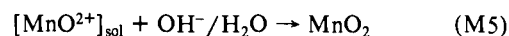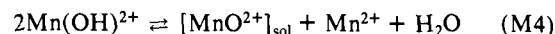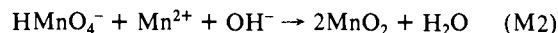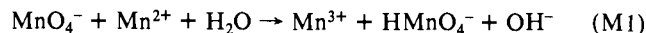**Figure 2.** Phase diagram in the input $[KMnO_4]_0$ – $[MnSO_4]_0$ plane showing the oscillatory domain at fixed inputs $[KH_2PO_4]_0 = 1.6 \times 10^{-3}$ M and $[NaOH]_0 = 1 \times 10^{-3}$ M. Along the broken line within the oscillatory region, the reciprocal residence time k_0 can be varied from 0.005 to 0.020 s⁻¹. At other points, oscillation occurs only for k_0 between 0.005 and 0.010 s⁻¹. Symbols: O, sustained oscillations; ⊘, damped oscillations; □, nonoscillatory steady state.

Phosphate ion (as $H_2PO_4^-$) appears to be essential for the minimal manganese oscillator. Efforts to replace this species with others known to form stable complexes with manganese intermediates ($P_2O_7^{4-}$, F⁻) were unsuccessful. We believe the phosphate

plays *two* key roles. First, it influences the formation of soluble Mn(IV) and its rate of flocculation to solid MnO_2, which serves as the autocatalyst, apparently via a surface effect. Equally important, because the rate of the Guyard reaction is extremely pH-dependent, the added KH_2PO_4 serves as a buffer, capturing the H⁺ formed in reaction 1 and maintaining the pH of the system close to 7.

Based on our experiments and Tompkins's proposed mechanism[12] for the Guyard reaction, we suggest the following skeleton mechanism to account for the oscillatory behavior:

$$MnO_4^- + Mn^{2+} + H_2O \rightarrow Mn^{3+} + HMnO_4^- + OH^- \quad \text{(M1)}$$

$$HMnO_4^- + Mn^{2+} + OH^- \rightarrow 2MnO_2 + H_2O \quad \text{(M2)}$$

$$Mn^{3+} + H_2O \rightarrow Mn(OH)^{2+} + H^+ \quad \text{(M3)}$$

$$2Mn(OH)^{2+} \rightleftarrows [MnO^{2+}]_{sol} + Mn^{2+} + H_2O \quad \text{(M4)}$$

$$[MnO^{2+}]_{sol} + OH^-/H_2O \rightarrow MnO_2 \quad \text{(M5)}$$

Steps M2 and M5 are slow, with M2 somewhat slower, so that the main source of MnO_2 precipitate is step M5,[12] the rate of which depends strongly on $[HPO_4^{2-}]$. Step M3 represents the partial hydrolysis of Mn^{3+}, which results in a soluble hydrated oxide that can be present as a dimer or in a polymeric form. The hydrated Mn(III) oxide undergoes disproportionation in step M4 to a soluble Mn(IV) species and Mn^{2+}. The $[Mn(IV)]_{sol}$ first forms a supersaturated solution and then generates MnO_2 precipitate autocatalytically as the result of nucleation and surface effects.[11,13] While using other reducing agents in place of Mn^{2+} can produce oscillators that are more robust in their pH or concentration ranges, they are likely to operate via the same overall dynamics. The key to understanding the behavior of the entire family of manganese oscillators will almost certainly lie in this minimal core system.

Computer Software Reviews

FitAll. Version 2.04. MTR Software: P.O. Box 902, Station P, Toronto, Ontario M5S 2Z2, Canada. List Price $40.00 + $5.00 S&H, no discounts mentioned.

Fitall is a general-purpose, nonlinear, least-squares regression analysis program that can be used to fit a set of experimental data to any one of up to 20 defined functions of your choosing. Two-dimensional graphs of the original data, of the calculated best fit curve, and of the residuals can be displayed on the computer's monitor. It requires an IBM PC/XT/AT or "true" compatible computer with at least 512K RAM, one disk drive, a color graphics adapter, PC/MS DOS 2.0 or later operating system, and TurboPascal v3.0.

