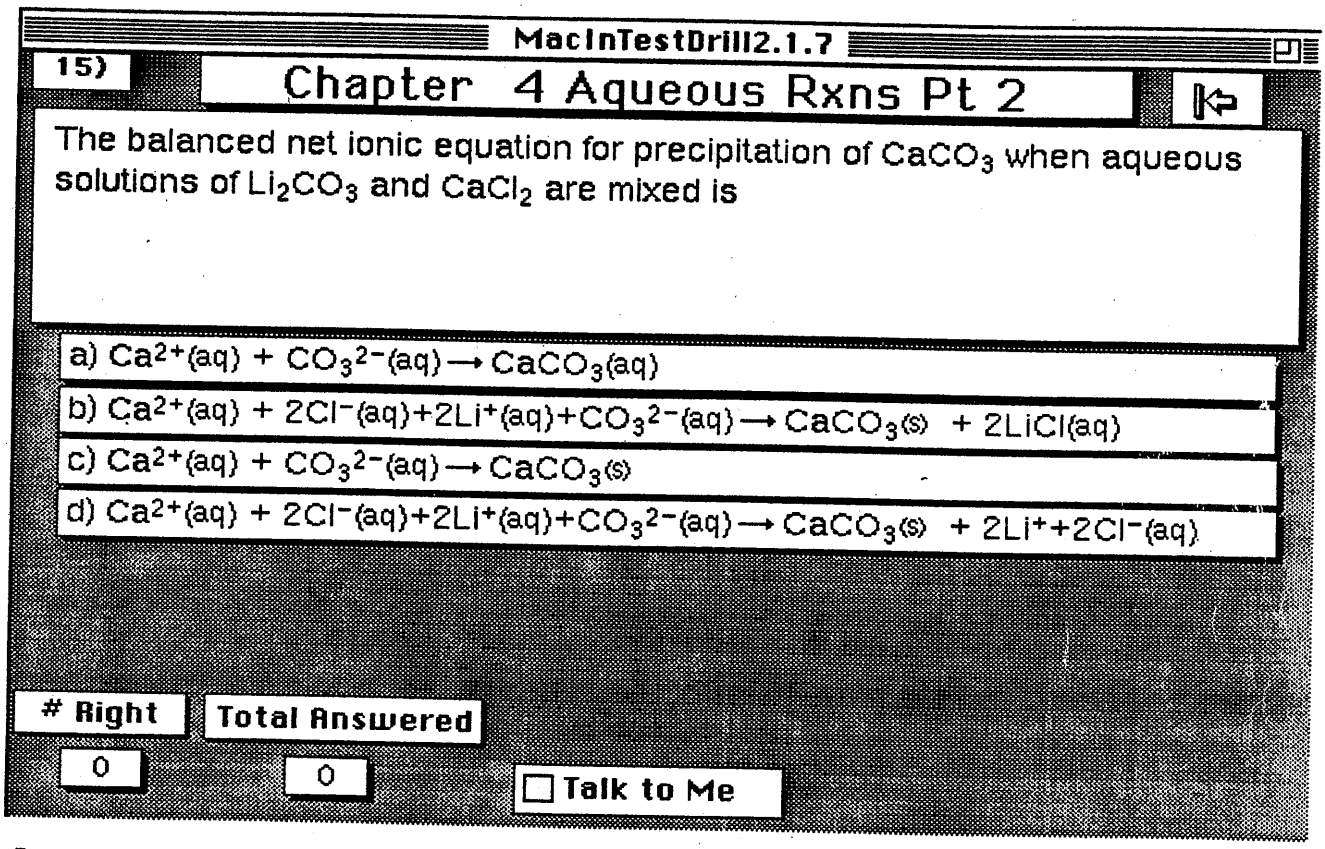
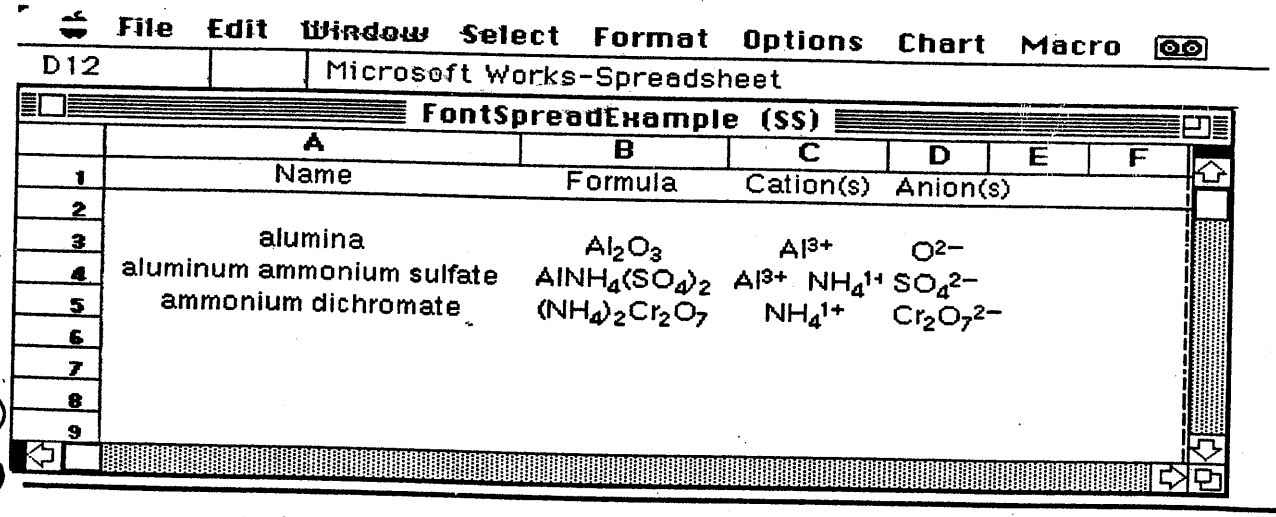
Computers in Chemical Education Newsletter

