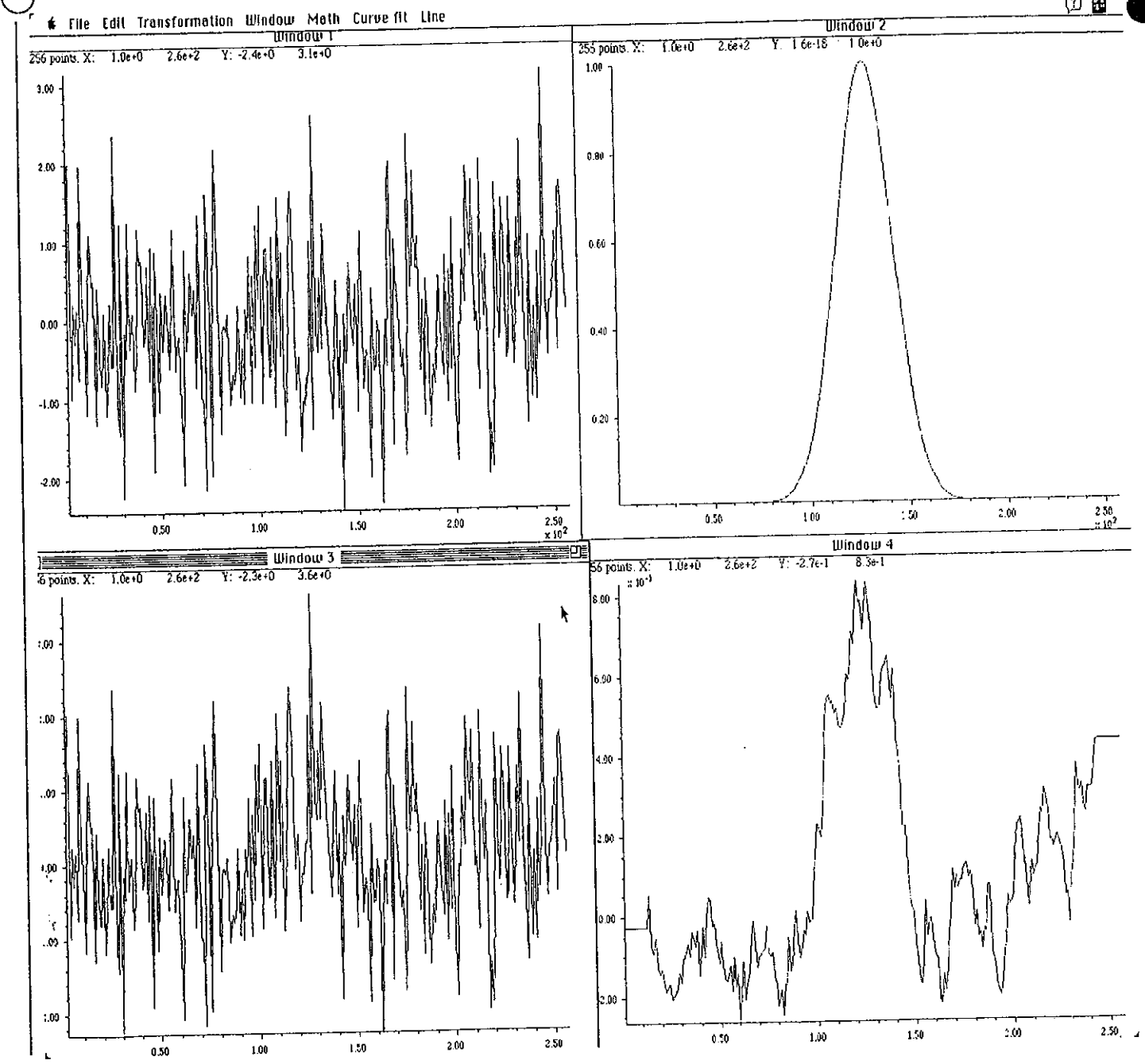
Computers in Chemical Education Newsletter

Spring 1993



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Don Rosenthal Chair

Editor Brian Pankuch, Department of Chemistry, Union County College, Cranford, NJ 07016

Submissions: General articles should be sent to editor Brian Pankuch at the above address. We would appreciate both 1) printed copy (hardcopy) and 2) a readable file on a Macintosh or IBM compatible 3 1/2" diskette. We have fewer problems with 3 1/2 " diskettes.
Submission deadlines: Fall issue - Sept. 25; Spring issue - March 15.

Some Supported Word Processors	File Format
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Microsoft Windows Write	.WRI
Microsoft Word	.DOC
MultiMate	.DOC
WordPerfect	.WP
WordStar 3.3	.WS
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For example if you use WordPerfect to make a file named foo send it as foo.WP. FOR OTHER WORD PROCESSORS SEE Aldus PageMaker 4.1. We can read ASCII FILES.

ALL NEW AND RENEWAL SUBSCRIPTIONS ; PLEASE SEND REMITTANCE TO M. Lynn James, Dept. of Chemistry, University of Northern Colorado, Greely, CO 80639.

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Cover: Playing with signal processing, courtesy of T.C. O'Haver, see Editors review.

The newsletter is done using Aldus PageMaker 4.2, and is printed using a LaserWriterII.

Contents

FROM THE CHAIR--
Don Rosenthal

The Committee on Computers in Chemical Education (C.C.C.E.) seeks to promote the use of computers and computing in chemical education. We do this by means of this Newsletter, by helping to organize symposia at National Meetings, by sponsoring new initiatives like the Computer Conference to be held this summer (described elsewhere in this Newsletter), by organizing workshops and by holding open meetings at the Biennial Conferences on Chemical Education. Let me describe some future activities and then indicate how you can help.

Symposia at National Meetings: A symposium entitle "Computers in Chemical Education" has been organized for the fall 1993 National Meeting in Chicago. Three half-day sessions will be held - "Computer Molecular Modelling" organized by James Beatty of Ripon College, "Interfacing in the Laboratory" organized by Robert Megargle of Cleveland State University, and "Personal Computers in Chemical Engineering Education" organized by Richard McCluskey of Clarkson University.

I am organizing a symposium on the use of computers in high school chemistry, undergraduate general chemistry, undergraduate organic chemistry and undergraduate analytical chemistry courses for the 13th Biennial Conference on Chemical Education being held at Bucknell University from July 31 to August 4, 1994. There will be a one and a half hour session devoted to each of the four topics. In each session there will be two invited speakers and a half hour devoted to discussion, questions and brief comments on the topic by member of the audience.

A symposium on "Computers in Chemical Education" is planned for the fall 1994 National Meeting in Washington, D.C. Thomas O'Haver (University of Maryland) is organizing a session on the use of Internet. Harry Pence is organizing a session on integrating computers into the undergraduate chemistry curriculum. A session on "What Chemists Need to Know About Computers and Computing" is being organized jointly with the Division of Computers in Chemistry.

How You Can Help:

We are always looking for material for this Newsletter. Send articles, paragraphs or suggestions to Editor Brian Pankuch. (His address is on the back cover.)

If you are interested in participating in any of our symposia, please contact the session chair. If you have suggestions for symposium topics, please send them to me.

If you have access to Bitnet or Internet, participate in our summer computer conference. If you are unable to participate in all sessions, select a paper or two to read and discuss.

If you would like to suggest some computer related activities or new initiatives, contact me.

We'd like to build our circulation. Share this issue with your friends and make the subscription form available to them.

IS ANYONE OUT THERE? LET US HEAR FROM YOU.