The program disk comes with a compiled version of the program that will run without owning TurboPascal v3.0. Nine of the 20 possible functions to choose for fitting are already defined, e.g., $Y + A + BX = C/X^2$ determines A, B, and C for your input set of X,Y data. The program works very well and has easily understood commands in the menus. The compiled version would be an excellent choice for analyzing data in an undergraduate physical chemistry laboratory or for standard fitting of data. A nice feature is the submenu that allows one to modify the data by taking the log, ln, sin, etc. of one or more sets of data. Inverting, scaling, and offsetting are also possible in the modify data submenu.

Data, both input and calculated, are claimed to be capable of being saved to disk in standard ASCII files (checked) or in Lotus 1-2-3 readable files (not checked). This will be an important feature because the autoscaled plots did not place the labels along the axes uniformly with respect to the tic marks. Thus, to prepare plots for publication, the data will have to be exported to a program that will drive a plotter or laserprinter; however, the plots produced by FitAll could be easily redrawn for publication by a draftperson.

The real power and versatility of FitAll is in the ability to input your own special mathematical relationships via the TurboPascal Editor and to fit functions with more than one independent variable. One must use v3.0. A later version did not work. This feature of FitAll allows it to be used in advanced research work where fitting to new relationships would be required. The procedure is relatively painless and is well documented in the usually well written but occasionally incomplete manual (provided on disk).

FitAll v4.0, the most current version of the program is now available in two versions: FitAll Standard v4.0, List price $50.00 (compiled, no source code), and FitAll Research v4.0, List price $75.00 (source code, not compiled, requires a high-capacity drive and TurboPascal v4.0 or 5.0).

James C. Howard, *Middle Tennessee State University*

PrintAll. Version 1.0. MTR Software: P.O. Box 902, Station P, Toronto, Ontario M5S 2Z2, Canada. List Price $50.00, S&H included, no discounts mentioned.

PrintAll is a screen dump utility for IBM-PC and compatible computers using MS-DOS or PC-DOS. It is not copy protected and claims to have been tested with DOS versions 1.11, 1.25H, 2.01, 2.10, and 2.11. It was used here with versions 2.11 and 3.20. It requires a computer with at least 64K of RAM and is installed in the computer's memory before you boot some other program. Once installed, PrintAll will print whatever is showing on the screen by merely pressing the PrtScn key. This feature makes it handy to get draft copies of graphs without moving around in an application program to get to a graph dump option or saving then exiting and booting a separate graphics dump program.

The manual is easy to read and well written. The MENU of printers contains 23+ printers. That is, there are 23 options some of which work for more than one printer. A note in the manual indicates that if the program does not work with your printer, you may call the authors to get technical support and/or an update that may work. The text dumps are standard and not the reason to buy the program. The graphics dump is restricted to one size and orientation, filling (1 in. boundaries left and right and 1.5 in. top and bottom) an 8.5 × 11 in. sheet of paper and rotated −90°. If you have some graphics programs that give limited printer support, this would be a reasonable, inexpensive alternative to buying a new graphics program with extensive printer support included.

James C. Howard, *Middle Tennessee State University*

STN Express. Version 2.01. STN International: 2540 Olentangy River Road, P.O. Box 02228, Columbus, Ohio 43202. List Price $595.00. Available also at an academic rate of $476.00. Not copy protected.

Introduction. STN Express is a program for IBM-PC and compatible computers that is designed to aid in searching on line STN International scientific data bases such as CAS ONLINE. It provides automatic logons, the ability to carry out simple menu driven searches, a facility for drawing chemical structures for structure searches, a transcript of an on line session, a simple command language, and many other features.

STN Express is a large program requiring relatively expensive hardware. Our version came on ten 5.25-in. disks (it is also available on 3.50-in. disks), each of which is used in the installation. Simply backing up the original disks with the required diskcopy command is a time-consuming process. The recommended hardware requirements include an IBM PC-XT, PC-AT, PS/2 or 100% compatibles, 640K RAM (with a minimum of 510K free), a hard drive and one floppy drive, a graphics card, a mouse, a modem, and the MS-DOS 3.0 or higher operating system. A printer is optional (but highly recommended), and a number of dot matrix, ink jet, and laser printers are supported as well as some plotters. Included is a well-written manual in the traditional three ringed notebook format and two on-disk tutorials, STN Mentor and STN Express Mentor. We did not evaluate these tutorials in any detail. We used a Zenith 248 AT compatible computer with 640K memory, MS-DOS 3.3, a VGA graphics board, a hard disk, a Logitech mouse, a 1200 baud modem, and an Epson compatible dot matrix printer for this evaluation.