Spring 1992





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Don Rosenthal and Al Latta co-chairs

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 3 1/2 inch Macintosh or IBM compatible diskette. We have fewer problems with 3 1/2 inch diskettes.

We can read the files from Microsoft Word or Works,Aldus PageMaker 3.01, 4.0, for other word processors please send text or ASCII code files if possible. Hardcopy is fine if that is most convenient.. **Submission deadlines**: Fall issue - Sept. 25; Spring issue - March 25.

ALL NEW AND RENEWAL SUBSCRIPTIONS : PLEASE SEND REMITTANCE TO M. Lynn James, Department of Chemistry, University of Northern Colorado, Greeley, CO 80639.

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FROM THE CHAIR

The ACS Division of Chemical Education's Committee on Computers in Chemical Education (C.C.C.E.) seeks to promote and publicize the use of computers and computing in chemical education. We do this via this Newsletter, and by organizing and participating in symposia and workshops at regional and national meetings.

This Newsletter serves as a vehicle of communication with those interested in computing. Articles and information are provided for our readers. Ideally, readers communicate with each other by writing articles or short paragraphs describing their use of computers in chemical education. The QUERIES sections provide an opportunity for readers to ask and answer questions. The success of this Newsletter depends upon your willingness to participate in these activities.

Don Rosenthal (Department of Chemistry, Clarkson University, Potsdam NY 13699, 315-265-9242, ROSEN@CLVM.BITNET) is promoting symposia at National Meetings. Al Lata (Department of Chemistry, University of Kansas, Lawrence KS 66045, 913-864-4054, LATA@UKANVAX.BITNET) is assisting with the organization of symposia and workshops at regional meetings. Symposia are being organized by Harry Pence (SUNY Oneonta) and Tom O'Haver (University of Maryland) for the 1992 Fall Meeting in Washington, DC. Lynn James (University of Northern Colorado) and Henry Derr (Laramie County Community College) are organizing a hands-on computer session for the 1993 Spring Meeting in Denver. Jim Beatty (Ripon College) is helping to organize symposia for the 1993 Fall Meeting in Chicago. Al Lata has worked with Joe Casanova to organize a symposium on "Integrating Computational Chemistry Into the Curriculum" for the Biennial Meeting at Davis in August 1992. Don Rosenthal and Ken Ratzlaff (University of Kansas) are organizing symposium sessions for the 1994 Biennial Meeting at Bucknell University.

Over a dozen C.C.C.E. National Computer Workshops have been held. Workshops are planned for the University of Kansas in August 1993 and at Bucknell University after the Biennial Meeting in August 1994.

C.C.C.E. activities are designed to meet the needs of chemical educators. You can help in identifying these needs. An open meeting of the Committee is planned for the Biennial Meetings in Davis. You are invited to attend. We welcome your suggestions and participation. If you have suggestions or wish to volunteer to assist us, a form at the back of this Newsletter should be filled out and returned.