Donald Rosenthal Department of Chemistry, Clarkson University, Potsdam NY 13699 Phone: 315-265-9242 or 268-2352 ROSEN@CLVM.BITNET

EDITOR SPECTRUM--- A review by Brian Pankuch

This set of tools is primarily for use in analytical chemistry. I spent hours exploring and it is really interesting to use. Having done many of the operations by hand, well with a calculator point by point, it is a great feeling of power to run an absorption or NMR spectra through the many available operations and transformations. If you've done it by hand and haven't tried it by computer you are in for a treat.

By transferring the files on the program diskette to your hard drive and double clicking on the program icon you are up and running. I'd suggest going through a few pages of the instruction manual to get a feel for the program. The program is straight forward to use. It is very intuitive. The 97 page manual is excellent-mostly screen shots showing the before and after using a transformation or operation. The manual is very easy to read and follow.

Despite playing 'what happens if I do this?', I only got Spectrum to crash twice. Considering that I can do this with every program I've ever used without trying, this means that the program is quite stable and robust. Although primarily for those handling data from any type of spectra or graph it is easy enough to use that I'm considering using it for data manipulation and teaching some basics. Of course it would help if we had computers to use in the lab.

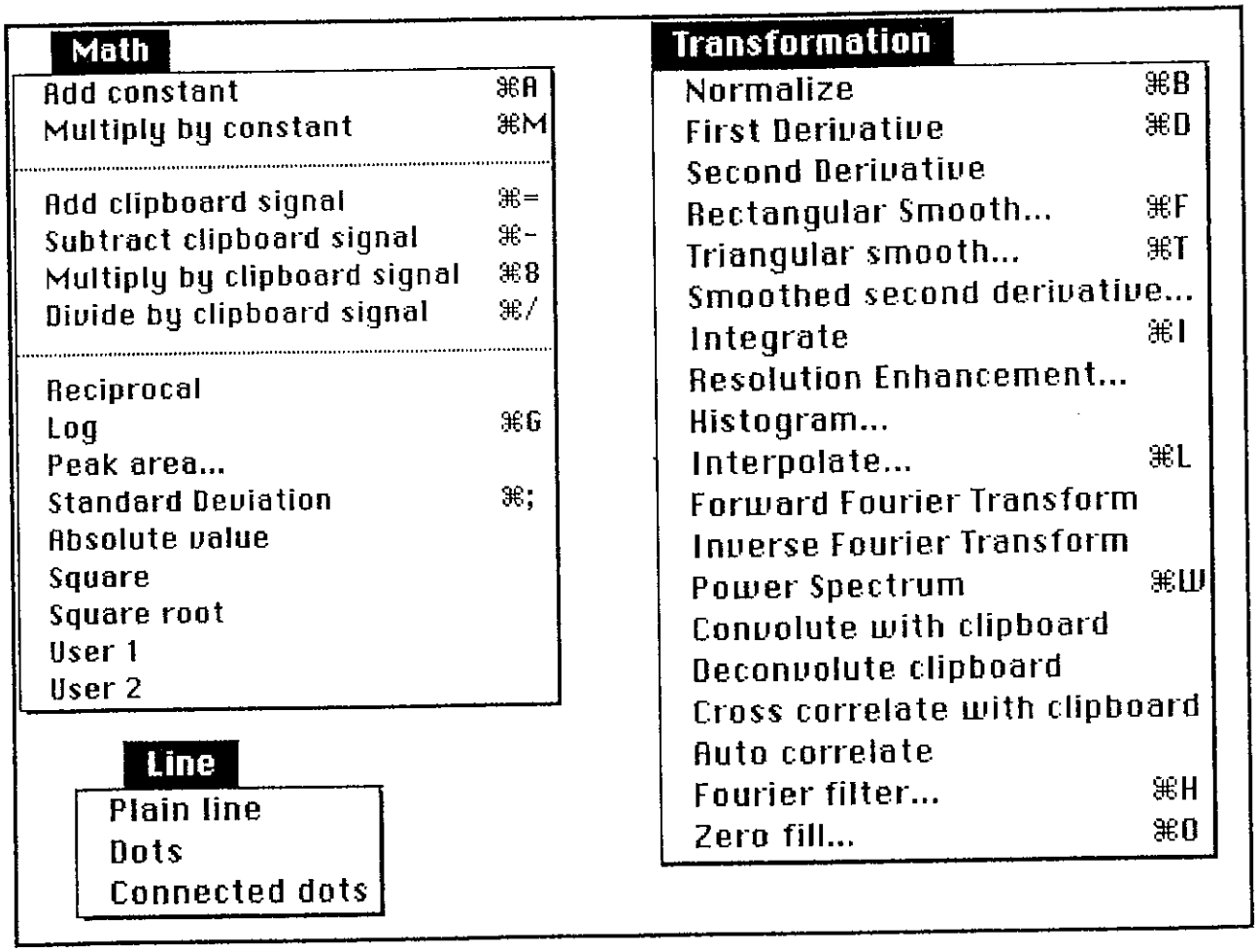
The program is designed for advanced and graduate level analytical courses. Strong organic students using gas chromatography, etc., would find parts of the tutorial quite worthwhile. If the data could be transferred directly from the instrument to Spectrum it would be worth spending sometime showing students some of the rudiments of cleaning up a signal. Although using and understanding all the features would

certainly take a lot of expertise, just using some of the basics shown in the following figures (from signals supplied with the program) with less advanced students would seem worthwhile.

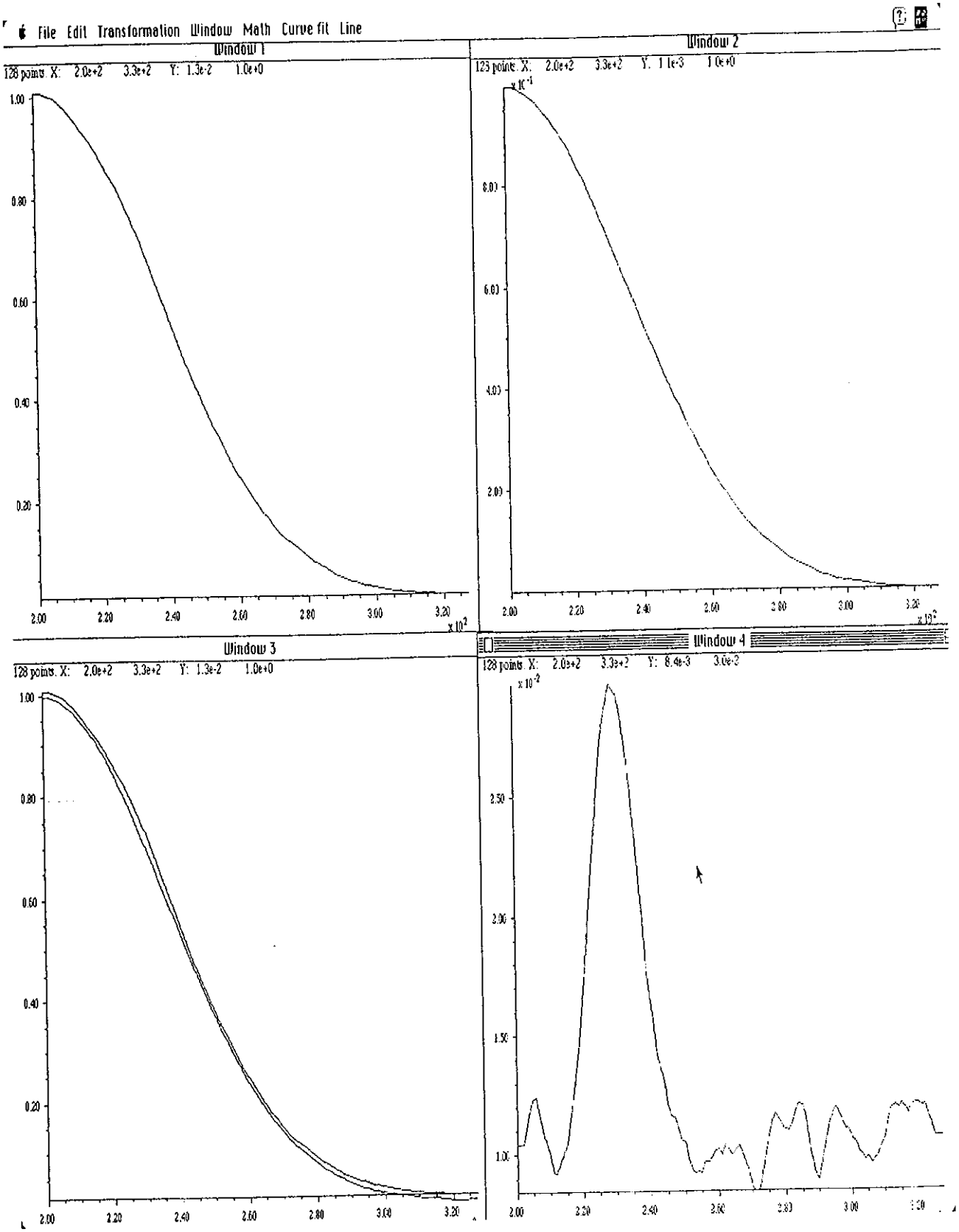
The tutorial has a variety of signals and suggested operations to demonstrate signal processing. The tutorial is informative. Having done some of these techniques by hand I can really appreciate the power at my fingertips. I'd recommend getting this program even if you don't have an immediate application. It is good enough and easy enough to use that you will minimally learn a bit and probably find some uses that I haven't thought of. Data files may be prepared in a text editor, spreadsheet, telecommunications programs, plotting or data acquisition program, and saved in ASCII (text only) format. You can also use the New command under File in the menu to generate synthetic signals. The signals can have optional noise on Gaussian, Lorentzian or sine waves.

