Computer Software Reviews

gNMR Version 3.6.5. Cherwell Scientific Publishing Limited, The Magdalen Centre, Oxford Science Park, Oxford OX4 4GA, England; http://www.cherwell.com/cherwell. Developed by Dr. Peter Budzelaar. Single-user list price $899; educational discount price $599. (Note: Some earlier versions of this program had the name geNMR.)

The NMR spectral analysis program gNMR is available for either Macintosh or IBM compatible computers (Windows 3.1 or higher). The Mac version requires a PowerMac with System 7.1 or higher or a Mac with MC68020 or higher CPU with MC68881 or higher math coprocessor (though a non-FPU version is also available) and 4MB RAM and a minimum of 5MB hard disk space. This reviewer examined the native PowerMac version of the program.

A flexible and powerful program, gNMR is capable of a wide range of NMR spectrum simulation and analysis functions from simple spectrum simulation (for single molecules or mixtures) to full line shape analysis. The program handles fitting of calculated spectra to experimental data by either assignment iteration or line shape analysis and is also capable of chemical exchange calculations. gNMR recognizes a large number of NMR-active nuclei (and isotope mixtures) up to spin $^9/_2$ and can simulate both isotropic and anisotropic spectra.

Installation of gNMR is straightforward. The program is not copy protected; the license allows creation of a single backup copy. I found a few scenarios that caused gNMR to crash but the program is generally robust. The gNMR manual is clearly written, thorough, and relatively free of typographical and other errors. Some apparent errors in the manual probably stem from minor changes to the software that escaped the manual editors eye. The manual does a good job of providing background on spectrum simulation and related issues in a way that would help users who want to explore applications beyond those that motivated the original purchase of gNMR. A tutorial covers simple simulation of spectra of single molecules, mixtures, natural abundance isotopomer mixtures, exchanging systems, and approximate calculations for polymers. Another nice feature of the manual is that there is strategy and advice provided throughout on how to overcome some of the difficulties presented by certain systems and even on evaluating the quality of the solutions arrived at by gNMR. A more complete index would be useful but overall the manual is very helpful and well-written.

It is not a trivial task to master the use of gNMR, but given the complexity of the operations of which it is capable, the learning curve is reasonable. Simple spectrum simulation can be learned very quickly, and the program could easily play a very useful pedagogical role at the advanced undergraduate level or above. Before looking at the program myself, I gave it to an undergraduate student who was working on a conformational analysis problem for her senior thesis. She was able on her own to learn the operation of gNMR and to work through the attendant problems of applying it to her own system for which she needed to establish coupling constants and exchange rates. This was an exceptional student but, with appropriate direction, most advanced undergraduates could acquire the necessary skills quickly. Another gNMR feature that might be useful with regard to applications in teaching is that data for simple spectrum simulation can be entered by reading in a ChemDraw (or ChemIntosh or Isis/Draw) structure from which gNMR does a primitive prediction of (^{1}H, ^{13}C, or ^{31}P) shifts and couplings. One might also use the program to help students explore the effects of changes in shifts, couplings, and field strength on the patterns displayed by various spin systems. Calculated spectra can be printed or added to other documents easily.

Two utility programs included with gNMR provide assistance in overcoming practical difficulties in the use of experimental data in a full line shape analysis or other application. Once spectra have been moved to the computer on which gNMR resides, gCVT accomplishes the conversion to gNMR format. This utility, at present, converts spectrum files from many Bruker, Varian, and GE NMR machines but can also convert Lybrics format or ASCII files. We used conversion from ASCII since our JEOL NMR file type is not yet supported. The second utility program, gSPG, facilitates editing, which might include, for example, adding/subtracting spectra or removing impurity peaks for the initial attempts at locating a line shape analysis solution. Both of these utility programs were fairly easy to use.

Overall, gNMR is a very nicely designed program. Industrial and academic chemists with serious interests in the analysis of 1D NMR spectra will appreciate the speed, versatility, and ease of use of gNMR.

