Computer Software Reviews

MacSimion. Version 1.0. Montech PTY LTD.: Monash University, Wellington Rd., Clayton, Victoria 3168, Australia. List price $399.00.

MacSimion is a program for the numerical simulation of the motion of charged particles in electric and magnetic fields. It is written in the C language for the MacIntosh family of computers. Two different versions are supplied on one diskette that is not copy protected. (Source code is not provided in the distribution package.) One version is for use with MacIntosh II computers, and the other is for use with MacIntosh SE and earlier MacIntosh machines. Implementation on a MacIntosh II with 16 color graphics is recommended.

Becoming facile with the use of MacSimion takes only a minimal amount of time—one or two hours. This ease of use is due to two factors. First, the program is very MacIntosh-like, making use of pull-down menus, icons, and the like. Thus, anyone familiar with operation of a MacIntosh should have little trouble adapting to MacSimion. Second, the operating manual is quite well organized and well written. It includes a tutorial section that steps one through the operation of the program, and it also includes a software reference section and a section that explains what calculations are actually being performed when the program is run.

MacSimion consists of three subprograms. The first is the "geometry" sub-program, which allows one to construct an arrangement of up to 127 distinct electrodes, each with its own electrical potential. This subprogram is interative and easy-to-use, resembling other MacIntosh graphics programs such as MacDraw.

The second, "refine" subprogram takes as input the electrode arrangement defined in the geometry subprogram, and by iterative application of Laplace's equation it solves for the electrical potential at all points in the two-dimensional array that represents the space in and about the electrodes. (Only two dimensions are needed because of the required symmetry in the electrode arrangement—see below.) On the MacIntosh II this refine procedure typically was completed very quickly (typically less than a minute). The result of the procedure is a contour map of the electrical potential in two-dimensional space. This contour map can be displayed directly on the MacIntosh monitor.

The "trajectory" part of the program takes as input the results of the refine procedure and, along with data specifying the initial conditions of an ion, calculates the trajectory of that ion in the vicinity of the electrodes. A choice of two algorithms for trajectory calculations is provided: (1) a "fast" algorithm, which uses linear field gradient interpolation and simple integration, and (2) an "accurate" algorithm based on the fourth-order Runge-Kutta technique which utilizes interpolation of the potential by means of a fitted fourth-order polynomial. Many other options are provided in trajectory mode, some for enhancing the speed or accuracy of the trajectory calculation (e.g. the option of fixed or variable time steps), others for modeling special physical situations (e.g. the fragmentation of an ion during its trajectory), and others for specifying the initial conditions of the ion. The output of the trajectory subprogram is an on-screen, real-time graphical representation of the trajectory, together with information pertaining to that trajectory (elapsed time, ion positions, ion energy, etc.). On a MacIntosh II, individual trajectories are calculated in times that are quite reasonable. On other MacIntosh machines trajectories may take about forty times longer than they do on the Mac II.

We found MacSimion to be a powerful easy-to-use program for the calculation of ion trajectories. Implemented on a Mac II the program allows one to modify electrode parameters and almost instantaneously see graphically the results of such modifications on electrical potentials and ion motion. One would expect the program to be very useful not only as a tool for the design of experimental apparatus but also as a pedagogical instrument. This having been said, it is also pertinent to outline some important limitations of the software package. First, the program allows only certain types of electrode arrangements to be constructed. In particular, only arrangements that have cylindrical symmetry or that extend infinitely in one direction are supported by the software. While the reasons for this limitation are clear, and while many electrode arrangements can be approximated within the confines of the limitation, one should be aware that is does exist. Second, the program can only handle temporally and spatially constant magnetic fields. Moreover, although ion trajectories are calculated in three dimensions, only two-dimensional trajectories are displayed. Third, the program can handle time-varying electrode potentials, but the time variations must be periodic and be either sinusoidal, square, or triangularly shaped waveforms. Fourth, the graphical output of trajectories, while providing very fast access to the calculated trajectory, also incurs some disadvantages. The screen resolution and size are such that convenient and accurate modeling of the electrodes is possible. However, viewing trajectories over distances much greater than the electrode system itself is difficult. This is unfortunate with respect to focusing systems which need to be characterized over the distance between lens and detector (e.g. a time of flight mass spectrometer system). Though this is an inconvenience, it is by no means fatal, as a good approximation of focusing behavior can be obtained over typical "geometry" dimensions, and far field behavior can be extrapolated in a straightforward manner. If one can tolerate these four principal limitations, the program's ease-of-use and speed make it quite attractive for ion trajectory calculations.

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Book Reviews*

Analytical Artifacts. GC, MS, HPLC, TLC and PC. Journal of Chromatography Library—Volume 44. By Brian S. Middleditch (University of Houston). Elsevier: Amsterdam and New York. 1989. xxiv + 1028 pp. $241.50. ISBN 0-444-87158-6.

