To emphasize the electrophilic character of the reagent, some competitive experiments were also performed. When an equimolar mixture of 4-methylcyclohexanol acetate (**11**) and methyl cyclohexane were treated with the oxidative solution made from F_2, the latter reacted about 8 times faster. This is largely due to the difference in the tertiary CH electron density, which is lower in **11** because of the proximity of the electron-withdrawing group.[5] If the distance between such a group and the tertiary hydrogen increases as in the pair (4-*tert*-butylcyclohexyl)methyl acetate (**13**) and **7**, again, in accordance with the electrophilic nature of the reaction, the former reacts considerably faster.

Of some importance is the use of this reaction to introduce the ^{18}O isotope into organic molecules. The most convenient source for this isotope is $H_2{}^{18}O$, and since, unlike any other hydroxylation method, the oxygen in the above process comes from water, introducing ^{18}O becomes a relatively simple task. For example, when adamantane is treated with the oxidizing solution originated from $F_2/CH_3CN/H_2{}^{18}O$, [^{18}O]-1-hydroxyadamantane was obtained in higher than 80% yield.

We are thus hopeful that F_2, now accepted by many fluorine chemists as an important fluorinating reagent, will also be considered by the general chemical community as a reagent that can perform some uncommon reactions leading to fluorine-free and difficult to obtain derivatives.

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(10) The spectral properties as well as the microanalyses of the new compounds are in excellent agreement with the proposed structures.

(11) Fluorine is of course a strong oxidizer and a very corrosive material. An appropriate vacuum line made from copper or Monel in a well-ventilated area should be constructed for working with this element. The reactions themselves can be carried out in glass vessels. If elementary precautions are taken, work with fluorine is relatively simple, and we have had no bad experiences working with it.

Additions and Corrections

X-ray Structures of Cubylcubane and 2-*tert*-Butylcubylcubane: Short Cage–Cage Bonds [*J. Am. Chem. Soc.* **1988**, *110*, 7232]. Richard Gilardi,* Michele Maggini, and Philip E. Eaton

Page 7232, second paragraph: the intercage bond length for *tert*-butylcubylcubane is misstated as 1.464 (5) Å. The correct intercage distance is 1.474 (5) Å as shown in Figure 2b.

Nephelauxetic Effect in Paramagnetic Shielding of Transition-Metal Nuclei in Octahedral d^6 Complexes [*J. Am. Chem. Soc.* **1988**, *110*, 8341]. Nenad Juranic

Page 8343: The last equation in the Appendix should read:

$$B(\zeta_i,\zeta_j) = 4180\ \zeta_i a^2\{1 - {}^{25}\!/_3 a^2[1 - (1 + a^{-1})^{-2}] + {}^{50}\!/_3 a(1 + a^{-1})^{-3} + {}^{1}\!/_3(1 + a^{-1})^{-4}[72 + 88(1 + a)^{-1} + 95(1 + a)^{-2} + 90(1 + a)^{-3} + 70(1 + a)^{-4} + 35(1 + a)^{-5}]\}$$

Multiphoton Ionization of Acetone Clusters: Metastable Unimolecular Decomposition of Acetone Cluster Ions and the Influence of Solvation on Intracluster Ion–Molecule Reactions [*J. Am. Chem. Soc.* **1989**, *111*, 6035]. W. B. Tzeng, S. Wei, and A. W. Castleman, Jr.*

Page 6039: The two sentences before the paragraph head (B) Studies of Metastable Processes, "When water is present... on site B in structure II. As a result, ... is quenched." should read "When water is present in the system, it can bond to either site A or site B. However, the dehydration reaction of the protonated acetone cluster is quenched if the water molecule is bonded to site A in structure II."

Ligand Oxidation in a Nickel Thiolate Complex [*J. Am. Chem. Soc.* **1989**, *111*, 5974–5976]. Manoj Kumar, Roberta O. Day, Gerard J. Colpas, and Michael J. Maroney*

Page 5975, Figure 1: In the figure caption the data refer to an oxidation (not a reduction) of **1** at −190 mV employing 0.1 M supporting electrolyte.

