Figure 2. Analysis of bromide ion release from p-(bromomethyl)-mandelate (**1**; 1 mM) in 0.1 M MES (pH 6.0) by mandelate racemase:[8] no racemase (■); racemase added (255 units; ●); difference curve (▲).

addition to **5**. The new product was determined to be p-methylbenzoylformate (**4**) based on λ_{max}, HPLC analysis (comparison of retention time with that of authentic **4**[4]), and its reaction with benzoylformate decarboxylase [EC 4.1.1.7].[3,7]

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(7) Our preliminary results suggest that k_{cat} for the formation of **4** from **1** is less than 1% of the estimated k_{cat} for racemization of **1**.

Bromide elimination was confirmed by analysis with a bromide ion electrode (Figure 2).[8] In the absence of enzyme, the release of bromide ion (closed squares) parallels the solvolysis of **1**; however, addition of the racemase results in an acceleration of bromide ion formation (closed circles). The difference curve (closed triangles) is consistent with the enzyme-catalyzed elimination of bromide to afford the p-xylylene derivative **3** which undergoes tautomerization to **4** (Scheme I).

The detection and chemical properties of xylylene derivatives have received considerable attention in recent years.[9] Their instability has largely precluded isolation. Our previous work with benzoylformate decarboxylase provided direct evidence for a thiamine-stabilized p-xylylene derivative generated from p-(halomethyl)benzoylformates.[3] The results reported here cleanly demonstrate a similar phenomenon for an enzyme which does not proceed through a covalent substrate–cofactor intermediate. The unique conversion of **1** to **4** by mandelate racemase provides compelling evidence for a carbanionic mechanism for this enzyme. Moreover, the indisputable formation of **3** as an obligatory intermediate suggests that enzyme-catalyzed halide elimination through an intervening aromatic ring may be a general method for the formation and analysis of a variety of unstable xylylene derivatives.

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(8) Bromide ion release was measured as described previously.[3]

(9) (a) Pollack, S. K.; Raine, B. C.; Hehre, W. J. *J. Am. Chem. Soc.* **1981**, *103*, 6308 and references therein. (b) Hersh, W. H.; Bergman, R. G. *J. Am. Chem. Soc.* **1981**, *103*, 6992. (c) Goodman, J. L.; Berson, J. A. *J. Am. Chem. Soc.* **1984**, *106*, 1867. (d) Trahanovsky, W. S.; Macias, J. R. *J. Am. Chem. Soc.* **1986**, *108*, 6820.

Computer Software Reviews

TrueSTAT. Version 1.0. TrueBASIC, Inc.: 39 South Main St., Hanover, NH. List price: $49.95. Educational discounted price: $19.95 (with a total of $500 purchase by institution).

TrueSTAT is an interactive, statistical simulation and data analysis system designed primarily as an educational tool. It incorporates a menu driven mode, a command mode, and a programming mode which allow several modes of graphical output (XY plots, Histograms, Box plots, Residual plots), the ability to generate test data from several types of distributions (normal, binomial, poisson, etc.), and some simple statistical routines.

Features: Versions of this program are available for the IBM-PC, XT, or AT, Macintosh, and Amiga. A version is in development for the Atari ST. The copy tested was for the IBM machines, and some of the following comments are specific to that version. The stated requirements for running this program include 256 Kb of RAM (the main program occupies 165 Kb), a graphics adapter, and DOS 2.0 or higher. This package is not copy protected and can be backed up with standard DOS commands.

The program was examined on a Heath-Zenith Data System Model 248 with an Enhanced Graphics Adapter and an IBM-XT with a Color Graphics Adapter. The latter was also equipped with a math coprocessor. No problems were encountered in operating this program in either of these environments. This included concurrent running of a memory resident program. The program automatically checks for the presence of the math coprocessor and utilizes it if available.

Overall, the program is easy to use and easy to learn. The manual is well-written and organized. A modest help facility is provided which provides information on commands and syntax. It fulfills nicely the stated goal of an instructional aid for anyone concerned with fundamental statistical analysis (i.e., courses in quantitative analysis, chemometrics).

The program features three methods of command entry: menu driven, direct command, and a programming language. With respect to the latter, a line editor is provided for generating code. While this is func-

tional for short programs, it is more convenient to use a full blown text editor/word processor if long procedures are to be written. In the menu mode, selections are made with the soft function keys. One awkward feature is that the various menu screens are not labeled and in one case the same command performs different functions within different screens ("PRINT" command). Data can be entered directly by the modes discussed above or by creating a suitable ASCII file. The latter is particularly useful for large data sets. While data can be saved to disk there are two annoying aspects. Contrary to stated claims files can only be saved on the default drive. In addition significant figures are lost in numbers with more than 6 significant figures when they are saved and then retrieved from disk. The only way to preserve these figures is to create data files external to the program.

