behave Ideally if they are Sufficiently Dilute
- 6.2 Nonequilibrium Isolated Systems Evolve in a Direction That Increases Their Disorder

This is a simple but effective device that should be used more widely.

This is a chunky book: more than 600 pages on thermodynamics sounds like pretty indigestible stuff, but it is surprisingly palatable. Sales may suffer from the reluctance of students to pay a fairly high price for a book that may appear to deal with only a small section of the syllabus (though the coverage is actually considerably broader than its title might suggest). Although *Molecular Thermodynamics* may not

appear on the shopping list of every chemistry student, it would certainly be a useful addition to the bookshelf of every physical chemistry lecturer.

Hugh Cartwright, Oxford University,
hugh.cartwright@chem.ox.ac.uk

S1430-4171(99)03307-6

ElemenTree: A 3-D Periodic Table. By Fernando Dufour available in two versions: 1. A transparent Vivak plastic periodic tree in pink, green, and black, 10-1/2 in. high, 8 in. at widest near base, US \$31.00. 2. A black-and-white Mini-ElemenTree, which fits into the pocket of a 3-ring loose-leaf binder, US \$18.00. Both kits include a 24-page instruction manual. Prices do not include shipping and handling or sales tax. Order as Catalog No. M2-84-0124 from Carolina Biological Supply Co., 2700 York Road, Burlington, NC 27215, Telephone: (800) 334-5551; FAX: (800) 222-7112; e-mail: dthomas@carolina.com or fcherry@carolina.com. <http://www.carolina.com>.

Readers of two recent articles by Eric Scerri on the periodic table (*American Scientist*, Nov.- Dec. 1997, pp 546 - 553 and *Scientific American*, Sept. 1998, pp. 78 - 83) may have seen colored pictures of a 3-dimensional periodic table and wondered if it is commercially available. The answer is a resounding yes.

According to the late American astronomer Harlow Shapley, the periodic table "is probably the most compact and meaningful compilation of knowledge that man has yet devised." Since Dmitrii Ivanovich Mendeleev first published it in 1869, more than 700 different graphical representations of this cornerstone of modern inorganic chemistry have been published (e.g., see Edward G. Mazurs, *Graphic Representations of the Periodic System During One Hundred Years*; University of Alabama Press, 1974, for a compilation). Each has advantages and disadvantages, and the quest for an "ideal" or "perfect" periodic table continues unabated.

Since he first saw an article featuring an adaptation of the 1925 Courtine model in the November 6, 1946 issue of *Popular Science* magazine, Fernando Dufour, chemistry professor at the Collège Ahuntsic, Montréal, Québec, Canada (now emeritus), better known to his friends and aficionados as "Nando," has been fascinated and obsessed by the idea of developing a 3-D color model table of his own.

He has described the genesis of his lifelong passionate preoccupation: "When I discovered the periodic table, I was awed to the ultimate heaven in thinking that this was knowledge so infinite it would unravel all the mysteries of nature - the blueprint of the universe itself. It was Archimedes' grain of sand - 'To understand a grain of sand is to understand the universe.'" Since then, for more than half a century, this septuagenarian, who humorously refers to himself as "a 74-year-old kid," has spent all his time developing version after version of a three-dimensional periodic table (first using cardboard and Styrofoam, and now plastic) designed for teachers, students, or for classroom use via an overhead projector, which makes one model sufficient for an entire class of students. In 1979 he received his M.Sc. degree from the Université Concordia in Montréal with the thesis topic, "An attempt to unravel atomic structure with a three dimensional model of the periodic table." In his opinion, "A third dimension [for the periodic table] is not an option but a necessity."

Easily assembled from 17 dismountable components, with s-block elements, the alkali and alkaline earth metals (pink),



Figure 1. Fernando Dufour with several versions of his ElemenTree.