Oxidation and Reaction of Trolox c, a Tocopherol Analogue, in Aqueous Solution. A Pulse-Radiolysis Study [*J. Am. Chem. Soc.* **1989**, *111*, 3315]. Michael J. Thomas* and Benon H. J. Bielski

Page 3316: The NMR and IR data for **5** and **6** are consistent with those previously reported by Cohen et al.[1] The melting point of **3** is identical with that reported by Cort et al.[2]

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(1) Cohen, N.; Lopresti, R. J.; Saucy, G. *J. Am. Chem. Soc.* **1979**, *101*, 6710.

(2) Cort, W. M.; Scott, J. W.; Araujo, M.; Mergens, W. J.; Cannalonga, M. A.; Osadca, M.; Harley, H.; Parrish, D. R.; Pool, W. R. *J. Am. Oil Chem. Soc.* **1975**, *52*, 174.

Computer Software Reviews

MassSpec. A Graphics-Based Mass Spectrum Interpreter. Version 1.0. Trinity Software: P.O. Box 960, Campton, NH. List Price $60.00.

MassSpec is a utility designed to aid in interpretation of mass spectra by identifying potential fragments from a user-entered chemical structure of up to 255 atoms. The program is available in both MS-DOS and Macintosh versions, which offer identical options and results with the exception of slight differences in the main menu structure. The MS-DOS system requires 256K RAM, mouse, and graphics card (CGA, EGA, or HGA) and a math coprocessor is recommended. The Macintosh version requires 512 K RAM and an 800K disk drive. Each version is supplied on a single disk along with a 29-page User's Manual. The Macintosh version was evaluated for this review.

The MassSpec utility can be broken down into two main functions: a structure editor and a fragment generator/locater. After starting the program, the user is given a blank work area in which a structure can be created, loaded, or saved to disk. Structures are created using menu options that include Ring (3–10 member and benzene), Bond (single, double, triple, and π circle), and Group, which can be any combination of elements up to atomic number 94, deuterium, tritium, a + or − charge, or a radical center. Options are also included to allow modification of various portions of a structure. After a structure is created, the user can make use of the Generate option to produce and display potential fragments based on up to three simultaneous cleavages. Only single bonds are selected for cleavage except for aromatic compounds with a molecular weight below 130 or when an atom is situated β to an activating group such as a multiple bond. After fragment generation, the user is permitted to display potential fragments. This is accomplished by entering a potential mass peak in a dialog box and having the system highlight, one at a time, the portion of the structure that could cause that fragment.

Overall, MassSpec is a somewhat disappointing program. In order to make use of this program, the user must have not only mass spectral data to evaluate but a reasonable estimate of the target compound which then must be entered with use of the structure editor. The structure editor had difficulty producing multiple ring structures. A biphenyl was more likely to be produced when a naphthalene was attempted or the rings were joined at the wrong locations. When a new structure was started, the screen was not properly cleared leaving bits of the former structure on the screen. After a structure is finally created and fragments generated, the user is not provided with a list of potential structures or masses but rather must still calculate potential values and then input them. Furthermore, while the system is referred to as a graphics-based system and the manual and product literature contain several mass spectra, the system offers no option for displaying graphics beyond the structure editor.

James K. Hardy, *The University of Akron*

ChemConnection Desk Accessory. Version 1.42. SoftShell International, Ltd.: 2754 Compass Drive, Suite 375, Grand Junction, CO 81506. List price $395.00; Educational and Government discount price $316.00; ChemIntosh owners price $100.00. Not copy protected. Recommended for use on an Apple Macintosh computer with at least 1 MB of RAM memory and a hard disk, or on a Lisa running MacWorks with at least 1 MB of RAM memory and a hard disk.

Structure searching with CAS ONLINE marks a new departure from traditional methods of searching *Chemical Abstracts*. For the well-established practice of searching subject, author, and formula indices, the computer provides convenience; but there is nothing in that part of the computer approach to the chemical literature which cannot be done with the printed addition of *Chemical Abstracts*. The application of Boolean searching techniques can narrow an otherwise broad search in ways that might be cumbersome with the printed edition, but the printed edition of *Chemical Abstracts* covers a much broader time span than does CAS ONLINE (at present), and use of the printed edition is free to the individual user (but not, of course, to the institution).

The revolutionary feature of CAS ONLINE is its capacity to search chemical structures—not only exact structures but also substructures—where the computer unearths the fragment of interest from larger molecules that one would not and often could not independently conceive of finding.