The program is extendible, i.e., you can add your own functions. On the Mac you would need Borland's, Turbo Pascal 1.1 and Turbo Pascal Numeric Methods Toolbox. Since I have neither of the above nor a copy of the source code (the actual line by line code for the program as opposed to the compiled code that is what we usually use) for Spectrum, I was not able to actually check the actual procedure. You would also need ResEdit from Apple. Suggestions for making changes looked straight forward if you are a Pascal programmer.

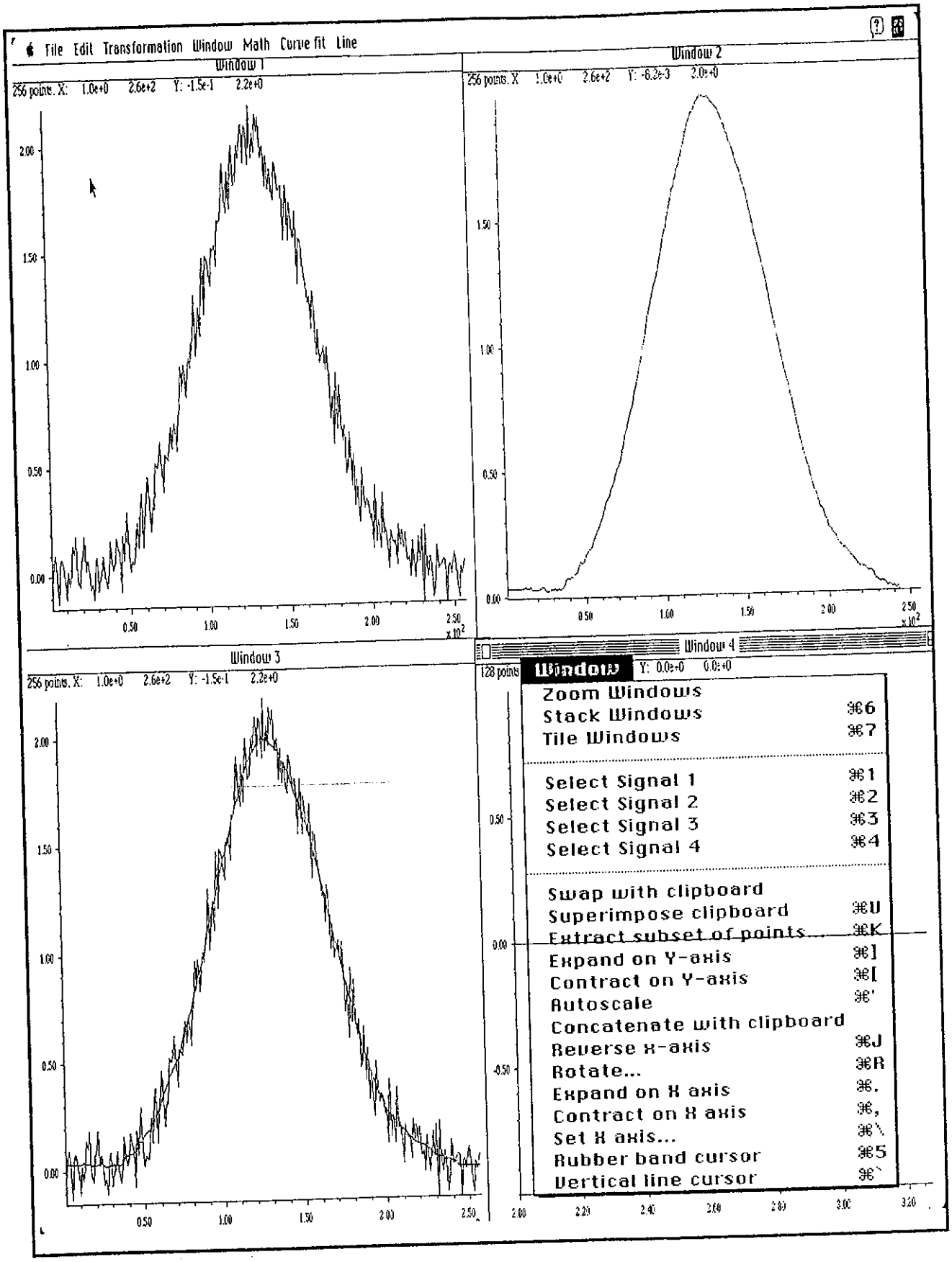
SPECTRUM was the 1990 NCRIPTAL winner. It is priced at $49.95 for a single copy, $249 for a department, $395 for all campus sites. It is available from: Academic Software Develpment Group, Computer Science Center, Room 3357, University of Maryland, College Park, MD 20742. Phone: 301-405-7600.