In addition to providing many fundamental statistical computations (i.e., mean, standard deviation, t-tests, confidence intervals, and linear regression) this program includes several interesting features particularly useful to an educator. Sets of random numbers can be generated from normal, binomial, Poisson, exponential, and uniform distributions. One can also generate random y values about a straight line for a corresponding set of x values. Datasets can be manipulated by arithmetic functions and operations (+, -, ×, ÷, square root, log, etc.).

One of the attractive features of this package is its plotting routines. These routines generate XY plots of datasets, histograms, a plot of the best fitting line for sets of ordered pairs, box plots, residual plots, confidence intervals, and a fit of a normal distribution to a dataset. It is a simple matter to simultaneously display several plots even of different type.

Overall, this program is a bargain at its modest price. The documentation is clear and concise and the program is easy to use. Despite some minor flaws, it would be a useful addition to the software collection of any educator or scientist concerned with the quantitative manipulation of data.

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ALCHEMY. Version 1.0. Tripos Associates Inc.: 6548 Clayton Road, St. Louis, Missouri 63117. (314) 647-1099. List price: $595 commerical; $350 academic.

ALCHEMY is a powerful desktop molecular modeling system designed for the IBM PC and MS-DOS compatibles. The elements of ALCHEMY are extracted from Tripos Associate's larger computer-aided molecular design software (i.e., SYBYL). ALCHEMY's major functions include the following: structure building, energy minimization, least-squares fitting of a series of molecules, and the generation of space-filling representations of molecules. The construction of a desired molecule is accomplished by hooking together molecular fragments in a manner analogous to a Drieding model. Energy minimization is via a molecular mechanics routine that uses analytical derivatives to find the local minimum. The molecular geometries of a series of structures can be visually compared by matching pairs of atoms with a least-squares fitting routine and viewing the superimposed structures. The overall shape of a structure can be viewed as a spacefilling model of the structure where the molecular surface is defined by its atomic van der Waals radii.

System Requirements: ALCHEMY requires an IBM PC, XT, AT, or compatible equipped with a minimum of 512 Kb of memory, one 1.2 Mb floppy disk drive or two 360 Kb floppy disk drives, one serial port, a mouse (Mouse Systems, Microsoft, or compatible) with software driver, an enhanced graphics adapter (or compatible) with 256 Kb of graphics memory, and an EGA monitor. Hardcopy of the molecular graphics requires a second serial port and a serial interface plotter which supports the HPGL-standard. A hard disk drive and/or a floating point (math) co-processor are strongly recommended. The program was evaluated on an IBM AT with an 80287 math co-processor, a 20 Mb hard disk drive, one 1.2 Mb floppy disk drive, one 360 Mb floppy disk drive, an IBM EGA card with enhanced color display, a Mouse Systems mouse, and a HP 7475A plotter.

Installation: The program is supplied on three floppy diskettes. Backup copies of the diskettes are made via the DOS diskcopy command. Diskette number 1 is a key disk (copy-protected) and gives an error during the copying process; however, the files are copied correctly. The program is installed on a hard disk drive by copying the contents of the diskettes into the appropriate subdirectory. For the program to run from the hard disk, the original ALCHEMY diskette #1 must be in one of the floppy disk drives. Once the program has started, diskette #1 can be removed and stored in a safe place. If diskette #1 is physically damaged, a replacement can be obtained from Tripos Associates for an unstated fee.

Before running ALCHEMY the first time, the configuration file ALCHEMY.CFG must be modified with an ASCII editor to indicate the type of mouse that will be used. Other options can be selected or changed within the program.

Features: ALCHEMY is a full-featured modelling package that is menu-driven and easy to learn. Commands are selected by moving the pointer to the desired "button" on the screen and clicking the mouse. The program is user-friendly with help available for the main menu and each sub-menu. The package is accompanied by a 122-page manual, which describes the display screens and all the commands. There is also a tutorial section in the manual that covers the basics of using ALCHEMY for molecular modelling. ALCHEMY can save and recall structures in SYBYL format, thus permitting ALCHEMY to exchange data with Tripos's larger modelling packages.