There are several ways to take advantage of this powerful new literature searching tool. One can go to Columbus, Ohio, and take a 2-day course from *Chemical Abstracts* to learn the complex but powerful verbal and structure drawing methods that make possible the submission of chemical structures to the computer for searching, or one can purchase a desk accessory for the Macintosh called ChemConnection.

ChemConnection is an extension/spinoff of a chemical structure drawing program called ChemIntosh (see the review of ChemIntosh by M. T. Crimmins, *J. Am. Chem. Soc.* **1987**, *109*, 6905). ChemConnection has the full ChemIntosh palette of structure drawing tools with additional telephone and preference buttons.

Having opened ChemConnection on your Macintosh, experiment for a few minutes following the straightforward drawing instructions. Draw the structure to be searched. After selecting the structure, click on the telephone button. The program will take over and in a second or so generate the appropriate CAS ONLINE code for the structure and place the code on the Macintosh clipboard. Using the instructions outlined on pp 71–73 of the ChemConnection manual, call STN International with a standard communications program such as VersaTerm Pro and log on to CAS ONLINE. At the end of the logon procedure CAS ONLINE will ask for a structure. "Paste" the structure in from the clipboard, and you are ready to fly with "sample" or "full"; "substructure", "family" or "exact" searches.

With the preferences button in ChemConnection one can specify partial ("normalized") bonds for resonance structures as demanded by CAS ONLINE. In addition, preferences permits highlighting (making bold or plain) certain atoms or groups of atoms not to be substituted in a substructure search. For example, you wish to learn about the existence of a compound containing an aromatic nucleus. You are interested only in the structure per se but are not particular about substituents on the aromatic ring. Make the atoms of the parent structure bold but allow the aromatic ring to be open to substitution by leaving it plain. CAS ONLINE will then find all examples of the structure of interest regardless of the substituents on the aromatic ring.

ChemConnection can be used in conjunction with a word processor in the same manner as ChemIntosh. Chemical structures are drawn the same way whether you are creating documents or searching the registry file of Chemical Abstracts. Since structures are built off-line, the expense of connect time is minimized. Once a chemical structure is drawn, it can be saved on a disk and later recalled for conversion to CAS ONLINE format. Valence errors are noted by the program, so the user can correct mistakes before starting a search.

The creative programming demonstrated in ChemConnection provides an idea of the improvements in ease of access to important data bases, such as CAS ONLINE, that are within reach.

No organic chemist can afford to be without ChemConnection. This powerful tool opens a new door to the chemical literature by facilitating the searching of chemical structures on CAS ONLINE.

Paul Dowd, *University of Pittsburgh*

Systat. Version 3.2. Systat, Inc.: 1800 Sherman Avenue, Evanston, IL 60201. (312) 864-5670. List price $595.00. Site licenses available. Not copy protected.

Systat is a comprehensive statistics and graphics software package available for the Macintosh, PC/MS-DOS, VAX, and UNIX systems. We reviewed the Macintosh 3.2 version. This package consists of 5 floppy disks, a looseleaf Systat statistics manual, a paper bound Sygraph manual (which describes how to use Sygraph, Systat's high-resolution graphics module), and a short document "Using Systat on the Macintosh", which contains installation and supplementary information. Systat 3.2 for the Macintosh is available in two versions: a 1-megabyte version and a coprocessor version that is designed for use with the 68020 processor and the 68881 coprocessor. We reviewed the 1-megabyte version. Evaluation was performed on both a 2-megabyte Macintosh SE with internal hard drive and a 1-megabyte Macintosh SE with a Jasmine 70Meg hard drive, using system 6.02. In addition, the Macintosh II's larger screen was found to be useful for graphics. The program documentation claims that it is functional with two 800K disk drives. However, since a set of application and work disks must be created and only a limited space is available for data, a floppy disk system would be very inconvenient. Initial booting of the program onto the 1-megabyte Macintosh SE resulted in a message indicating a need for more memory. After removing any extra INIT and CDEV programs from the system file and rebooting the computer, the program opened without a problem. However, this is inconvenient for users who normally use those extra programs on a 1-megabyte machine.

Systat consists of 12 separate modules: DATA, GRAPH, STATS, TABLES, CORR, MGLH, FACTOR, MDS, CLUSTER, NPAR, SERIES, and NONLIN. When a module is started, a text output window and a commands window are displayed. A Systat file can have up to 200 variables. However, since the data editor can only hold 100 variables, data sets can be merged if a large amount of data is to be analyzed.