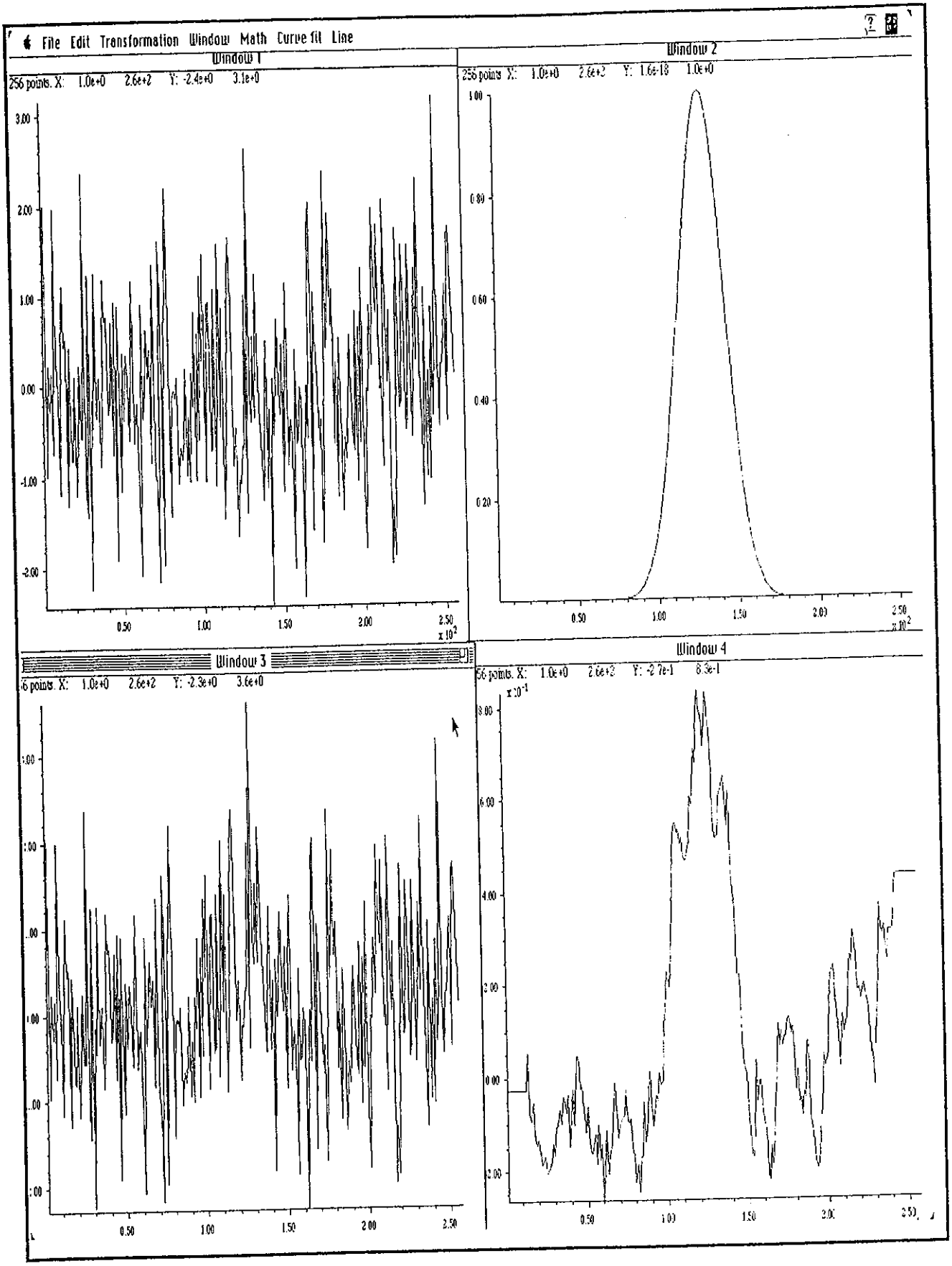
These are screen shots showing the wide diversity of functions available from the menus. Many other capabilities are available.



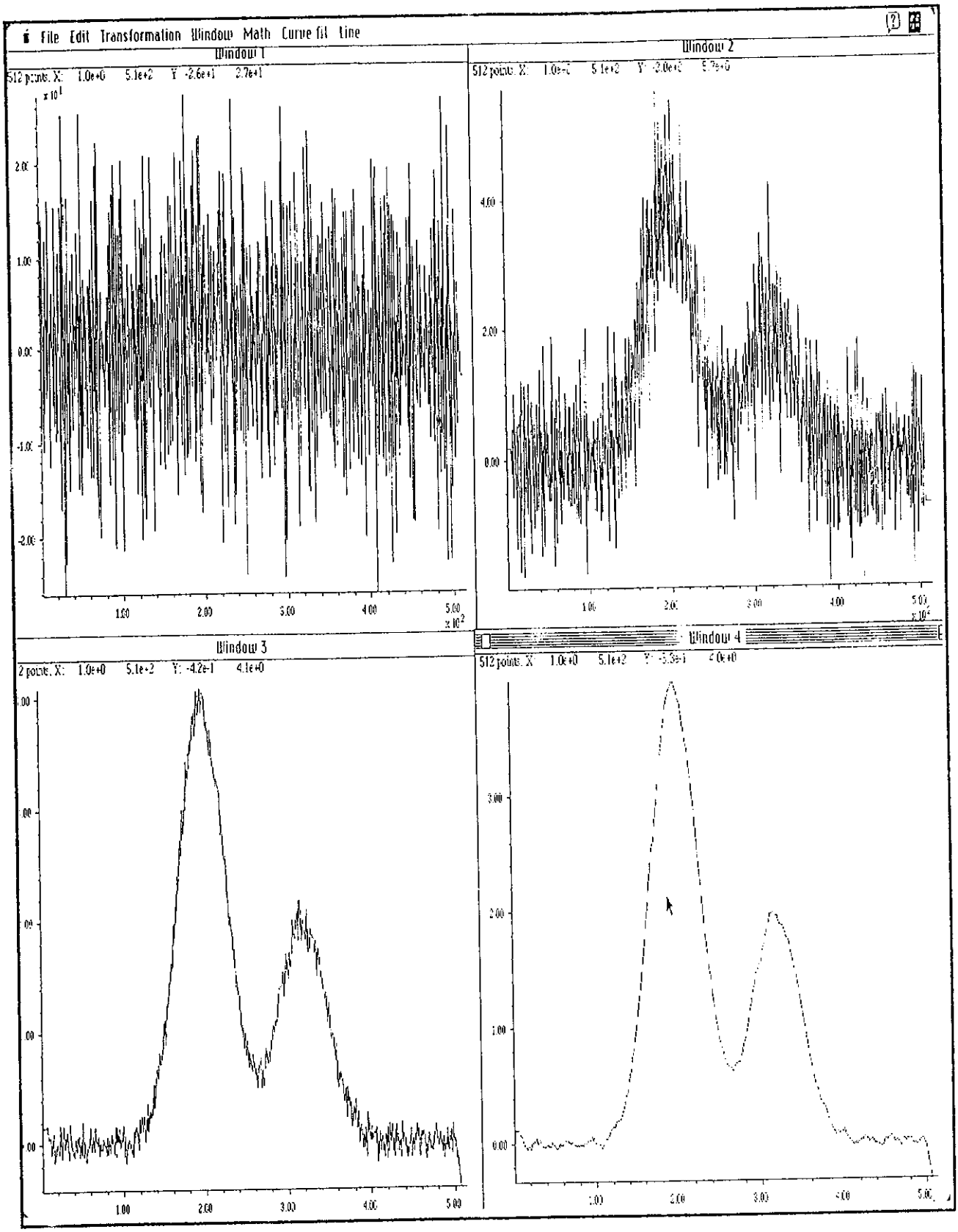
Window 1 is a signal, Window2-background, Window3- both signal and background, Window4-subtract background to get the actual signal that was buried under the backround. Amazing!