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Alchemy 2000 Version 1.1. Tripos, Inc., 1699 S. Hanley Rd., St. Louis, MO 63144-2913. Phone: (314) 647-1099. FAX: (314) 647-9241. List price $995.00 for personal or commercial use and $695.00 for academic use

Alchemy 2000 comes on a CD and runs under Windows 3.11 (with DOS 6.0 or higher), Windows 95, and Windows NT. It requires a minimum of an 80486 processor with math coprocessor, 8 Mbyte (16 recommended) of RAM, 40 Mbyte of hard disk space, VGA graphics, and a mouse. The programs are not copy protected; however, a computer dependent unlocking code is required. This code must be obtained from Tripos after installation before the program will execute. The documentation which accompanies the program is adequate and reasonably complete. There is a reference manual and a Getting Started manual as well as an addendum which contains the latest changes and additions to the program and a complete index to both manuals. The Getting Started manual is an excellent tutorial which leads the user through installation and introduces the various capabilities of the program. Some of the more complex capabilities of the program will require specialized knowledge of molecular modeling and molecular mechanics techniques; however, an appendix with references to articles and books is provided at the end of the manual.

Alchemy 2000 is an updated and greatly expanded version of Tripos' Alchemy III molecular modeling and computational chemistry program. Although this program replaces Alchemy III, it is essentially a new program with numerous additional capabilities not present in Alchemy III. The program's capabilities include the ability to build molecules including proteins, optimize the geometry of small molecules and peptides up to 500 atoms, compute point charges and determine bond distances, bond angles, and torsion angles. In addition the program features a customizable user friendly interface, batch mode calculation capability, 2D to 3D conversion routines, and multiple methods for geometry optimization of structures. Routines are also available to determine a variety of molecular parameters including surface area, volume, and molecular formula. All of these routines work as described and provide a wide variety of tools for analyzing and studying the structure and properties of complex molecules.

Alchemy 2000 also contains a module for display and manipulation of protein structures. Although this module does not provide routines for geometry optimization of complete proteins, it does do a very excellent job of displaying and manipulating protein structures. In addition to the ability to construct proteins from amino acid residues, it will import protein structures in various 3D formats including PDB. Primary structure may be modified by changing, inserting, or deleting amino acids. Amino acid secondary structure can be selected for each amino acid, and when the protein is built, the appropriate bond angles will be assigned. The only drawback is that amino acids in random coils are assigned random bond angles and there is no convenient way to designate specific bond angles although you can modify the angles using the twist function. This characteristic of the program also affects modifications to proteins imported from the protein data bank. Although you can mutate an amino acid without losing the tertiary structure after rebuilding, whenever a deletion or addition is made, all tertiary structure is lost from the point of change to the C terminal end of the protein. With the exception of this one drawback, this module is an excellent program for the study, display, and manipulation of peptide and protein structures.

Alchemy 2000 also includes a module to create presentation reports about a molecule or collection of molecules. The presentation can contain structures, additional information imported from Alchemy 2000, information imported from other Windows programs, and objects generated by the user. These reports as well as any other information

generated by Alchemy 2000 can be printed to any printer installed in the Windows environment.

Overall this is an excellent program, and I would recommend it to any scientist or student interested in gaining a better understanding of chemical compounds at the molecular level. It is also an excellent program for calculating molecular parameters and preparing databases for comparison and graphing of molecular properties. Application

modules which plug in to Alchemy 2000 are available for carrying out complex analysis of data generated by Alchemy 2000.

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Book Reviews

Dynamics of Molecules and Chemical Reactions. Edited by Robert E. Wyatt (University of Texas–Austin) and John Z. H. Zhang (New York University). Marcel Dekker, Inc.: New York. 1996. ix + 667 pp. $150.00. ISBN 0-8247-9538-5.

Chemistry as seen through the eyes of a physicist is both complex and difficult. The forces that hold molecules together, govern their vibrations, and determine the outcome of chemical reactions are highly nonlinear and nonseparable. The dynamics that ensue from these forces are as complex as any found in nature. Their study is not for the faint-hearted, yet great as the challenges are, so are the rewards in being able to understand and predict complex chemical interactions from first principles.

This book is a collection of chapters by expert members of that fearless group of theoretical chemists who have taken on the challenge of describing chemical dynamics from first principles. For those students and researchers who are also willing to be challenged by the subject, this book is highly recommended. The chapters are all well written, and up to date in both content and literature citations.

The book is divided not quite equally into two parts; the first deals with intramolecular dynamics, and the second deals with chemical reactions. A very nice pedagogical overview is provided by Remacle and Levine in the first chapter. Following that Wyatt and Iung review their work on computational methods to obtain vibrational eigenvalues, eigenstates, and spectra for polyatomic molecules. Shofield and Wolynes review their work on intramolecular vibrational relaxation using formal concepts of diffusion and localization, and relate some of their findings to unimolecular reactions. McCoy and Sibert review their work on developing and applying unitary perturbation theory to the efficient calculation of vibration/rotation eigenvalues, and the adjustment of potentials to improve agreement with experiment. In a translational chapter placed between the two parts of this book, Kosloff reviews state-of-the-art grid-based methods to obtain wave functions and their time evolution.