The molecular display options really distinguish ALCHEMY from other packages (see, for example: ChemCad review, *J. Am. Chem. Soc.* **1987**, *109*, 2229). Structures may be viewed in mono or stereo; the stereo view can be projected in either a relaxed or a crossed mode, and the stereo separation can be increased or decreased, as needed. In all display modes,

ALCHEMY performs real-time translations and rotations; the screen updates are fast and provide smooth movement of the structure. The movements can be either global (affects all the molecules displayed) or relative (affects only the molecule selected). The direction and amount of movement (rotation or translation) is selected by positioning the cursor on the appropriate axis of an x–y grid in the lower right portion of the screen.

The display limitations of ALCHEMY are not stated in the manual; however, Tripos says the program can display ca. 1000 atoms with a comfortable viewing limit of approximately 300 atoms. Several molecules can be displayed at once, which is useful for manual or least-squares fitting. When viewing several molecules simultaneously, each molecule may be individually assigned one of 15 colors; the default setting colors each molecule by atom type (chemical element). ALCHEMY has a chiral/invert option that locates and assigns all chiral centers in a molecule. The chiral centers are assigned by the Cahn, Ingold, Prelog rules. Once the chiral centers are assigned, the molecule can be inverted (all the chiral centers are inverted) or a single chiral center can be inverted.

ALCHEMY optimizes the geometry of structures via a molecular mechanics procedure using analytical derivatives; the minimizer is derived from Tripos's larger mainframe packages. The size limitation of the minimization is not mentioned in the documentation; however, Tripos reports that molecules of ca. 130 atoms are the upper limit. We were able to optimize structures of ca. 150 atoms; experimention found that the upper limit is 200 atoms. The form of the equations used for minimization are clearly described in the manual. In addition, the manual provides clear instructions on how to modify the force field; the various parameters are stored in several files which are easily changed with an ASCII editor. Geometry optimization is rather fast with a math co-processor (8087 or 80287) which is a recommended hardware option.

ALCHEMY also has the ability to compare two structures manually or via a least-squares fitting method. The least-squares method requires picking a minimum of three linearly independent sets of atoms from each molecule; the fitting process results in a root mean squared distance which is an indication of the quality of the fit.

ALCHEMY allows the user to access another program through an external command. This command temporarily halts execution of ALCHEMY, creates a file (EXTOUT.MOL) containing the coordinates of the current molecule, then executes the user supplied routine (which must be named EXTERN.EXE). When the external program has terminated, control returns to ALCHEMY which reads the molecular coordinates from EXTOUT.MOL, if it exists.

The molecular displays may be produced as hard copy by use of an HP-GL compatible plotter. The output may be a stick drawing analogous to the display on screen, or a space filled drawing where each atom is represented by a sphere with a radius equal to its van der Waals radius. The space filled drawing is a nice feature, but the plotting time is rather long.

Summary: In conclusion, ALCHEMY is a versatile desktop modelling package. The structure display options are diverse and useful. The real-time rotation (translation) of structures is fast and smooth, which permits viewing the structure from any perspective. Structure minimization for most molecules is reasonably fast for a microcomputer, especially with the suggested math coprocessor. The program interface is straightforward and easy to learn. The menu approach and on-screen help reduces the use of the manual. The space-fill display is nice, but very slow. The only output device supported is a plotter, since ALCHEMY is very color oriented. Support for other output devices (dot matrix printers, laser printers) would be nice since not everyone has access to a plotter.

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Book Reviews

Industrial Applications of Surfactants. Edited by D. R. Karsa (Lankro Chemicals Limited). The Royal Society of London: London. 1987. VIII + 352 pp. $65.00. ISBN 0-85186-666-2

The term surfactant has been identified in the past mostly with household cleaning and personal care applications. However, surfactants exhibit versatile characteristics due to their amphipathic behavior, which enables them to be employed in other than domestic usages. As the editor of *Industrial Applications of Surfactants* points out, approximately 40% of worldwide surfactant production is consumed in the industrial domain.

This monograph highlights a diverse number of industrial applications which require surfactants. It is based on papers presented at an international conference held in April 1986.

Topics are divided into the following categories: main surfactant groups (Anionics, Cationics, and Nonionics), specific surfactant compounds (Copolymers, Fluorochemicals, and Silicones), and applications (Antifoams in Gas–Oil Separation, Antistatic/Conductivity Additives in Paints and Plastics, Coal–Water Slurries, Concrete Industry Applications, Emulsion Polymerization, Enhanced Oil Recovery, Fire Fighting