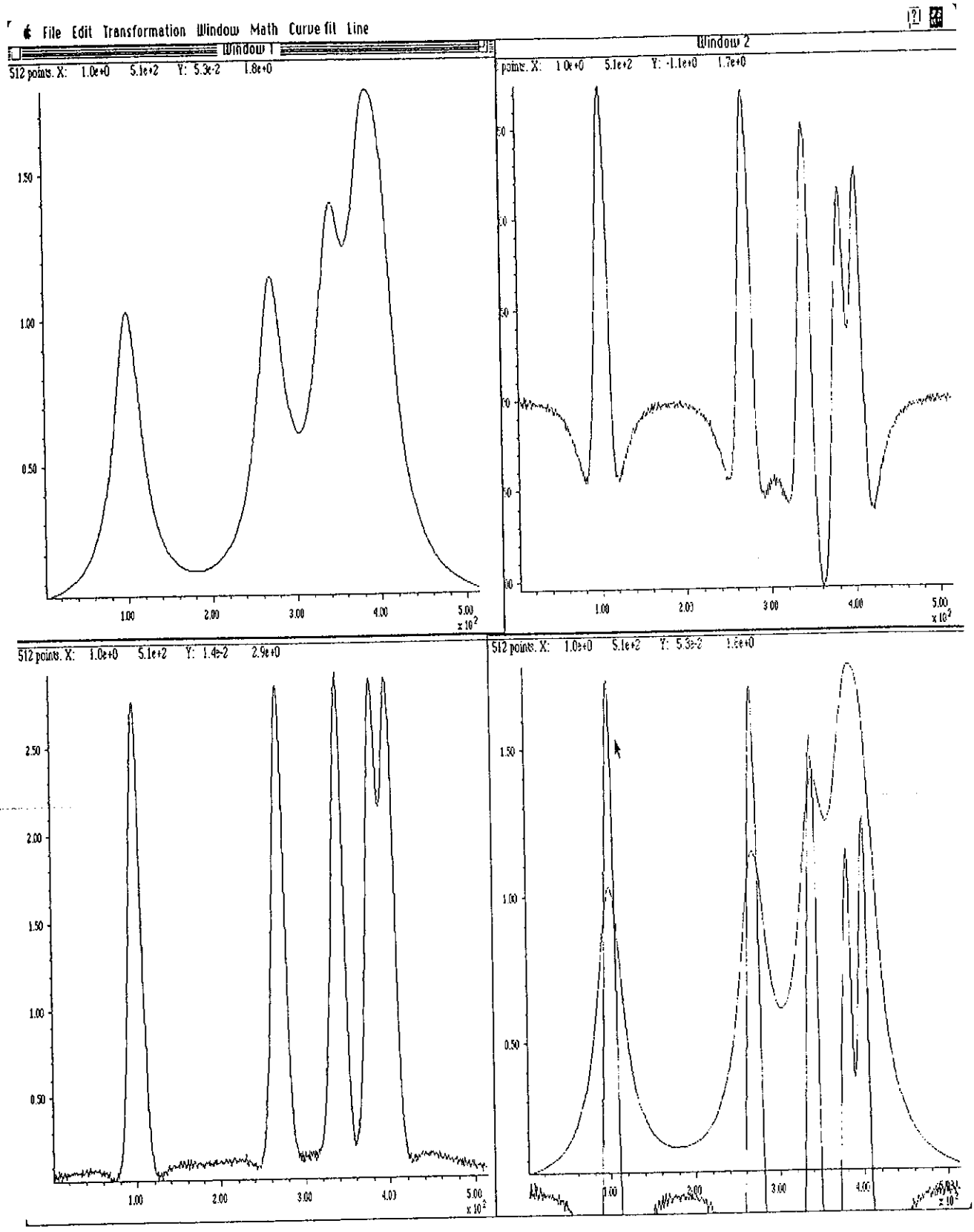
Window1 shows noise , Window2 shows gausian, Window3 shows both combined, Window4-some window transformations available from the menu.



Window 1 shows noise , Window 2 shows gausian, Window 3 shows both combined, Window 4 shows the combination -smoothed with rectangular smooth.



Window 1a very noisy signal, Window 2-rectangular smooth using 11 points, Window 3-two rectangular smoothes using 11 points, Window 4-four rectangular smoothes using 11 points, notice how each smoothing improves the signal.



Enhancing resolution- Window 1 shows five bands, with low resolution. Window 2 shows the second derivative with a multiplier of -700 notice the extraneous positive lobes around the peaks. Window 3 shows the addition of Windows1 and 2. Window 4 superimposes Windows1 and 2.

ELECTRONIC CLASSROOMS

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Chemistry is probably the best discipline which could be taught in an electronic classroom. There are two reasons for this - the nature of the material and the availability of software. Chemistry is complex, abstract, and often needs to be visualized in three dimensions. In organic chemistry and biochemistry more than one level of visualization may be essential for understanding. There are many excellent molecular modeling programs that can supplement the normal array of animation and authoring programs.

As a part of the design of the J. Joseph Moakley Center for the Application of Technology which is being constructed at Bridgewater State College, we have examined existing electronic classrooms at a variety of colleges and universities in the northeastern United States. As a result of this study, we have identified the following categories of electronic classrooms:

1. the two microcomputer classroom. Although there is no reason why only one microcomputer cannot be used, the use of a high level Macintosh **and** a 486 IBM/ clone allows full access to a larger base of software. A computer projection device, which may vary from a LCD panel on an overhead projector to a sophisticated video projection system, completes this model. We were surprised to find that departments which could afford more sophisticated setups often chose this model.

2. the desktop microcomputer model. The addition of ten to thirty microcomputers and a local area network (LAN) which is often connected to the institutional backbone, converts the two-microcomputer classroom into this model. A number of colleges have found that two students per microcomputer works better than one; hence fifteen is a popular number for student stations. It is essential that such a classroom be tiered so that the computer monitors do not interfere with the view of the projection TV screen. Although one would think that this type of classroom could be used as a computer laboratory (if adequate security is provided), many institutions found that interest in using the electronic classroom as a classroom did not leave much time for student use outside of class.

3. the maximalist model. The addition of screen control and screen sharing from a "master" microcomputer is relatively easy to implement in software. Some faculty object to the "control" implications of this model; others like the software control system.

4. the workstation model. At least one university in the northeast has an electronic classroom that uses UNIX workstations. The decreasing cost and increasing power of workstations may make this the choice of the future. An easy to use graphics user interface (GUI) can hide the complexities of the UNIX operating system and provide Macintosh-like ease of operation. If such a system is networked properly it can provide enormous computing power at very reasonable cost.

EDITOR: Bill is willing to set up a bulletin board about electronic classrooms at his college. Please send any suggestions for the format and other subjects of interest to Bill. This sounds like a great idea for getting ideas for those of us who are in the process of introducing electronic classrooms to our colleges.

HyperChem for Windows, Release 2. Reviewed by: **Andrew N. Welch and Yuzhuo Li**, Clarkson University, Potsdam, NY 13699. E-mail: welchan@craft.camp.clarkson.edu

Autodesk, Inc.: Scientific Modeling Division, 2320 Marinship Way, Sausalito, CA 94965. List Price $3500; educational discount price $595.

HyperChem for Windows is a powerful molecular modeling program that performs calculations using *ab initio* and semi-empirical quantum mechanical methods. HyperChem is designed in such a way that all of its commands and output can be controlled externally by other Windows programs, such as Excel or Visual Basic. In order to run HyperChem, the following is required: an IBM-PC compatible computer with an 80386 CPU and an 80387 math coprocessor, or an 80486 or higher CPU, 4 megabytes of memory, a hard disk with at least 5 megabytes free, a VGA or better video display, a parallel port for the locked version, a pointing device compatible with Windows 3.0 (such as a mouse), MS-DOS Version 3.1 or higher, and Windows 3.0 or higher.

HyperChem was tested on both a 486-25 and a 386-33. Installation was quick and easy and was completed in under ten minutes. There are two versions of HyperChem, an unlocked version and a locked version. The unlocked rendition requires no special action. However, the locked version demands that a hardware key be continually present in the parallel port. This form of copy protection does not permit simultaneous use of the software on different machines.