The installation is rather time consuming (it took us about 40 min). A number of questions are asked concerning the exact hardware configuration and the location of certain files. For the casual computer user some of this information may take time to locate. Installation can be aborted at any time, but doing so requires you to start the whole process over. Some, but not all, of the choices made can be changed later by using the setup function within STN Express. It would be helpful if all of the information supplied during installation could be modified from within the program. (The installation program modifies your DOS environment by inserting some SET commands and modifying your autoexec.bat and config.sys files. It also sets up several subdirectories on your hard disk.) Although it is possible to use multiple LOGINIDs with STN Express, this requires the cumbersome use of DOS batch files with SET commands to start the program. It would be much more convenient if the Logon or Setup portion of the program allowed a choice of different LOGINIDs.

The Program. STN Express is invoked from the DOS command line by typing "express". Inside the program a menu line at the top of the screen lists the following "drop down" menu choices: Guided Search, STN, Query, Results, Housekeeping, Setup, Terminal, and Exit. These can be selected by using either the mouse or the arrow keys on the keyboard. The center of the screen shows the session status: on line or off line, session capture, and printing (active or not active). A status line at the bottom of the screen indicates how the keyboard can be used to position the cursor and select an item. It also shows that the Help function is available by pressing F1. At other points in the program a variety of other information appears on the status line. The menu choice STN initiates the logon process. Setup allows changes to be made in preferences, vendors, printers modem protocols, etc. Terminal allows the

use of STN Express with services other than STN (such as BRS, DIA-LOG, or manual emulation). Housekeeping provides methods for deleting files generated by STN Express or ordinary DOS files. The remaining choices are the heart of the program and are described in more detail below.

Guided Search. Guided search allows the user to prepare a search while off line without using the standard STN International command language (if you do know the STN International command language it can be used to advantage in the Guided Search). It is menu driven and allows you to save the search strategy in a file for use when on line or for later modification. You are led through a series of "index cards" on which you make choices as to the nature of your search (e.g., topic, author, substance, structure, registry number). When you have finished defining the search strategy you can perform the search, save it for later use, print it, or review the STN commands that it has generated. You can also specify what kind of information you want in the results of your search and the name under which you want the transcript of the search saved. The Guided Search is useful mainly for persons who wish to perform only simple searches and who will only rarely carry out a search. In spite of the ability to review the STN commands generated, the use of the Guided Search will be of little aid in learning more than the rudiments of search strategies and the STN International command language.

Query. The Query section is the most powerful and most useful portion of the program. While off line you can prepare and/or print a chemical structure query, prepare and/or print a command file, print a predefined search strategy, or set a structure collection name. While you are on line you can upload structure queries, run command files, or use predefined search strategies. For those who often carry out structure searches, the ability to build structures off line and later upload them for a chemical structure search is a powerful tool. In preparing a structure query you are presented a large blank area on the screen on which you can "draw" your structure. The menu across the top of the screen allows you to choose the atom (element) you wish, choose shortcuts (abbreviations such as Ph for a phenyl group or *t*-Bu for the *tert*-butyl group), variables (e.g., X for halogens, A for any atom except hydrogen), templates (predefined ring systems, e.g., cycloalkanes, bridged rings, nitrogen-containing rings), and bonds (e.g., single, double, unspecified, and various stereochemical features), draw (e.g., draw rings, chains, move atoms or fragments of molecules, fuse rings, assign charges), edit or make changes in a structure, and utilities (save the structure, recall a saved structure, print a structure, repaint a structure). On entering the draw mode the default atom is carbon and the default bond is a single bond. The mouse is used to advantage in preparing these structures and very complex structures can be built. The drawing of the structures at first seems somewhat awkward (e.g., it is more difficult than using ChemDraw on a Macintosh computer), but with a little practice structures can be quickly prepared. This is clearly far superior to trying to prepare structures while on line to CAS. We occasionally had difficulty viewing multiple bonds on screen (e.g., a double bond would appear as a single bond even though we had chosen a double bond), but if the structure was printed out it was clear that the double bond was really there. We recommend that complex structures always be printed out and checked for accuracy before using them in a structure search. The error trapping in the drawing module is quite good; for example, you are warned if you attempt to build structures that violate valence rules. Once a structure is completed and you are on line, the structure Query can be uploaded to the CAS Online REGISTRY file and the structure search is carried out. If you display the information retrieved, the structures are nicely displayed on the screen and can be printed out satisfactorily even on dot matrix printers. We consider this portion of the program to be excellent.