Don Rosenthal - Co-Chair with Al Lata of the C.C.C.E.

EDITOR---Brian Pankuch

USING A QUADRA 700: The Quadra 700 is one of Apple's latest systems. It comes with a Motorola 68040 processor. Mine has 20 Meg of ram memory, a 520 Meg Fujitsu hard disk and a RasterOps 21 inch monochrome monitor. The operating system is updated 7.01. Since I used four suppliers for the different items my, first surprise, a rather pleasant one, was that all the hardware worked when I assembled it.

After hearing so much about System 7, Apple's latest operating system, I was eager to try it. My first impression on bringing it up was--where is it? My usual manipulations looked and felt the same. After hunting I did notice a few improvements. Balloon Help is one. To give you an example of how this works, I'm writing this column using Micosoft's Word 5. I can check spelling and grammar within this program. After checking I get a table of statistics giving me information about the column. The different indexes shown are not familiar so I click on Balloon Help, move the mouse pointer to each entry and a balloon similar to those used in the newspaper comics comes up with information about what I'm pointing to. This is much easier than looking it up in over a thousand pages of manuals.

Now imagine a large number of students unfamiliar with either the Mac or the program you want them to use. Balloon Help is a potential time saver. A student can move the mouse to what they want to know about and have the information balloon right up! System 7 gives help on the major features of the Mac interface up on the screen. Not being magic, help for a specific program has to be programmed in by the programs author and many have done this. For instance Word 5 and PageMaker 4.2 have Balloon Help, Hypercard 2.1 does not.

The Quadra comes with a microphone which attaches anyplace convenient and with a simple click of the mouse I can record up to a minute of sound and include it with this column. I could send it to you, and you could read and hear. Neat but I don't personally see much use for it unless I want to practice a few German phrases.

Quicktime is an extension for System 7. The examples I have allow me to open a window and play a 'movie' with sound. One example is a wind surfer bouncing along in rough water during a thunderstorm. You can see the lightning and hear the thunder. This becomes interesting when you realize you could be watching a chemical reaction occurring in color on the screen. You stop, step,

go backwards as often as you want. About 10 seconds of the wind surfer requires about 500 K of storage. Not bad, but we won't be showing movies this way for a while. The ability to have moving picture included in an interactive chemistry program is very intriguing.

Apple supplies a utility with System 7 that checks all the programs on your hard disk and estimates compatibility with System 7. I was happy to find that the estimated compatibility was usually conservative and almost every program I had still worked despite warnings. If you don't need maximum speed from the system, it is wise to shut off the cache switch and 32 bit addressing. With them off everything I've looked at worked, except Mathematica. When both are on older programs such as Microsoft Works and Word 4 would crash, when both are off Works and Word 4 are OK.

One surprise I got was with Symantec's Think Pascal. I use this program about 30 hours a week and called Symantec technical support to check the compatibility before I got the new Quadra. They assured me that Think Pascal 4 worked fine. It didn't, so back to tech support, who at first claimed yes it did. A few exasperating days later they admitted a patch was needed. It seems that Apple made a few 'improvements' in the newest Quadra's and neglected to tell Symantec.

Symantec was kind enough to Express mail the patch to me. I still couldn't get it to work. Back to tech support, yes it should work, no one else is having problems, did I try..., etc. After a couple of hours of going through every permutation I could think of, tech support admitted something must be wrong plus I had noticed the dates on all the programs were 1988. Odd for a 1992 update. They sent a second patch that had the same problems.

On my final try the head of tech support personally copied the patch on to a diskette and mailed it to me. It worked! It seems that Symantec was recycling diskettes of old unsold programs and someone was putting a new label on but was forgetting to put the new programs on. Some days....

In general I seem to find it easier to customize and make changes under System 7. Adding new fonts or sounds, changing the appearance of folders or the screen are easier. I'm lucky it works because the Quadra won't allow you to use any older system like 6.07. Overall once things are working it's a fun adventure exploring the innovations that are available and experimenting with new tools.

Several new programs I've tried have been from diskettes in compressed form. They had automated installers but this seemed quite time consuming. The only real problem I had was getting the laser printer to work after automated installation of System 7. The system installed the wrong software. Luckily I had several sources available, and found one that worked on a CD from Apple.

Introducing computers to freshman classes:

After 3 years of experimenting with using the Mac in our four beginning courses we found the results were quite positive. We now introduce the use of chemistry programs to all freshman, taking about 30 minutes during the first lab period to move each lab class to a separate Mac lab. We share the computer's with the rest of the college and have had a few problems with scheduling.