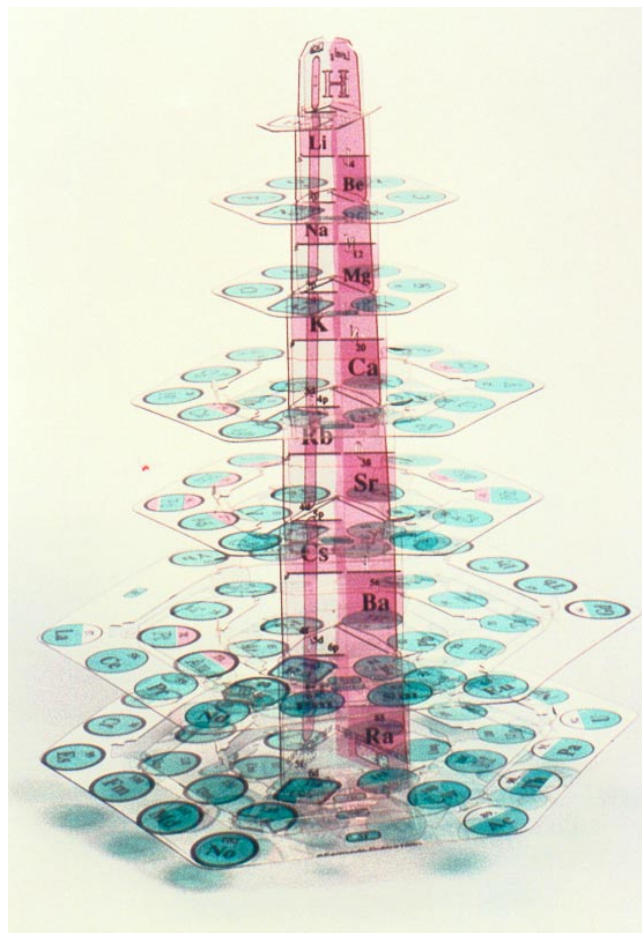


Figure 2. The ElemenTree.

forming the trunk and the p-, d-, and f-block elements (green) arranged concentrically as hexagonal branches, this latest version of Dufour's model resembles a stylized Christmas tree (*sapin périodique*). Used in the first Chemical Heritage Foundation - Woodrow Wilson Summer Institute on the History of Chemistry at Princeton University (July 5-31, 1992) by Susana S. Suarez, it was displayed at the Annual Chemistry Congress held in Manchester, England and has been featured in numerous newspaper and magazine articles.

As students assemble the tree, they effortlessly apply the *Aufbauprinzip* and can simultaneously visualize and trace

trends, similarities, and differences in a variety of fundamental concepts such as the continuity and periodicity of an unbroken sequence of elements from hydrogen (atomic no. 1) at the top to ununoctium (atomic no. 118) at the base, Pauli's exclusion principle, Hund's rule, vertical and horizontal symmetry (groups and periods), quantum numbers, valence, order of orbital energies, types of orbitals involved, atomic radius, ionic or covalent bonding, sigma-pi bonding, metallic or nonmetallic character, ionization potential, electronegativity, and electron affinity. Many chemical or physical properties of the elements that are discerned only with difficulty or not at all with the traditional two-dimensional periodic table are readily perceived and correlated by use of the 3-D periodic tree; the accompanying instruction manual describes how, with both its vertical and horizontal axes, the ElemenTree expands visual access from the three periodic features of the two-dimensional table to 42 features. By removing the central support, the preassembled parts fit into a book-size (8-5/8 in. x 9-1/2 in.) folder, ready to be "recycled" from one classroom to another or to be stored on a bookshelf.

This useful educational and research tool suitable for high school through college and university level courses in chemistry and related fields has been sold in 26 countries, 46 of the United States, and 10 Canadian provinces. To the best of my knowledge there is no other product like it on the market. Indeed, Sherlock Holmes may have anticipated Dufour's pedagogically ingenious, user-friendly, hands-on interactive 3-D periodic table when he said to Dr. Watson, "ElemenTree."

George B. Kauffman, [California State University Fresno](http://www.csufresno.edu/~george.kauffman)
george_kauffman@csufresno.edu

S1430-4171(99)03308-5

Introduction to Organic Spectroscopy. By Laurence M. Harwood and Timothy D. W. Claridge, Oxford University Press, Oxford, 1997. ISBN 0-19-855755-8.

This brief textbook of under 100 pages contains a wealth of information in a tiny package. It is one of the *Oxford Chemistry Primers* series. While it might not fit the classic definition of a primer, a first book introducing a topic, it certainly is a valuable resource to the student of organic chemistry who wishes to have a brief, clear, and well-written introduction to the subject of spectroscopy. This is a compilation of information about the methods and applications of spectroscopy to the identification and structural elucidation of organic compounds.

The book begins with an introduction to the basic theory of spectroscopy, explaining the electromagnetic spectrum, developing Beer's law, and defining many of the important terms used in spectroscopy. The mathematics throughout the book is kept to a minimum, with verbal explanations and analogies substituting nicely for mathematical derivations.

UV-visible and infrared spectroscopy are each covered in one chapter. NMR spectroscopy is treated in two chapters, one on the basics and one with more advanced topics. The advantages and applications of Fourier transform spectroscopy in both IR and NMR spectroscopy are described, again in a nonmathematical way. A chapter devoted to mass spectrometry completes the book. In each case, the major emphasis is on the interpretation of data. However, basic instrumentation is also described for each method. For instance, in the MS chapter,

magnetic-sector quadrupole and time-of-flight mass spectrometers are described, and several types of ionization systems are briefly treated.