Within the Query section it is possible to upload prepared command files to carry a variety of types of information retrieval. The command file can be prepared either within the program or outside of the program with any editor or word processor that can prepare standard ASCII files. The options available in command files are relatively rudimentary and require that you be familiar with the STN International command language, but the examples in the manual and on disk are very helpful. Although not emphasized in the manual, the proper placement of spaces is often crucial for a command file to run properly. Certain variables are provided to allow for unknown features such as the number of answers that will be obtained in a given search. It is also possible to write the command file such that the user will be able to enter requested information at the STN prompts. These command files are powerful and one can quickly logon, carry out a series of operations, and logoff.

Under the Query menu STN Express provides a few predefined search strategies applicable in a variety of disciplines. These appear to be of very limited general utility.

Results. The Results section of the menu provides commands for capturing all or a portion of the session to a disk file referred to as a

transcript. One can use the default name for this ("session") or choose another name. One unusual, and at first confusing, aspect of this is that the name you choose for the transcript is actually the name of a new subdirectory that will be created and will contain a file called "trans". We at first thought we had lost the transcript of one of our sessions when we could not find a file with the name we had selected for the transcript. We would prefer that the transcript be a file with the assigned name. The transcript can be printed when you are off line and will print both the text of your session and any graphics (structures) produced. You can also choose to print the session directly while on line, with or without saving it to disk. It would be useful if the status line at the bottom of the screen always indicated whether capture and/or printing was on. This does appear in the center of the screen in some instances but is not always visible. Because printing does not start until the program has queued a whole page and you can toggle printing on and off with a function key it is easy to think that you have not turned printing on and accidentally toggle it off. Another menu item under results allows you to use continuous scrolling or have the screen display occur one screen

at a time. If you do use continuous scroll you can easily stop the scrolling at any time. STN Express allows you to scroll back through the last 30K of information that has appeared on the screen. This is a very useful feature. When you are off line you can also browse any transcript by having it displayed on the screen rather than printing it. It is also possible to irreversibly split the transcript into separate text and graphic portions.

Support. STN International has a toll free number to reach their Search Assistance Desk. Our calls with questions about STN Express were answered immediately or we were called back and provided with the information we needed.

Recommendation. STN Express is a very useful program. It does exactly what it is claimed to do. In the hands of a chemist or information specialist it can greatly decrease on line time and simplify searches, particularly structure searches. For persons or organizations who do extensive on line searching this relatively expensive program will pay for itself many times over in decreased connect time and on line charges.

Robert G. Carlson and John A. Landgrebe, *University of Kansas*

Book Reviews*

Quantum Theory of Polymers as Solids. By Janos J. Ladik (University of Erlangen-Nurnberg). Plenum: New York and London. 1988. xiv + 417 pp. $69.50. ISBN 0-306-42434-7.

The aim of this book is to present "a unified approach in one volume to the quantum theory of polymers and its applications". The theoretical chemist will find it an informative, albeit incomplete, survey of polymer calculations performed over the last 20 years. Used in this way, the book suffers by not having an author index.

The experimentalist may find it of more limited value. Although the author requires "only a knowledge of elementary quantum chemistry and linear algebra", he has adopted a rather liberal interpretation of the word "elementary". It is a pity he has chosen to use the vector notation of the physicist rather than the secular notation more familiar to the chemist. The physicist language tends more to mystify than enlighten the chemist. Thus the chemist who wishes to gain an understanding of calculation may well not, but example, reach Chapter 4 and thus miss an excellent treatment of aperiodicity in polymers. This difficulty in communication has been recognized by the *Journal of Chemical Eduction*; it has recently published a series of articles on the calculation and interpretation of polymer properties (**1988**, *65*, 319, 379, 513) written specifically for the nonspecialist. The present book would find a wider audience were secular notation to be used and the vector formulation presented as an appendix.

Brian O'Leary, *The University of Alabama at Birmingham*

Thermodynamic Data for Pure Compounds. Part A (Hydrocarbons and Ketones) and Part B (Halogenated Hydrocarbons and Alcohols). Physical Sciences Data Series. Volumes 25A and 25B. By Buford D. Smith and Rakesh Srivastava. Elsevier: New York. 1986. Volume 25A: x + 883 pp. Volume 25B: x + 999 pp. $294.50 (set). ISBN 0-444-42579-9 (set).