Since the computers are sometimes down it would help if to have a second group of Macs in our academic learning center. They will also provide additional tutoring when our human tutors get swamped by students wanting to learn the last month's material an hour before their test.

We have over a thousand students a year who are exposed to using Macs for drill and practice, tutorials and simulations. We have a large number of students for whom English is not their native tongue, and another group who are returning to college to make themselves more competitive in the job market. Both groups are finding the programs a helpful bridge to the textbooks.

As I reported in the last issue we've had very good results in increased student ability to do chemistry problems and a concomitant increase in test scores for those students who use the programs more than a few hours. This year I have shown an overhead to my students indicating the better student results here at Union and other colleges by those who use computer programs. I have had student use of the programs jump from the 30-50% of a class to 76-92% of a class. The ability to have much of the basic drill, practice, and tutorials available on the Macs has had the pleasant side effect of having more penetrating and interesting questions asked in class. Since the programs also seem to increase student confidence in their problem solving ability more students are tackling problems beyond just those assigned. A number of students are doing all the problems at the end of each chapter in their text.

Except for the initial introduction to the Macs, use is voluntary. We make it convenient by having the Macs available from 8 AM to 11 PM and on Saturdays.

We are looking for more high quality programs that work. If you have come across any, how about reviewing it and sharing it with the rest of us.

Below are the results of putting four articles from this edition of the Newsletter through Word's grammar checker.

ARTICLE	1	2	3	4
Passive Sentences	35%	10%	4%	16%
Flesch Reading ease	35%	28%	66%	61%
Flesch Grade level	15	17	8	9
Flesch-Kincaid	13	11	8	9
Gunning Fog Index	16	10	10	12

Flesch Reading ease and Flesch Grade level are based on the average number of words per sentence and the average number of syllables per 100 words. Standard Reading ease is 60-70% at a 7-8 Grade level.
Gunning Fog Index is based on the overall sentence length and the number of words per sentence that contain more than one syllable.

"Where Chemical Formulas Never Dared to Go"
or
"Numbers as superscripts/ subscripts in spreadsheets, databases, HyperCard, ..."
Henry R. Derr, Laramie County Community College

Which of the following chemical formulas do you find more pleasing to your eye:

(1) Al2(PO4)3
or
(2) $Al_2(PO_4)_3$

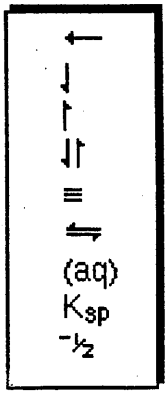
If you greatly prefer (2) and only use form (1) when you have no other choice, then read on. How about this set

(1) (SO4)2-
or
(2) SO_4^{2-}

if again you like (2) then stay tuned. Have you ever been working with a spreadsheet and wanted to place a chemical formula in a cell and had to resort to version (1)? I have, and every time I looked at it something in the back of my mind kept bothering me about it. How about a chemical database. The database applications out there do not generally support subscripting and superscripting of numbers. How about when you are using a word processor and you have to go though some kind of two or even three key sequence to activate the subscripting, you type your subscripts and then its another sequence to get back to normal text. If you have typed chemical formulas this way you know it can be a very tedious proposition.

I have found a way to type a subscripted $_2$ for example by holding down the option key and typing a 2. The technique is to use a font set which has the number already positioned as a superscript or subscript. Two different sets of modified Haber bitmapped fonts have been used. The font HaberDown will convert any number typed as normal text into a subscripted number. This has been primarily useful in converting all our chemical formulas for our inventory. The formulas are correctly displayed and printed by just changing the font used for that field. HaberOSupOdown will display a superscripted number by holding down the Option-Shift key combination and typing the number. A subscripted number is entered by holding down the Option key and typing the number.

The font set was prepared by modifying an existing font using ResEdit. Using ResEdit(available from most Mac retailers or Mac user groups), additional character types can be added or modified to suit individual needs. Characters such as those shown below can be produced using a single key stroke.



Hardware: The fonts have had been used successfully on a Mac Plus, Portable, SE20, SE30, IIci, IIcx, and IIfx computers. System software from 6.0.2 to 7.0.1 has been tested.

Problems encountered: In some applications if the unmodified Haber font is installed a conflict occurs between the modified and unmodified font.