This encyclopedic volume is a compilation of information on artifacts in the determination and identification of chemical substances. It includes generous doses of analytical folklore, arcana, gossip, and uncommon wisdom as well. The volume is thus invaluable to help the analytical chemist keep a watchful eye on artifacts of the analytical process ("artifact" wins handily over "artefact", according to the detailed statistics presented: 2447 to 648 overall, 556 to 123 in *Chemical Abstracts*, and 1048 to 437 in *Excerpta Medica*). Containing over 1100 entries from abietic acid to zinc dialkyl dithiophosphates and nearly 1000 complete literature citations, this is a labor of love (and determination) that few would be capable of undertaking and even fewer capable of completing. It is entirely a single-minded affair: there are no coauthors and no effusive/perfunctory acknowledgments to associates/graduate students. Rather there are cautionary notes under the entry "Literature Surveys" to never trust a librarian to do one's computer-assisted searches and to always follow up computerized searches with manual ones. Chemical Abstracts Service (CAS), recently chosen to devise a way to classify and modernize the retrieval of the holdings of the U.S. Patent and Trademarks Office, would be well advised to seek the services of the author to ensure that they are indeed doing a thorough job. The magnitude of this effort boggles the reviewer's mind; he can only offer his respectful tribute to the author and confess his total lack of jealousy of this achievement. Any criticism offered hereunder should thus be taken not as indices of diminution of the value or the scale of the undertaking, but as the duties of a critic.

The entries are in alphabetical order. The title for each entry contains the common name (not necessarily the CAS name), the molecular formula, and the mass spectroscopist's molecular weight (based on the most prevalent isotopic composition). The mass spectrum is then given (70 eV electron ionization throughout) in frames 200 amu wide. The chemical structure, CAS name and registry number, and the Merck Index reference number follows. Synonyms are given next. [Reader, are you informed enough to know what compound bears the synonyms (partial

*Unsigned book reviews are by the Book Review Editor.

listing): aceticyl, acetilum acidulatum, acetol, acetophen, acetosal, acetosalic acid, acetosalin, acylpyrin, ASA, aspro, asteric, empirin, helicon, measurin, rhodine, salacetin, salcetogen, saletin, and xaxa (no relation to the Gabors)?] Now follows the main text, preparations in which the entry occurs as an ingredient or impurity (in the former category, 179 pharmaceuticals, ranging from ACA to zactirin, are listed for aspirin; yes, you guessed correctly) and impurities which occur in the title compound, including any added stabilizers, are listed. Further, all such subentries are dutifully and painstakingly cross-referenced. Potential problems from losses or artifact formation during analysis, complete with literature citations, are discussed whenever such information is available. If the title compound can lead to the formation of other compounds during the analysis, this is also discussed. Mass spectra of derivatives are given in a number of cases.

The volume primarily addresses chromatography (almost exclusively gas chromatography) and mass spectrometry. This reviewer, being interested in atmospheric analysis, was pleasantly surprised to note that the formation of artifact sulfate during the sampling of ambient air was dutifully catalogued and so were the contaminants in FEP Teflon bags commonly used in air sampling. The myth about the virginity, inertness, and pristine behavior of Teflon is firmly disposed of under "Teflon". With equal resolution, under "glass-lined steel tubing", Middleditch dispenses with the mass spectroscopy community gossip relating the occurrence of a m/z 418 peak as due to cracks in such tubing as precisely that, gossip. The information presented on chromic acid makes it clear that, unless the analysis is totally immune to the residual presence of this material, it should never be used: 12 sequential water washes failed to remove the adsorbed chromic acid; it apparently penetrates glass!

It is a pleasure to thumb through this volume even if one has no great interest in analytical artifacts. It may not be comforting to know that all of us are involved in passing one another illicit drugs (in 90% of the sampled U.S. currency from several major cities, cocaine residues were detectable in denominations of $20 and above, and quite possibly in smaller bills as well), but this reviewer will decidedly sleep better knowing that perfluoroethers are not being produced in quantity in Martian factories; their presence in Martian soil samples was due to contamination. It is impossible to disclose in this review all such interesting morsels that are generously interspersed between the more prosaic entries; the reviewer therefore leaves it to the interested reader to find out what connections analytical artifacts may possibly have with Napoleon's alleged arsenic poisoning, Legionnaire's disease, chameleons, or "purple beards and black spots".