Upon loading HyperChem, the screen resembles that of other Windows programs. There are pull down menus, buttons for moving and scaling both the molecule as well as the entire HyperChem win-

dow, and the blank workspace.

Drawing molecules in HyperChem is uncomplicated. A default atom is first selected then bonds are drawn to form a skeletal structure. The default atom is selected by double clicking an icon and then using scroll bars to select an element. Atom charge and constraint of atomic geometry, bond length, angle and torsion angle can all be specified. The angle as well as stereochemical conformations, such as *cis-* or *gauche-*, can be specified. For a biochemist, databases of standard amino acid residues and nucleic acid residues can be employed to make macromolecules. A user selects the conformation and presses buttons labeled with residues to make a molecule. Zwitterions and counter ions can be specified. Once a molecule is created, a residue can be treated as a unit. It is not difficult to mutate a specific residue.

Once a molecule is drawn, a user typically invokes the so-called Model Builder. This section of HyperChem changes the entered 2-D representation into a 3-D drawing. This feature makes it easy to spot errors in input and change them. On the 386-33 and 486-25, the Model Builder worked essentially instantaneously. Once the model is built, the user is able to use many of HyperChem's features.

The display of molecules is flexible. Color can be used; atom labels range from the common element name to its chirality and a residue can be displayed with its name and/or position. Hydrogen bonds can be displayed. There are five rendering options: sticks, dots, sticks and dots, spheres, and disks (a "flatter" version of the sphere). Sphere rendering was very quick compared with other molecular modeling programs. Several molecules may be displayed together, superimposed if desired, to show the differences between them, such as what is different between an optimized and an unoptimized molecule.

There are several different methods of selecting certain parts of a molecule. Atoms, residues, or entire molecules may be selected and manipulated as units. A sphere may be used to select objects encompassed in the 3-D area. There is a NOT operation that will select what is currently unselected, and that which was currently selected becomes deselected. Backbones, side chains, and rings may be selected without having to select each individual element. You can even extend a selection along a chain until you get to an sp^3 carbon atom. A group of selections may be named and used later. Additionally, certain selection names are used in changing the molecule. For example, if the PLANE selection is input, the user may carry out a molecular reflection across the plane. Selection is very well supported in HyperChem.

There are four molecular mechanical force fields available: MM+, AMBER, BIO+, and OPLS. In general, these methods are designed for macromolecules, nucleic acids and proteins. However, although MM+ was originally designed to be used with organic molecules, the scheme was modified to broaden its potential use. Dielectric interaction (epsilon) and nonbonded interactions can be scaled and changed from what they would normally be when the molecule is a gas. Geometry constraints for bond length, angle, and torsion angle are able to be defined. Semi-empirical methods available are Extended Hückel, CNDO, INDO, MINDO3, MNDO, and AM1. Options include convergence criteria, charge, spin multiplicity, spin pairing, electron excitation state, and the DIIS procedure which can accelerate convergence. For each method, there are tables of data that contain information such as ionization energy and Slater exponents; numbers come from values obtained in literature. These parameter tables may be edited and recompiled to fit special applications. A periodic box may also be specified to represent solvent effect. Geometry may be optimized by the steepest descent, Fletcher-Reeves, or Polak-Ribiere methods. Geometric optimization and single point calculations were compared with results obtained with the Gaussian 90 program running the same type of calculation, and the results were essentially the same. The speed of these calculations is not slow for a PC. Nitrobenzene was optimized in 36 seconds and azidoadamantine was optimized in 43 seconds. There appear to be no significant computational discrepancies between the two programs.

HyperChem, because of its integrated nature, deviates from the traditional method of log file output from calculation stages. Contour plots, superimposed on the molecule, can depict electrostatic potential, spin density, charge density, and orbital information. Molecular dynamics can be animated. A temperature routine can be used to monitor the effects of heating on the screen. Snapshots may be saved for later study. Additionally, there is a facility where graphs of different energies, such as kinetic and potential, may be plotted during the run.

There is a log file facility used to store commands. It is useful and flexible. Events are saved and the user may put comments into the file at will. Unfortunately, there is no facility for datafile conversion. This means that a user must write his own converter program if he wants molecules created in HyperChem to be used with external computational programs. The only filetypes supported are .HIN, which is the proprietary format, and .PDB, the Brookhaven Protein Data Base format. The documentation describes the use and the method of obtaining .PDB files. Pictures of the HyperChem workspace can be saved to the clipboard as a Windows Metafile (.WMF) or as a Windows Bitmap (.BMP). These pictures are easily inserted in other documents.

Probably the most useful aspect of HyperChem, and that which separates it from other pro-

grams, is its ability to be controlled externally by other programs. The tutorial provided describes using Excel to drive HyperChem. The torsion angle in hydrogen peroxide is changed by an Excel macro and the new energy is recomputed. Cells are automatically filled with the appropriate data and a graph can be plotted. There is considerable potential for user interaction in the program. A user is able to write routines in any language that is able to provide DDE (Dynamic Data Exchange) links to Windows. If desired, additional optimization or other kinds of manipulation of molecules is able to take place outside of HyperChem.

The online help is sufficient. There is a glossary that assists beginners in learning specific terms. Details on using the program's features are suitable. The documentation is superb. The tutorial does not take longer than a work day to complete and yet it illustrates most of HyperChem's capabilities. There is a guide for novices that explains much of the theory of computational chemistry. The language is comprehensible even to a beginning chemist. This guide explains which method and parameter set is best for each type of calculation. The reference guide is very complete and discusses not only program operation but also methods of interfacing HyperChem externally.

This program would be of considerable use to a first year chemistry, organic chemistry, biochemistry, or physical chemistry student. Because of the ability to show molecular geometry, concepts having to do with structure, bonding, interactions, and polarities become much easier to learn. The Windows platform allows the user to install many special devices that aid the learning process. For example, a projector can be used to show an entire classroom clearly what is on the computer monitor. These devices, sold by third party vendors, resemble overhead projectors that have a wire that connects to the computer.

Many students have difficulty visualizing the three dimensional shapes of molecules. With HyperChem, a large number of molecules may be drawn, optimized, and displayed on the screen. A lab could be designed where each student is assigned several molecules and asked to use Hyperchem to predict what the molecular shape would be. Different groups of students may be assigned different sets of molecules generating a larger database of structures. Students then would be able to deduce empirical rules on how to determine shape. Alternatively, the teacher may program the molecules and optimize them as a batch job with an external program. Then another program could be written that presents the data as a sort of "slide show." Students are then able to discover the correlations themselves and deduce the rules that determine molecular geometry. Another opportunity to use HyperChem for first-year students is when gases are studied. A sample of some gas may be heated and students can watch its effects on potential and kinetic energies and on the molecule itself. For the Organic Chemistry student, HyperChem can be very useful in teaching stereochemistry. It is easy to build molecules with different chirality, label each chiral atom, and rotate each to demonstrate the difference between the two molecules.

For more advanced students, the use of HyperChem can demonstrate the concepts of computational chemistry. Typically, one would have to use many programs to show differences between the different algorithms. However, because HyperChem has such a large array of methods, only one program needs to be learned. Additionally, the traditional text-based computational systems are ineffective in motivating students because the interface is more cumbersome to use.

In conclusion, HyperChem was found to be a very powerful tool. There is a new version that is currently in the process of being tested that includes several more computational methods including configuration interaction, better support for metals and inorganic compounds, more options for specifying stereochemistry, a floating element selection box, UV/VIS and vibrational analysis, and more extensive orbital analysis. HyperChem is quick, accurate, and, for the most part, easy to use. As an educational and research tool, the reviewers recommend this software.