The DATA module contains a spreadsheet-like data editor that should be familiar to anyone who has used a Macintosh spreadsheet. Data can be entered directly, pasted in from the clipboard, or read in from Text-only data files. Once the raw data is entered, the user has the option of sorting, transforming, or manipulating the data in a myriad of different ways. Sorting the data is imperative since a number of the statistical tests require a sorted data file. Transforming the data can be accomplished by using either the programs built in Systat BASIC language or a menu option. Although the transformation menu is easier to use at first, the BASIC language is just as easy once one is familiar with its structure. In addition to sorting and transforming the data, Systat allows manipulation of the data using the BASIC language. These manipulations include regrouping based on specific criteria, selecting out subsets of data based on specific criteria, and transforming specific data points that meet certain criteria as well as many other manipulations. The data-handling capabilities of the program are quite impressive once some of the BASIC language functions, which are thoroughly explained in the manual, are learned.

On the negative side, data can only be manipulated in the DATA module. Therefore, after exiting the DATA module, if the user wants to change something in the data file, a transfer must be made back to the DATA module. The Transfer command is provided for this manipulation. The need to transfer to the DATA module occurred quite often while learning the program, but it decreased as experience was gained. This may be considered part of the learning curve for the program.

Basic summary statistics (mean, standard deviation, skewness, kurtosis, min, max, range, variance, sem, and sum) are calculated in the STATISTICS module. All calculations are performed by first identifying a data file to be examined; this is accomplished by selecting the file with the Use command in the file menu. Once a file is selected, appropriate commands can be entered in the Systat command window to achieve the desired computation. There are no menu choices to perform the calculations, only help menus for guidance. A useful characteristic of the help window is that it can remain open while a command is entered in the commands window permitting comparison of syntax. The command line interface takes some time to learn. The program enables the user to choose the specific summary statistics desired on the variables of interest. This module also allows the user to perform T-tests (paired and unpaired) as long as only two independent variables exist in the data file. If more than two variables exist, it is necessary to go back to the DATA module and select out the two independent variables one wishes to examine. In addition, the user can calculate an ANOVA (factorial design) with or without post-hoc contrasts (Duncan's multiple range test, Tukey's HSD, or Newman-Keul's test). The ANOVA feature automatically calculates Bartlett's test for homogeneity of group variances, a convenient feature since many people forget to check this assumption before using an ANOVA. If a more sophisticated ANOVA design is needed, it can be calculated in the MGLH module (Multivariate General Linear Hypothesis Module).

A criticism about the statistical modules concerns the output of the results. If the P value of the calculated statistic is less than 0.001, then Systat will report the P value as 0.000. Even though it is possible to change the format of the remainder output (mean, standard error, etc.) to as many as 9 decimal places, it is not possible to change the format of the P value output. When Systat was contacted about this problem, they indicated that it would be corrected in the next version (Version 4.0). It should be noted that they were very happy to assist users as much as possible.

The MGLH module allows the user to calculate an ANOVA, MANOVA, linear regression, multiple linear regression, and ANCOVA. The data are analyzed by defining an appropriate model statement. MGLH can perform an ANOVA on balanced and unbalanced data with use of the following models: one-way ANOVA, two-way ANOVA, randomized block designs, incomplete block designs, factorial designs, mixed models, nested designs, split-plot designs, repeated-measure designs, and Latin-square designs, to name a few. Regression coefficients can be analyzed in the graph module as can residuals from a regression model and plots of interactions from factorial designs. For an ANOVA, post-hoc tests are performed by specifying the effect variable and using the contrast statement. The program will compute an F-test for the desired contrast. Multiple comparisons are performed by employing the C Matrix command and defining the desired contrasts. If Systat prints out the long format, additional information necessary to calculate Scheffe's multiple contrast tests as well as other types of comparisons can be obtained. Overall, the MGLH module is extremely powerful and easy to use. The manual does an excellent job explaining how to use the program as well as giving the user a lesson in statistics. In some places the manual discusses how the program differs from some of the mainframe statistics programs like SAS. Those familiar with these mainframe programs will appreciate this touch.