This is a computerized critical compendium of thermodynamic literature data for pure compounds: 263 hydrocarbons (methane through indene), 131 ketones (acetone through 34-benzoyloxy-2,6-dimethyl-2,5-heptadien-4-one), 91 halogenated hydrocarbons (bromomethane to 1,1,2,3,3,3-hexafluoro-1-propene), and 359 alcohols (methanol through 3-(phenylazo)phenol) for the literature up to 1983. The data are the following: vapor pressure, saturated liquid volume, second virial coefficient, enthalpy of vaporization, and saturated vapor volume as functions of absolute temperature, plus melting and normal boiling temperatures, and the critical constants (temperature, pressure, and volume), the compressibility factor, the dipole moment, and the radius of gyration, and the coefficients for the equations of state for the vapor and the liquid. The relevant literature references are given, but only the final results of the critical comparisons are shown. As discussed in the Introduction, this was to be part of a massive work for mixtures of compounds, but that task proved to be too monumental.

This reviewer would have liked to see also the enthalpies of formation, but for those there is, of course, already the excellent, if dated, compendium by J. D. Cox and G. Pilcher, *Thermochemistry of Organic and Organometallic Compounds* (Academic: New York, 1970).

The novelist hopes to entertain. The compiler of scientific data, like

the lexicographer, must hope not to mislead. The novelist, like Homer, can often doze off a bit. The presenter of data must be forever watchful.

Robert M. Metzger, *University of Alabama*

Comprehensive B₁₂. Chemistry-Biochemistry-Nutrition-Ecology-Medicine. By Zenon Schneider and Andrzej Stroinski (Academy of Agricultural Sciences, Poznan). Walter de Gruyter: Berlin. 1987. xi + 409 pp. $149.50. ISBN 0-89925-312-1.

The title of this treatise on vitamin B_{12} is somewhat misleading. The book is too brief to be a comprehensive treatment of vitamin B_{12}. However, it is a useful handbook of vitamin B_{12} chemistry and biochemistry. It is replete with useful leads to the literature and tables of data and is, in short, a rich and compact reference work for those whose needs impinge on vitamin B_{12}. The subject index seems to be reasonably complete; the absence of an author index is a drawback. An index of microorganisms is included.

The first chapter opens with a brief historical synopsis of the vitamin B_{12} field with a helpful chronological outline of major developments. Chapter 2 provides a summary of the nomenclature of vitamin B_{12} and its derivatives.

The chemistry of cobalamins with a listing of vitamin B_{12} derivatives, their structures, spectral absorbance, occurrence, biological activity, and a discussion of their properties forms the core of chapter 3. Tables include cobalamins substituted with alkanolamines, first-order rate constants for the spontaneous decomposition of alkylcobalamins in acidic and neutral solution, vitamin B_{12} labeled with cobalt isotopes, polarographic half-wave potentials, equilibrium and rate constants for β-ligand substitution and pK_a values.

Chapter 4 deals with the biosynthesis of vitamin B_{12} and contains a catalogue of the effects of growth media and aeration on cobalamin products and vitamin B_{12} analogues. No structures are given for guidance in this chapter, except for a page of heterocyclic bases at the end of the chapter. However, there is a large, loose, folded chart at the end of the book that provides a flow-sheet diagram of the biosynthesis of vitamin B_{12}.

Purification and estimation of vitamin B_{12} are covered in the fifth chapter. Following a short section on the extraction of corrinoids by organic solvents, other purification techniques including paper and thin-layer chromatography, ionophoresis, column chromatography, adsorption on charcoal, adsorption on immobilized B_{12} binding proteins, and high-pressure chromatography are described. Estimation of corrinoids by microbiological assay is buttressed by tables on the response of test microorganisms to complete and incomplete corrinoids and a table on bacterial vitamin B_{12} and analogues containing nucleotides other than 5,6-dimethylbenzimidazole. Radioisotope dilution and enzyme assay methods for the estimation of nanomole to picomole quantities of vitamin B_{12} are described together with spectroscopic assays, neutron activation assay, and chemical methods. Procedures for microbial production and purification of vitamin B_{12} and other cobamides and cobinamides are included. Among the spectroscopic methods there is only brief mention of NMR, and there is no mass spectral information. Thus, the recent development of the powerful FAB and field-desorption methods have been overlooked.

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*Unsigned book reviews are by the Book Review Editor.