The volume is thoroughly indexed, bearing a subject index, author index, molecular formula index, and a mass spectral index (six most useful peaks), facilitating the retrieval of the massive amounts of information that it contains. The entries are thoroughly cross-referenced. The latter leads to some amusing results, however. Under each of the three entries ammonia, carbon dioxide, and carbonyl sulfide, the sole textual information states: formed when the insecticide thiofanox is heated in the presence of stainless steel. (Thiofanox may be quite useful as a condensed form of a library of chemicals on an intergalactic voyage; no less than 26 compounds are listed as being formed when it is heated in the presence of stainless steel!) The only incorrect information this reviewer spotted includes the description of a number of Amberlite and Ambersorb resins as ion-exchange materials.

In summary, no library can afford to be without this volume. As far as GC/MS practitioners are concerned, defer buying your next column until you have acquired your laboratory copy!

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Introduction to Microwave Sample Preparation: Theory and Practice. Edited by H. M. Kingston (National Institute of Standards and Technology) and L. B. Jassie (CEM Corporation). American Chemical Society: Washington, DC. 1988. xxii + 263 pp. $49.95. ISBN 0-8412-1450-6.

Kingston and Jassie have put together a valuable collection of chapters that introduce the practicing analyst to the fundamentals of microwave sample dissolution and preparation. In addition to a short introductory chapter, which presents a brief historical review of this newly emerging field, the volume includes several excellent chapters of general utility that cover theoretical concepts (Chapter 2), parameter monitoring and prediction (Chapter 6), and safety considerations (Chapter 11). These chapters provide just the proper amount of background on how and why microwave heating works, and its safe, practical utilization. The remaining seven chapters present tested applications by practicing analysts involving geological, metallurgical, biological, pharmaceutical, and radioactive samples. The various applications demonstrate that the microwave methodology permits major improvements in sample throughout with no loss in analytical precision. It is clear also that the procedures are ideally suited to automation, including robotics, so this will certainly be an important future trend.

The editors have performed a very useful service in pulling this compact volume together in a timely fashion, concurrent with the developments in commercial instrumentation. Anyone who has performed a conventional Kjeldahl determination will surely become a convert when he learns that sample digestion is 20 times faster with microwave heating than with traditional methods.

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Volumes of Proceedings

Nonlinear Optical and Electroactive Polymers. Edited by Paras N. Prasad (State University of New York, Buffalo) and Donald R. Ulrich (Air Force Office of Scientific Research). Plenum: New York and London. 1988. ix + 454 pp. $85.00. ISBN 0-306-42768-0.

This volume of typescript papers is represented as a treatise. It consists of review papers and reports on original research, derived from a symposium held at the National American Chemical Society Meeting in Denver in 1987. The breadth of the concerns may be judged by the group headings under which the papers are arranged: Nonlinear Optical Polymers, Electroactive Polymers, Theory, Synthesis, and Devices. The index is just over three pages long and includes a heavy helping of acronyms and abbreviations, from "ABPO" to "SSH".

Unconventional Photoactive Solids. Edited by Harvey Scher (BP Research International). Plenum: New York and London. 1988. ix + 259 pp. $62.50. ISBN 0-306-43025-8.

The typescript papers in this volume were given at the Second International Conference on the subject, held in Cleveland in 1985. They are grouped into eight categories: Fractals in Disordered Media, Spectral Hole-Burning, Exciton Transport: Experiment and Theory, Electron Transfer in Disordered Media, Energy Transfer in Organic Solids, Silica Glasses, Carrier Dynamics in Amorphous Semiconductors, and Devices and Applications. The index of a little over two pages has some fascinating entries, such as "photohole capture", "reacting walker", and "hopping rate".

Redox Chemistry and Interfacial Behavior of Biological Molecules. Edited by Glenn Dryhurst (University of Oklahoma) and Katsumi Niki (Yokohama National University). Plenum: New York and London. 1988. xi + 659 pp. $115.00. ISBN 0-306-43038-X.

The Third International Symposium on the title subject was held in Honolulu in 1987, in conjunction with the 172nd meeting of the Electrochemical Society. A large number of papers (the Table of Contents covers five pages) were presented, and they are reproduced from typescript. There is much to interest the organic electrochemist, the pharmaceutical chemist, and bioorganic chemists. The index is commendably thorough.

Surface and Interface Characterization by Electron Optical Methods. NATO ASI Series B: Physics Volume 191. Edited by A. Howie (University of Cambridge) and U. Valdre (University of Bologna). Plenum: New York and London. 1988. viii + 319 pp. $75.00. ISBN 0-306-43086-X.

A striking color plate of silicon and iron surfaces begins this volume of proceedings of a conference held in Sicily in 1987. There are 16 typescript papers, preceded by an obituary and photograph of the late Wolfgang Telieps. The papers deal with both transmission and reflection, and with static and dynamic phenomena, including catalytic activity. There is a three-page subject index.