Computer Software Reviews

Chemcal. Program Version 2.01.00. Copyright 1985 by B&B Scientific Software: 1124 East Portland Street, Phoenix, Arizona 85004. $89.95.

Chemcal is a single-disk, noncopy-protected program that is most useful for the calculations needed for chemical analyses. The software is IBM compatible. (This reviewer found that it will also run on a Texas Instruments Professional Computer with use of the "Emulate" program provided on MS-DOS.) From the main menu that appears after loading the program, one has a choice of four subprograms: one that allows the calculations of elemental percent weights from a molecular formula, one that allows the reverse process, a third that is a slight variation of the latter, and a fourth subprogram that is a listing of atomic weights. The calculations are most readily done for programs containing any of the following elements: C, H, N, O, S, P, Cl, F, Br, and I. (Although slightly more tedious, it is possible to make determinations when other elements are present.) The software also allows one to take into account in such calculations the presence of solvent molecules.

This reviewer found the program to be simple to learn and use. If one has a compatible computer readily available, the program can easily take the place of a tabular listing of the elemental percent weights for various molecular formulas or of a calculator needed to make such calculations.

David Wenkert, *North Texas State University*

Book Reviews*

Progress in Analytical Atomic Spectroscopy. Volume 7. By C. L. Chakrabarti (Carleton University). Pergamon Press: Elmsford, NY. 1986. v + 421 pp. $132.00. ISBN 0-08-034141-1.

This volume is a compilation of papers originally published in 1984 in the journal of the same name. This journal is aimed at the rapid publication of comprehensive reviews authored by some of the leading analytical spectroscopists in the world (Note: As of 1986, the journal has broadened its scope to include analytical molecular spectroscopy and has, thus, changed its name to Progress in Analytical Spectroscopy). Since its inception in 1978, this journal has been an authoritative reference guide for analytical spectroscopists—this volume is no exception. Although the nine review articles included in this volume range from 13 to 71 pages in length, all present a detailed account of their respective subjects. Generally, the articles are more than just reviews based on previously published papers and include a wealth of previously unpublished data from the authors' laboratories as well.

Two of the most popular high-power transient plasma sources (spark and laser plasmas) are covered separately by Scheeline (High Voltage Discharges: Diagnostics and Opportunities) and Dittrich and Wennrich (Laser Vaporization in Atomic Spectroscopy). Scheeline limits his presentation primarily to modern spark source production and diagnostics, but he closes with a discussion of some of the more promising new transient plasma sources produced by high-voltage capacitive discharges. Dittrich and Wennrich's treatment of laser atom/ion cells is exhaustive in its scope, including no less than 432 references!

An excellent review/tutorial on microwave plasma sources is presented by Matousek, Orr, and Selby (Microwave-Induced Plasmas: Implementation and Application). Coverage of electrothermal atom cells includes theoretical modeling of platform atomizers in a paper by Paveri-Fontana and Tessari (Models in Electrothermal Atomization: The Platform Atomizer) as well as Sedykh and Belyaev's discussion of the use of molecular absorption measurements for graphite furnace diagnostics (A Study of Sample Volatilization in a Graphite Furnace by Means of Atomic and Molecular Absorption Spectra).

A comprehensive tutorial on noise and noise reduction schemes in optical spectroscopy is given by Epstein and Winefordner (Summary of the Usefulness of Signal-to-Noise Treatment in Analytical Spectrometry). A detailed theoretical treatment of the technique of laser-enhanced ionization is given by Travis and co-workers (Principles of Laser-Enhanced Ionization Spectrometry in Flames) along with a discussion of the future prospects of the method.

Finally, the volume contains two articles on detection strategies in analytical spectroscopy. McGeorge and Salin (Image Sensor Applications in Analytical Atomic Spectroscopy) present a framework for the evaluation of multiwavelength detection systems with discussion of a variety of electronic multichannel detection devices. A very different perspective is presented by Dittrich and Niebergall in their comprehensive presentation of an extremely powerful plasma diagnostic technique called equidensitometry (Equidensitometry—A Method for Plasma Diagnostics in Atomic Spectroscopy). This method is actually just a means of presenting spatially resolved spectrographic information, but its visual impact is impressive—the potential of equidensitometry as a plasma diagnostic tool is amply demonstrated by the authors.

Unfortunately, space limitations preclude more than a terse commentary on the papers included in this volume—suffice it to say that this compilation is an essential addition to the library of any analytical atomic spectroscopist who is without access to the original journal.

Joel M. Goldberg, *University of Vermont*

Practical Organic Mass Spectrometry. By J. R. Chapman (Kratos Analytical Instruments Ltd.). John Wiley & Sons: New York. 1985. ix + 197 pp. $34.95. ISBN 0-471-90696-4.

This book is directed toward the practicing mass spectrometrist and aims to review the principles, practical details, and applications of a number of newer methods. Theoretical presentation is deliberately limited to providing the basic understanding necessary for employing or evaluating a technique.

The first chapter (24 references) is an introduction covering the standard instrumentation. Included in this chapter is a discussion of multiplier gain measurements and methods for determining the basic instrument sensitivity. There is no discussion of FTMS or TOF instruments or their performance relative to the more common types of mass analyzers.

The second chapter (56 references) deals with sample introduction and concentrates on GC and probe inlets. The major LCMS systems are concisely described in this chapter, but the reader is referred to other literature for applications and practical details.

The third and fourth chapters give authoritative yet concise reviews of the major ion–molecule reactions employed in positive and negative chemical ionization methods, respectively. Practical details are presented on CI operation and the introduction of reagent gases into high-voltage sources of magnetic instruments. Both chapters give separate tables listing applications along with reference lists organized by the reagent gas employed and the compound classes studied. Chapter 3 contains 69 general references plus 276 application references while Chapter 4 gives 49 and 80 references, respectively.

Chapter 5 covers methods for analysis of labile molecules including FC, DCI, DEI, and FAB. The theoretical and practical discussion emphasizes FD following the author's belief that this technique provides a common background in ion formation processes and sample preparation methods for the use of other, newer methods. This chapter contains 121 general plus 46 DCI and DEI application references.

Chapter 6, on metastable ions, gives a complete set of equations describing the required field relations for implementing various metastable scans on magnetic instruments. A lucid discussion is given on the precursor or fragment ion resolutions obtained with these scan modes. While some bias may be noted in the author's preference for IFFR studies on forward geometry magnetic instruments, the treatment of the advantages of triple-stage quadrupole instruments is brief but objective. A table with 98 references summarizes analytical applications to 1983 and 84 references are given.

*Unsigned book reviews are by the Book Review Editor.