Multi-way tables can be produced with the TABLES module and subsequently fit to a log-linear model. The correlation module, CORR, can compute symmetric triangular matrices of correlation and similarity. Principal components analysis with optional rotations and factor scores can be obtained with the FACTOR module. Time series can be analyzed with the SERIES module. Models available include Fourier analysis, Box-Jenkins ARIMA, and linear and non-linear filtering.

The GRAPH module can be a stand-alone software package. Its ~900 page manual describes how to prepare bar graphs, scatterplots, function plots, vector, dot, bubble, and quantile plots, stem-and-leaf diagrams, histograms, as well as 2- and 3-D plots. Rectangular or polar coordinates can be used as well as log and power scales. A variety of graphical symbols can be used to display multivariate data. Characters can also be used as symbols; symbol size can be varied. The Vendor says that in the upcoming Version 4.0, Systat will support color graphics and color mixing specified by wavelength.

The PPLOT (probability plot) function can be used to graph data against a theoretical normal distribution. It is helpful to test whether or not data are normally distributed before running a parametric statistical test. A useful feature that is documented in the manual, but can easily be overlooked, is that *any* graph can be saved as a PICT file. By saving a graph in the PICT file format, the user can open the graph in MacDraw or any other program that can open PICT files. This feature allows complete customization of a graph.

Since a command line interface is used rather than the Macintosh interface, graphing is also less straightforward than in graphing programs like CricketGraph. A plot command must be issued from the commands window. A significant amount of control over the appearance of the output is possible, but it must be specified in the plot command. The graph is then displayed in a view window. It is possible to resize the graph using the usual click and drag method; however, the resultant changes in graph size are not visible until after the next plot command is executed. In addition, the size of the graph is limited by the size of the view window; no full-page resizing of the graph is available. The Macintosh II's larger screen was therefore convenient for creating larger graphs.

Not only can graphs be plotted in a 3-dimensional perspective, but orientation and position of text written on each face of a 3-D cube can be controlled. The text on three faces of a cube is angled to appear 3-dimensional. This is only possible with the Systat fonts, which are included with this package. In order to produce a smooth 3-dimensional function plot, it is necessary to use the Laserwriter option. Otherwise a more jagged version is displayed. This option requires more time and memory. A complex 3-D plot with smoothing using the Laserwriter option requires 10–15 min to be displayed on the screen and an additional 2–3 min to be printed with the Laserwriter. However, the results are well worth the wait.

It initially took some time to become familiar with how to list data in the DATA module in order to be able to plot the desired 3-dimensional results. Thinking in 3-D is not necessarily intuitive. Overall, Systat offers an enormous diversity of graph types. The manual also offers a nice chapter on cognitive science and graphic design.

The tutorials in the manuals are clear. However, the manuals are written from the view of non-Macintosh users, i.e., all instructions in the manuals are for commands to be entered in the commands window. The "Using Systat on the Macintosh" document attempts to cover the additional possibilities afforded by the pull-down menus and the abilities of the mouse, but the use of more than one manual is somewhat inconvenient when the software is first being utilized.

A significant disadvantage, or inconvenience, for Macintosh users is that this version of Systat does not make full use of the Macintosh interface. For example, graph commands must be entered line by line. The vendor was quick to emphasize that version 3.2 was an interim release. Version 4.0 (to be released by the end of 1989) will take full advantage of the Macintosh interface, as illustrated by the Mystat package that was included with version 3.2.

Mystat is promoted as educational software. It is a scaled down version of Systat, limited to 50 variables, but it makes full use of the Macintosh interface and is easy to use. Statistical analyses available include multi-way tables, correlation, and regression. Overlay plots, histograms, and stem-and-leaf plots are available. The vendor indicated that single copies are distributed free upon written request from individuals. Multiple copies are available at $5.00 each. Since the capabilities of Mystat itself are significant, it is better than a demo (which is often not totally functional) and is a bargain at this price, although it is limited in its capabilities.

In summary, Systat is a very complete statistical program. This type of capability comes at the cost of a steep learning curve. It takes some tinkering to get accustomed to the interface. The lack of the Macintosh-like interface sorely hampers the program's usefulness. Systat is not for the beginner. It is overkill for simple statistical designs. If your work calls for a complete statistical package including the ability to handle large data files and/or 3-D graphics, this program may be worth the investment after version 4.0 is released.