Each chapter contains a set of exercises for the reader, mostly focused on interpretation of various spectra, and a short list of further readings. The answers to the exercises are also provided. The book would serve as a useful supplement to an undergraduate organic chemistry course, or to an instrumental analysis course. Students will appreciate the way it condenses the important points, with many easily located definitions of terms and good analogies to explain what might be difficult concepts. In addition, it would be a useful reference on the shelf of the graduate student or organic chemist who occasionally needs to interpret spectroscopic data or to determine what sort of spectroscopy should be done to obtain needed information.

Barbara B. Kebbekus, [New Jersey Institute of Technology](http://www.njit.edu/~barbakeb)
BKebbekus@aol.com

S1430-4171(99)03304-9

Thermodynamics of Chemical Processes. By Gareth Price. Oxford University Press (1998), 86 pp.

This short book is no. 56 in the Oxford Chemistry Primers Series. The author's aim is to introduce the concepts needed to treat energy changes during chemical processes and reactions and to explain how these concepts are used to discuss chemical reactivity. The margins, which take up almost one-third of each page, are used to explain mathematical concepts such as integration and differentiation, to show diagrams of apparatus such as a bomb calorimeter, to show schematics such as representation of fluid densities below and above the critical point, and to show tables and graphs. The scope of the book is suggested by the titles of its five chapters:

1. Preamble: Energy in Chemical Systems
2. Enthalpy and Thermochemistry
3. Entropy in Chemistry
4. Free Energy and Equilibrium
5. Phase Equilibrium and Solutions

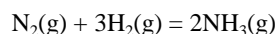
This book is meant to be used for a short introductory undergraduate course for students who have taken A-level mathematics in the British system. This is equivalent to a U.S. sophomore course for students who have been exposed to some calculus. Freshmen taking a concurrent calculus course would also be able to use this book. The text is developed in an understandable fashion with many worked example problems and a few additional problems. I would personally be tempted to use this volume as a supplemental text for freshman chemistry. I must admit at this point that I teach at a technical college at which the freshmen have either been exposed to calculus in high school or are taking calculus at the same time as freshman chemistry. Although some calculus is explained in the margins of this book, most students would not be able to learn enough from these margins to understand the text.

The text contains very few mistakes or misprints. One of the few that I could find is the statement that the First Law of Thermodynamics is

$$U = q + w$$

for an *isolated* system, not a *closed* system. Since the author makes a point of stating that the most common type of system is *open*, it would also be worth stating that it is very difficult to state the First Law mathematically for an open system, but that this can be done in a number of ways.

This brings me to one of the common oversimplifications made in this book, unfortunately almost standard in explanations of thermodynamics at this level. This is the following statement of the Le Chatelier Principle: "If a system is subjected to a constraint, it will react to minimize the effect of the constraint." This is wrong when stated in this way. As usual, however, the Principle is used correctly in the examples in the text even though the constraints are, again as usual, not stated. For example, when discussing the change in the equilibrium of an exothermic or endothermic reaction when the temperature is changed, the constant pressure constraint should be stated. The Le Chatelier principle should not be stated in the general fashion quoted from this text. It is very specific and should be stated specifically for the types of examples given. It is not difficult to provide specific examples that contradict the general statement. For example, if we assume that the gases involved in the reaction



are ideal gases, then, if the mole fraction of the $\text{N}_2(\text{g})$ in the undisturbed equilibrium mixture is greater than 0.5, and if the mixture is kept at constant temperature and pressure, then the addition of a small amount of additional $\text{N}_2(\text{g})$ will result in a new equilibrium mixture in which *even more* $\text{N}_2(\text{g})$ has been produced. This is a consequence of the second law of thermodynamics; the proper use of the Le Chatelier principle is a consequence of the second law of thermodynamics; it is not an additional thermodynamic law.

Since this otherwise excellent little book errs only in the ways in which most books at this level err, I would recommend it for beginning courses that use calculus. It is much more readable than most books written at a comparable level.

Sonja Krause, [Rensselaer Polytechnic Institute](mailto:krauss@mail.rpi.edu)
krauss@mail.rpi.edu

S1430-4171(99)03309-4

Mathematica Programs for Physical Chemistry. By W. H. Cropper, Springer, New York, 1998, ISBN 0-387-98337-6.

William H. Cropper's book and CD-ROM of Mathematica programs elegantly demonstrate what he asserts in his preface: with modern software tools "the tedium of calculation work [in physical chemistry] has largely been overcome." The Mathematica programs are easy to execute, and many take full advantage of the impressive graphical capabilities of this software package. Designed to be used as a companion volume to a regular textbook, this book covers a wide range of topics in physical chemistry, including many examples in thermodynamics, kinetics, quantum chemistry, spectroscopy, and statistical mechanics. The presentation is clear; each equation explored in the CD-ROM is introduced succinctly in the text. The programs can be run as is, or are easily altered as interactive exercises, most-obviously by introducing new parameters. The book contains many exercises based on the programs; the results are included on the CD-ROM. The depth

of coverage in many areas often goes beyond most conventional junior-year physical chemistry courses, but this allows instructors to go more deeply into their favorite topics. I believe that any physical chemistry instructor will enjoy using the programs.