Their first chapter on reactions is provided by Zhang and Zhang, who review their work on time-dependent treatments of gas-phase and gas-surface bimolecular and unimolecular reactions. Next, Mandelshtam and Taylor review their work on time-independent propagators and stabilization methods to describe reactions and resonances, i.e., quasibound vibrational states. The description of novel time-independent methodology continues in the chapter by Kouri, Huang, and Hoffman, who describe in detail their Distributed Approximating Functional representation of the Hamiltonian operator. Chatfield *et al*. present results of rigorous characterizations of the vibrational states of the transition state of a chemical reaction, based on an analysis of the cumulative reaction probability. Theories to obtain the exact cumulative reaction probability (from which the thermal rate constant is obtained via a simple Boltzmann average) are reviewed by Miller, along with applications to several reactions. The Geometric Phase and its place in the theory of reactive scattering is reviewed by Kuppermann, who also gives extensive comparisons of results for the famous H + H_2 reaction with and without consideration of this phase. Nakamura reviews advances in methods to describe chemical interactions that involve multiple electronic states. Billing, Balakrishnan, and Markovic present a review of hybrid classical/quantum approaches to reactive scattering, with several applications. Purely classical approaches to unimolecular and bimolecular reaction dynamics are reviewed in the chapters by Hutchinson and Mayne, respectively. Last, but by no means least, is the chapter by Pollak on the theory of reaction rates in the condensed phase. This is an excellent review with a nice historical perspective.

This book is so good it is on my desk, and the desks of graduate students here at Emory, and I am sure elsewhere. Although it will ultimately make it to the bookshelves, I expect it will spend more time on desktops for quite awhile.

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Olefin Metathesis and Metathesis Polymerization. By K. J. Ivin (The Queen's University of Belfast) and J. C. Mol (University of Amsterdam). Academic Press: San Diego. 1997. xvi + 472 pp. $70.00. ISBN 0-12-377045-9.

This book is essentially an update of an earlier work by K. J. Ivin entitled *Olefin Metathesis* (*OM*; Academic Press, 1983). In the time that has past since the publication of *OM*, advances in the field have been profound and mainly in the area of applications to polymerization processes, as the expanded title of the new book suggests. Like the original book for its time, this treatment is a comprehensive look at all aspects of olefin metathesis. Coverage of the literature is up-to-date (more than 1900 references up to mid-1996), and the book is very well-indexed; there is no difficulty in finding your way to a topic of interest. Equations, chemical structures, and figures abound, and a random check unearthed no errors, suggesting that the chemistry is reported accurately and reliably.

Although portions of the original book are presented verbatim, the new knowledge accumulated in the intervening years is seamlessly woven into the original text, and the book reads as though this were the first writing. Structurally and organizationally, the new book follows closely the format of *OM*. The first chapters, which deal with topics such as the historical and mechanistic aspects of olefin metathesis, a catalyst survey, and metathesis reactions involving simple olefinic substrates, are augmented but not significantly different from those found in *OM*. The major changes (and the additional 100+ pages) come mainly in later chapters covering metathesis reactions involving acyclic dienes (both polymerization and ring-closing processes), acetylene substrates, and ring-opening metathesis (ROMP) reactions (including monocyclic and polycyclic alkenes). These changes reflect the many exciting developments that have occurred in these aspects of the olefin metathesis field, particularly applications of ring-closing metathesis to synthetic organic problems and the development of new, functional group tolerant ROMP catalysts. The final two chapters update the environmental aspects of olefin metathesis in its use for polymer degradation and summarize the current applications of metathesis-based processes in the chemical industry.

As a document of an important branch of organometallic chemistry, this book is complete and should satisfy all chemists with an interest in olefin metathesis and related reactions. Given the substantial advances that have taken place over the past 15 years, the book renders the original *OM* obsolete and is therefore a valuable update which research libraries will want to include in this year's purchases. For the specialist, it would likely be consulted frequently and is worthy of consideration for a personal book collection. Fortunately, the very reasonable price of $70.00 makes both types of purchases possible even in the current era of library cutbacks and shrinking professional development allowances.

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