G. A. Arbuckle and A. B. Bocarsly, *Princeton University*
M. Feldman and P. A. Fitzgerald-Bocarsly, *University of Medicine and Dentistry of New Jersey*

DIPPR Pure Component Data Compilation. Version 1.0. Technical Database Services, Inc.: 10 Columbus Circle, New York, NY 10019. List price $850.00; educational discount 20%. Various site licensing agreements available.

The Design Institute of Physical Property Data (DIPPR) is an AIChE-sponsored research organization that is supported by industry and several engineering/scientific societies. A major DIPPR project, housed in the Department of Chemical Engineering at Pennsylvania State University, is the development of the DIPPR Pure Component Database, a critically evaluated, self-consistent databank of thermophysical properties for common industrial chemicals. The DIPPR databank is updated annually and made available to the public in several forms, including computer tape for mainframe use, and distributed by NIST, and a version searchable through STN International. The current program represents a third alternative for access and consists of the database and associated software for searching, display, printing, and file creation. The database includes 766 pure elements or compounds, and data are available for the following properties: molecular weight; critical temperature, pressure, volume, and compressibility factor; melting point; triple point temperature and pressure; normal boiling point; liquid molar volume; ideal gas enthalpy of formation, Gibbs energy of formation, and entropy; enthalpy of fusion at the melting point; enthalpy of combustion; acentric factor; radius of gyration; solubility parameter; dipole moment; van der Waals volume and area; refractive index; flash point; lower and upper flammability limit; autoignition temperature; solid and liquid density; vapor pressure; heat of vaporization; solid, liquid, and ideal gas heat capacity; second virial coefficient; liquid and vapor viscosity; liquid and vapor thermal conductivity; and surface tension.

The program requires an IBM XT or AT compatible computer with at least 256 Kb of RAM and 4 Mb of hard disk capacity. A math coprocessor is required, indeed the setup routine will not run without one being present. A graphics terminal is required, and CGA, EGA, VGA, or Hercules graphics cards are supported. Installation is simply accomplished. The search routines are straightforward, and there are terse, but useful help screens to provide reminders (although occasionally it is necessary to search for the help screen that applies to the particular task you may have forgotten how to do). The printed documentation provided with the program is also brief, but quite adequate.

The database itself consists of numerical data, a four-character quality code (for instance, XE2Z means the following: an experimental value, from a critically evaluated source, with accuracy better than 1%, with accuracy assigned by the author of the evaluated source), notes, and references. There is also a reference to the existence of environmental data, which is not part of this database but is available to DIPPR project supporters. The data include 13 temperature-dependent properties along with equations for calculation of the properties as a function of temperature. The manner in which the calculations are done is well documented.

The database can be searched by "identifiers", including class, name, molecular formula, or CAS Registry Number. Under name and molecular formula searches, embedded substrings can be used as the search items; e.g., "BrCl" as a search item will return the three compounds in the database containing one Br and one Cl. Searching under "bromochloro" returns bromochlorodifluoromethane but not bromotrichloromethane. The second class of searches is based on properties. In such searches, the property (or properties) is chosen, and the program prompts for the numerical range to be specified, e.g. mp between 300 and 400 K. The property searches and identifier searches can be combined in several ways to either "or" or "and" the queries, and the list of hits can be pruned after it is generated.

Once a single entry or set of entries has been identified, data relating to that compound or set can be selected and then displayed on the monitor or sent to a dot matrix printer (either with or without accompanying notes and references). Alternatively, an ASCII file can be generated and saved by specifying a pathname. The data can be displayed or printed in SI, CGS, or English units, but disk files are always created in SI units. For the temperature-dependent data, displaying or printing the data includes the value at 298.15 K, as well as equations and coefficients for calculating data at other temperatures. A further alternative is to calculate the value of a property at a specified temperature or to create a graphical representation of the data over a specified temperature range. The data or plot can be displayed or sent to a dot matrix printer.

Two FORTRAN modules are provided as a means to copy data directly from the database to an external FORTRAN application. For a single component in the database, the routines supply either a value for a single designated property or an array containing regression coefficients for calculation of a single temperature-dependent property.

TDS reports that an expanded version of the program will soon be available with additions to the database to bring the total number of components to 1023. The program itself is reported to have some "cosmetic" changes and some enhancements in search options, and the new version will not require a math coprocessor. Owners of version 1.0 may trade-in for version 2.0 for the difference in selling price ($400.00). The DIPPR database is augmented with annual releases, and TDS indicates that future annual updates to the database will be available without purchase of the entire software package.