But how well will it work for students? Here I am a little less confident. Some of this comes from my own experiences writing educational software. Something I find challenging, interesting, and great fun to prepare, all too often doesn't excite the students nearly as much as it did me. Why? Because when they use it, the process is all too automatic. I found this to be the case with some of Cropper's 140 Mathematica programs. Take, for example, the program "Acetate." Using extended forms of the Debye-Hückel theory to obtain the activity coefficients, it calculates pH values for acetic acid-acetate buffers. This is a tedious hand calculation. Instead you open the notebook, execute the program, and the result appears. But if you are not familiar with or not interested in Mathematica, you are not likely to examine the underlying code to see how it all works, and you simply have a pH calculator, which is convenient but not particularly instructive.

Mathematica's excellent graphics make the curve displayed in a program like "Morse" pretty to look at, but not more informative than a graph found in a textbook. Some students may benefit from seeing the curve change as the parameters are altered, but each plotted separately on differently scaled axes looks pretty much the same. Many of the 2-D graphical results (in programs like "X-ray1", "Leps", or "Aorbital") are lovely. Is seeing them at the end of a Mathematica notebook more instructive than seeing the same equations and figure in a book? For some students, the answer will be yes.

It is often argued that to motivate a student, a computer exercise should be interactive, dynamic, seriously use the computer's power, or be an obvious timesaver. Many of the Cropper's Mathematica examples nicely satisfy one or more of these criteria.

Some of my favorites:

- The program "Patterns" gives a pretty and very clear graphical explanation of the relationship of peak-to-lattice positions in a Patterson map.
- The pair of programs "Symtop1" and "Symtop2" effectively use color graphics to explain the pattern of overlapping P, Q, and R branches, which explain the bandshapes in perpendicular and parallel transitions in the IR spectra of symmetric tops.
- "Coil1" generates a polymer random coil; it is fun to see the different coils generated each time the program is executed.
- "Nmrft" and "Irf" use the computer's power and nicely demonstrate the concept of Fourier transforms.

I experienced only a few problems.

- Two versions of each program are included, "name.ma" for Mathematica 2.0, and "name.nb" for Mathematica 3.0. If Microsoft Windows 95 is set to not display filename extensions (often the default), this can be confusing since the files then appear to be the same.
- When using the programs, one frequently has the opportunity to alter data: the program instructs the user to change the data in line *n*. I found it a little frustrating that one had to guess how the unnumbered lines were being

counted. On the other hand, it is pretty easy to figure out where to make changes.

- Some of the programs use separate data files on the CD-ROM. When I tried to run these by first starting Mathematica and then loading the programs, they failed to run, since the program looked in the wrong place for the data. The problem disappeared when Mathematica was launched using the program name on the CD-ROM.

I am only an occasional Mathematica user, so these minor and easily resolved problems suggest that this collection of programs is very user-friendly. I didn't have the software to run the QuickBasic programs.

I used the CD-ROM on a 200-MHz Pentium machine with 32 MB of memory. It still took a little time to display some of the graphics. My previous experience with Mathematica on slower machines suggests that some of these programs might try the patience of the user. But given the cost of Mathematica, chances are good that people using it today are probably also using quite new hardware.

Instructional programs written in languages like Fortran or Basic can be designed so users can be totally unaware of the underlying code; they simply execute the application. With

Mathematica programs the opposite is true; the code is always there. This is a mixed blessing. On the one hand, one could argue that this is better pedagogy; the package is not a mindless black box. But it can also be imposing; if you are not familiar with Mathematica, there is a lot of code, some of it quite imposing, between you and the answer. Some is important to understanding the chemical problem, but quite a bit is not. Looking at it may be a good way to learn Mathematica, but if that is not the objective, it may be an unfortunate distraction. Nevertheless, Mathematica is being used as an important instructional tool in many disciplines. Students in a modern physical chemistry lecture or laboratory may be perfectly comfortable scrolling through the code, and will probably learn a great deal as they do so. Where physical chemistry students are already familiar with Mathematica, this book is a natural and very welcome contribution. But even for those for whom Mathematica is new, it is well worth the effort to use at least some of these lovely programs.

Sally Chapman, [Columbia University
schapman@barnard.columbia.edu](mailto:schapman@barnard.columbia.edu)

S 1430-4171(99) 03306-7