THE COMPUTER CONFERENCE ON APPLICATIONS OF TECHNOLOGY IN TEACHING CHEMISTRY - THE FEBRUARY TRIAL SESSION AND THE SUMMER CONFERENCE

by Donald Rosenthal, Department of Chemistry, Clarkson University, Potsdam NY 13699 (ROSEN@CLVM.BITNET)

and **Thomas O'Haver**, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 (TO2@UMAIL.UMD.EDU)

INTRODUCTION

The summer computer conference is the first such conference sponsored by the Division of Chemical Education's Committee on Computers in Chemical Education. Articles on the summer Computer Conference and Computer Conferencing appeared in the Fall 1992 issue of this Newsletter.

We view this conference as an experiment and have tried to design the format to take advantage of the unique features of computer conferencing. We decided to test the format and other aspects of the computer conference by scheduling a trial session during February. The purpose of the trial session was to determine how well the proposed format worked and to obtain feedback from participants which might be used to modify the format and instructions to participants and authors. PRE-TRIAL ACTIVITIES

Upon registration for CHEMCONF ten pages of INSTRUCTIONS FOR PARTICIPANTS were sent to each participant. Twelve pages of INSTRUCTIONS FOR AUTHORS were sent to each author. Just prior to beginning the trial session there were over two hundred registrants from twenty-four countries.

Three papers were selected for the trial session:
Paper 1: "How to Make Computer-Assisted Instruction Fail" by Stephen K. Lower, Simon Fraser University, Canada (three pages),

Paper 2: "Windows and Networks: Lowering the Activation Energy for a Chemistry Department Microcomputer Facility" by Thomas O'Haver (eight pages),

Paper 3: "Some Computer Graphics Examples" by Thomas O'Haver (seven pages plus twenty-five figures each converted and transmitted as a separate text file).

These three papers were selected because each was quite different from the other. Paper 1 was similar to a paper which Professor Lower distributed at the 12th Biennial Conference on Chemical Education at UC Davis last summer. Paper 2 appeared in the Fall 1992 issue of this Newsletter. Paper 3 was prepared specifically for the trial session and was designed to provide participants with examples of graphics and to provide practice in downloading and viewing figures.

Prior to the beginning of the trial session the abstracts of the three papers were distributed. The trial session schedule was sent out a few days before the beginning of the session. TRIAL SESSION.

The papers and figures were distributed on Monday, February 1. Each paper contained questions intended to stimulate discussion by the participants. Short questions were sent by participants to the authors or to other participants during the next three days, i.e. questions for Paper 1 were sent on Tuesday, questions for Paper 2 were sent on Wednesday and questions for Paper 3 were sent on Thursday. In the second and third week two days were devoted to the discussion of each paper. The authors answered short questions directed to them at the beginning of the discussion of their paper. An evaluation form was distributed on February 16 and was to be returned to Thomas O'Haver via electronic mail before the end of February.

How well did the trial session and the proposed format work? Participants were generally enthusiatic. There were some problems. These will be discussed later. The following are some of the comments received:

* Great conference... I hope more are in my future. Mike Whitbeck, University of Nevada at Reno
* So far I have enjoyed the discussion and also learned a lot. It is great. Angelo R. Fernando, University of Alberta
* ... many (messages) are immensely helpful and thoughtful. Allan Smith, Drexel University
* We're all operating . . on the cutting edge of a new form of information and idea exchange. Carl H. Snyder, University of Miami
* I've learned and had fun. Paul Edwards, Edinboro University of Pennsylvania
* It feels like a real conference. You get snippets of conversations and ideas which add up to a coherent whole after some time. Dan Bearden, Clemson University
* I have found this trial session at once informative, energizing mind-boggling, fascinating and a tremendous source of ideas. The mind-boggling fascination is, that from the computer in my office, I am in contact with people all over the world -- doing exactly the same thing I am. ... a chance to learn, a chance to share new information. Elisabeth T. Kintner, University of Pittsburgh - Johnstown
* ... the excitement of developing ideas, clarifying points, getting to the position where I better understand what should happen in my classes ... Charles Sundin, University of Wisconsin - Platteville
* I think it has the potential for making us all feel a little less isolated. Robert Brown, Douglas College, Canada
* There was ample time for discussion. Papers and discussion could be examined in a leisurely manner. Participants were able to ask short questions of authors and obtain well thought out answers. Donald Rosenthal, Clarkson University
* . . thoughtful responses (keyboard is better than just discussing, since you do have to think . . about what you are writing.) Frank Darrow, Ithaca College
* Allowed everyone to have a voice. Doug Williams, Kalamazoo College
* The entire concept was wonderful. Opens new horizons. Howard Dess, Rutgers University .

One question that was asked on the evaluation form was "What did you like most about the Computer Conference?" Some of the above comments were made in response to this question. Other comments occurred spontaneously during the trial session.

Considerable discussion was generated during the conference with

many of the registrants participating. One participant reported the trial session had generated over two hundred pages of print out. (This does not include 80 pages of evaluation from 34 participants.) The papers and full discussion are available and can be accessed via electronic mail. (If you are interested, contact Thomas O'Haver at T02@UMAIL.UMD.EDU.)

Participants were asked to provide an overall evaluation of the papers, discussion and meeting on a scale from 1 to 5 where 1 is poor, 3 is average and 5 is excellent. The overall evaluation of the papers ranged from 3 to 5 with an average of 3.7. The discussion was rated from 2 to 5 with an average of 3.5. The trial session was rated from 3 to 5 with an average of 4.1.

Paper 1 listed eleven things a teacher could do to make computer-assisted instruction (CAI) fail. The paper was written in an ironic style and generated the most wide-ranging discussion, including the use of CAI, simulation and the role of more traditional teaching methods in a course which uses CAI.

Paper 3 contained examples of black and white, gray scale and color graphics. Some participants identified difficulties in the transmission of graphics and offered solutions and suggestions for the better handling of graphics. Some participants didn't even try to work with the figures. This discussion was most useful. As a result, some modification in the instructions and in the handling of graphics will be made for the summer conference.

Another question which was asked on the evaluation form was "What did you like least about the conference?" Many of the responses to this question reinforced comments made during the session. Rather than listing individual comments, we will summarize some of the conclusions.

"Noise" was generated by some participants due to a lack of familiarity with electronic mail and LISTSERV, a lack of discipline on the part of some registrants and inadequate instructions. Some registrants when they discovered more about the nature of the trial session and the volume of mail it would generate decided to sign off CHEMCONF but did not know how to do it properly. We all received the message "I want out". A few other extraneous messages added "noise".

The first week was designed for SHORT QUESTIONS to the authors or participants. All such questions were to be sent to CHEMCONF so that all participants would know what questions the authors were being asked. Private messages were to be sent to the authors identifying grammatical or other errors, or messages to Tom O'Haver asking for technical assistance. Some participants used the first week to begin discussion. This was not our intention. The first week was to be used for reading the papers, asking short questions and preparing for the discussion.

Some participants introduced "noise" by discussing one paper during the time allocated for discussion of another paper. Another problem was that even though a specific two days was allocated to the discussion of a particular paper several threads of conversations intertwined. Even if the thread can be identified, the segments of the thread are not necessarily received sequentially. The labeling of the message was not always sufficient to identify the thread nor indicate where the message fit on the thread.