The database itself is the product of a great deal of careful evaluation, and the current software allows one to exploit that database in a number of very useful ways. Clearly, however, the average chemist who needs this kind of physical and thermochemical data on an occasional basis will continue to rely on a handbook, not this program. The audience for the program is likely to be industrial chemists and engineers who deal with a variety of common industrial chemicals on a regular basis.

F. K. Cartledge, *Louisiana State University*

Book Reviews *

Photochemistry. Volume 19. Edited by D. Bryce-Smith and A. Gilbert. The Royal Society of Chemistry: London. 1988. xviii + 580 pp. $239.00. ISBN 0-85186-175-X.

This ambitious attempt to summarize the literature from July 1986 to June 1987 for an increasingly diverse field continues its invaluable service to the photochemical community. The reviews are laid out in the now familiar format, with Part I covering photophysical processes, Part II covering transition metal and main group photochemistry, Part III covering organic photochemistry, Part IV covering polymer photochemistry, and Part V covering solar energy conversion. Particularly extensive are the seven chapters on organic photochemistry in Part III, which includes treatments of ketone and enone photochemistry, aromatic and aliphatic hydrocarbon photochemistry, photoredox chemistry, photochemistry of heteroatomic compounds, and photoeliminations.

Part I, by Cundall, is the least satisfactory of the reviews. In addition to a rather terse coverage of an enormous body of work in time-resolved spectroscopy, it is encumbered by a type font that does not print well in condensed form and by a total lack of figures, which makes "browsing" impossible. Part II, by Cox, has a more acceptable number of figures, although the shortness of the chapters again contributes to a terse coverage of the field of inorganic photochemistry. This is further hampered by a rather artificial division into photochemistry of transition metal complexes and transition metal organometallic compounds, which inevitably produces redundancies. The chapters by Horspool, by Cox, and by Reid on organic photochemistry in Part III are the most readable and enjoyable of the lot. Extensive use of figures makes browsing facile, and the extensive coverage of this area—over half the monograph—provides reassurance that the preponderance of the relevant literature has been cited. The depth of coverage also allows some analysis of the conclusions drawn by the cited authors, where differences in interpretation are possible. The treatment of polymer photochemistry by Allen (Part IV) is heavily and appropriately referenced, although the brevity of the chapter provides little evaluation of the material, and reference to the primary literature is necessary. Finally, Part V on solar energy conversion, by Harriman, is a welcome summary of recent developments in this important, if somewhat moribund, area.

Returning with this volume is the "Introduction and Review of the Year", by Bryce-Smith and Gilbert. Although necessarily selective, this observation of the "highlights" provides a welcome analysis of areas for further reading in later chapters.

In summary, this report provides a useful and in-depth compendium of developments in organic photochemistry. Organic photochemists can certainly profit by its depth, although its high cost serves as an enormous barrier for its inclusion in personal libraries, where it rightfully belongs. Inorganic, physical, and polymer photochemists will find it of more limited utility, although it can provide an extensive source of references for the years in question.

Laren M. Tolbert, *Georgia Institute of Technology*

Rubberlike Elasticity, A Molecular Primer. By James E. Mark (University of Cincinnati) and Burak Erman (Bogazici University). John Wiley & Sons: New York. 1988. viii + 196 pp. $135.00. ISBN 0471-61499-8.

This book is an introductory level, thoroughly referenced presentation of rubberlike elasticity in a concise but clear manner. The material should be understandable to chemists with a solid undergraduate physical chemistry background. Molecular concepts, explained with simple physical models and analogies from other fields of science, are emphasized throughout the text. The division of the book into two parts will help the average reader to gain a gradual understanding of the material.

Part A, Fundamentals, defines rubberlike elasticity, lists its molecular requirements, and describes the origin of elastic force. The analogy between a gas and an elastomer, i.e., both pressure and retraction are entropy driven, is expertly presented. A chapter on the fundamental features of stress–strain relationship follows. The third chapter describes the preparation of networks, and the most important structure-related concepts, such as functionality, dangling chain, loop, cycle rank, etc. The next two chapters deal with statistical theory for idealized and real

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*Unsigned book reviews are by the Book Review Editor.