We sought to obtain information on the degree of participation by each registrant in the trial session. We consider this evaluation to be an important aspect of the trial session (and summer conference) experiment. Several registrants indicated that February was a busy time for them. When someone goes to a meeting the participant frequently makes a definite commitment to participate. We are interested in learning how much of a commitment of time and effort registrants will make to a conference which extends over TWO MONTHS in the summer. The results of the trial session survey indicated that those participants who returned the survey:

1. accessed the discussion from zero (only read the papers) to seventy times. The average was 24 times.
2. Devoted from 2.3 to 28 hours to the trial session. The average was 9.5 hours.

Those who participated in the evaluation process probably devoted more time to the trial session than the average registrant.

The trial session evaluation form contained the question: "What changes can be made to improve the computer conference?" Some suggestions were made during the trial session. Some of these suggestions have already been mentioned. The suggestions were not always consistent. Some participants wanted more structure, others wanted less. Some participants wanted more than two days devoted to discussion of each paper. Other participants were afraid that additional discussion time might result in too much discussion. If three papers generated 200 pages, will fifteen papers generate 1000 pages! Who wants to wade through so much discussion? There was an appeal for brevity in discussion. It is obvious that some participants are addicted to electronic mail. The suggestion was made that we impose voluntary limits on the number of times participants can submit discussion on any one paper. Registrants will need to exert more self-discipline and the conference manager may need to play a more active

role in managing the summer conference. In order to reduce the noise, the conference manager (Tom O'Haver) will announce the beginning and end of each session. This will avoid confusion associated with different time zones. Registrants will be asked to limit themselves to the designated activity, e.g. SHORT QUESTIONS for Paper 1 or DISCUSSION for Paper 2. Time for GENERAL DISCUSSION may be available on another LISTSERV or at other designated times. Discussion of papers will generally be for two days, but where discussion is scheduled for Friday and Monday the weekend will be available. This effectively provides four days.

Additional details will be provided for registrants just prior to the summer conference. SUMMER CONFERENCE - June 14 through August 20, 1993.

Abstracts for the following fifteen papers have been received and the tentative order of presentation is as indicated:
SESSION ONE

1. CULTURAL DIFFERENCES REFLECTED BY AN INTEGRATED MEDIA CHEMISTRY COURSE - AN AMERICAN/ISRAELI PERSPECTIVE. Nava Ben-Zvi, William S. Harwood, Ahuva Leopold, and Lisa L. Ragsdale Hebrew University, Israel and University of Maryland

2. FOR LANS SAKE: SUGGESTIONS FOR THE USE OF NETWORKED COMPUTERS IN CHEM ED B. James Hood, Middle Tennessee State Unversity

3. WHY DO ELECTRONS AND NUCLEI FORM ATOMS AND MOLECULES?: A GUIDED, INTERACTIVE EXPLORATION IN QUANTUM MECHANICS John P. Ranck, Elizabethtown College

4. THE USE OF COMPUTERS IN A JUNIOR-LEVEL ANALYTICAL CHEMISTRY -PHYSICAL CHEMISTRY LABORATORY COURSE Donald Rosenthal, Clarkson University

5. IT'S HOW YOU PLAY THE GAME: DESIGN OF AN ELECTRONIC ASSISTANT FOR ORGANIC QUALITATIVE ANALYSIS Joyce C. Brockwell, Northwestern University SESSION TWO

6. INDIVIDUAL COMPUTER-GENERATED GRAPHICAL PROBLEM SETS Frank M. Lanzafame, Monroe Community College

7. INTEGRATING COMPUTERS INTO THE HIGH SCHOOL CHEMISTRY CLASSROOM William J. Sondgerath, Harrison High School, West Lafayette, Indiana 8. USING THE AIRWAVES: A SATELLITE M. S. FOR INDUSTRIAL CHEMISTS. K. J.Schray, N.D. Heindel, J. E. Brown, and M. A. Kercsmar. Lehigh University

9. APPLICATIONS OF NETWORKED COMPUTERS AND ELECTRONIC MAIL IN A CHEMISTRY COURSE FOR NONSCIENCE STUDENTS Carl H. Snyder and James Shelley, University of Miami

10. COMPUTATIONAL CHEMISTRY AS A CENTRAL FEATURE IN THE TEACHING OF ORGANIC CHEMISTRY Joseph Casanova, California State University at Los Angeles SESSION THREE.

11. STAFF DEVELOPMENT IS THE BIGGEST COST IN COMPUTING David W. Brooks, University of Nebraska-Lincoln.

12. THE COMPUTER CO-OP: TEACHING ORGANIC CHEMISTRY ON A CONFERENCE IN AN INTERDISCIPLINARY MACINTOSH LAB Carolyn Sweeney Judd and Robert G. Ford, Central College, Houston Community College System.

13. FINITE DIFFERENCE SOLUTION OF THE DIFFUSION EQUATION ON A SPREADSHEET Douglas A. Coe, Montana College of Mineral Science and Technology.

14. CHEMULATE! A SIMULATOR OF UV/VIS KINETICS EXPERIMENTS FOR THE MACINTOSH Richard S. Moog, Franklin and Marshall College.

15. MENU DRIVEN PROGRAMMING FOR STUDENTS AND TEACHERS Reed Howald, Montana State University.

Those wishing to register for the Computer Conference must send the message: SUBSCRIBE CHEMCONF <your name> to LISTSERV@UMDD.UMD.EDU before June 1, 1993. Detailed instructions will be sent via electronic mail to registrants.

The success of any conference depends upon the quality of the papers and of the discussion. We hope YOU will help us make the summer conference a success.

DEMO OF THE NEW VERSION OF MOBY VIA ANONYMOUS FTP

Wilmon B. Chipman
Dept. of Chemical Science
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Bridgewater, MA 02325
CHIPMAN@TOPCAT.bsc.mass.edu

The demonstration version of MOBY, version 1.5, may be obtained via anonymous FTP from benny.bsc.mass.edu(or 134.241.41.5). If you have access to a computer on the Internet which supports FTP (file transfer protocol), log on to the computer and use

the following sequence of commands (use lowercase throughout):

ftp benny.bsc.mass.edu
anonymous <cr>

your_email_address <cr>
cd pub <cr>
cd moby <cr>
binary <cr>
get mobyread.me <cr>
get mobydemo.exe <cr>
get manualps.exe <cr>
quit <cr>

At this point you will have the binary version of the files in your directory on the computer that is connected to the Internet. Your local information services folk can advise you on the best way to transfer these files to your microcomputer. MOBY version 1.5 runs best on a 486 or 386. The 386 will require a math coprocessor. MOBY requires 530 K of RAM to be free. The mouse driver must be installed before running MOBY. If you have a problem with the local file transfer, it will probably be that the files are not being transferred as binary files.

mobydemo.exe is a self-extracting archive file that contains the demo version. manualps.exe is a self-extracting file that contains a postscript version of the demo manual. Make a directory called c:\MOBY and copy the files to it. Then run the files and they will self-extract.

If you have problems with this process, you can email to CHIPMAN@TOPCAT.bsc.mass.edu

The demonstration of MOBY, version 1.5, can also be obtained by writing to

Raye Scovern Hazan
Electronic Media Dept.
Springer-Verlag New York, Inc.
175 Fifth Avenue
New York, NY 10010

Prices for the complete new version of MOBY are in the file READ.ME which you can find in the directory c:\MOBY after you install the program. The site price for 10 or more copies is quite attractive.

Please read both:
MOBYREAD.ME and
READ.ME
for further information about MOBY.

I have a spelling checker.
It came with my PC.
It plainly marks four my revue
istake I cannot sea.
I've run this poem threw it.
I'm sure your please to no.
It's letter perfect in its weigh;
My checker tolled me sew.

from Communication Briefings
November 1992

On this note fromthe Chair have a great summer.