If you would like a copy of the fonts, send a check for ~~$1000~~ $6 (NO Purchase Orders Please) to cover the cost of a 800K disk, shipping and handling to Henry R. Derr, Laramie County Community College, Cheyenne, WY 82007-3299.

The following are examples using Microsoft Works, HyperCard and Wingz.

EDITOR'S NOTE: If you're interested learning more about ResEdit, the program Henry used to make his fonts, the book 'ResEdit Complete,' by Alley and Strange, Addison-Wesley, 1991, is readable and comes with a copy of ResEdit version 2.1.

File Edit Window Organize Format Report Macro

MicroSoft Works

FontDBExample (DB)

Name	Formula	Cation	Anion
alumina	Al_2O_3	Al^{3+}	O^{2-}
aluminum ammonium sulfate	$AlNH_4(SO_4)_2$	Al^{3+} NH_4^{1+}	SO_4^{2-}
ammonium dichromate	$(NH_4)_2Cr_2O_7$	NH_4^{1+}	$Cr_2O_7^{2-}$

Henry'sHardPlace:Classes: CHM101:MolarMass

A47 Wingz

Al_2O_3	101.94	$Ca(ClO)_2$	142.99	$La(NO_3)_3 \cdot 6H_2O$	433.03	K
$AlNH_4(SO_4)_2$	237.14	$Ca(NO_3)_2$	164.10	$Pb(C_2H_3O_2)_2$	325.28	KA
$AlCl_3$	133.34	CaO	56.08	$PbCl_2$	278.12	
$Al(OH)_3$	77.99	$CaHPO_4$	136.06	$Pb(NO_3)_2$	331.23	
$Al(NO_3)_3$	213.00	$CaH_4(PO_4)_2$	234.06	PbO	223.21	
Al_2O_3	101.94	$CaSO_4$	136.14	PbS	239.28	
$AlK(SO_4)_2$	258.20	C	12.01	Pb_3O_4	685.63	

File Edit Window Select Format Options Chart Macro

D12 | Microsoft Works-Spreadsheet

FontSpreadExample (SS)

	A	B	C	D	E	F
1	Name	Formula	Cation(s)	Anion(s)		
2						
3	alumina	Al_2O_3	Al^{3+}	O^{2-}		
4	aluminum ammonium sulfate	$AlNH_4(SO_4)_2$	Al^{3+} NH_4^{1+}	SO_4^{2-}		
5	ammonium dichromate	$(NH_4)_2Cr_2O_7$	NH_4^{1+}	$Cr_2O_7^{2-}$		
6						
7						
8						
9						

MacInTestDrill2.1.7

15) **Chapter 4 Aqueous Rxns Pt 2**

The balanced net ionic equation for precipitation of $CaCO_3$ when aqueous solutions of Li_2CO_3 and $CaCl_2$ are mixed is

a) $Ca^{2+}(aq) + CO_3^{2-}(aq) \rightarrow CaCO_3(aq)$

b) $Ca^{2+}(aq) + 2Cl^-(aq) + 2Li^+(aq) + CO_3^{2-}(aq) \rightarrow CaCO_3(s) + 2LiCl(aq)$

c) $Ca^{2+}(aq) + CO_3^{2-}(aq) \rightarrow CaCO_3(s)$

d) $Ca^{2+}(aq) + 2Cl^-(aq) + 2Li^+(aq) + CO_3^{2-}(aq) \rightarrow CaCO_3(s) + 2Li^+ + 2Cl^-(aq)$

Right: 0 | Total Answered: 0 | ☐ Talk to Me

MOLECULAR MODELING WITH MOBY

Wilmon B. Chipman
Christopher White
Bridgewater State College
Bridgewater, MA 02325

For several years, students at Bridgewater State College have used PCMODEL (Serena Software, Box 3076, Bloomington, IN 47402-3076) as a part of the laboratory in the introductory organic chemistry course. We have found that PCMODEL helps students to visualize molecules in three dimensions; the program also serves as an excellent introduction to the use of molecular mechanics to calculate molecular geometry and NMR coupling constants.

Recently we have obtained a copy of a new molecular modeling program, MOBY, and a CD-ROM containing all of the structure files in the Brookhaven Protein Data Bank (both MOBY and the CD-ROM are available from Springer-Verlag NY, Inc., 175 Fifth Avenue, New York, NY 10010). This year we used MOBY to teach protein structure in a senior biochemistry course. MOBY is a powerful tool for helping students get a feel for the complexity of biopolymers.

Each student was given the amino acid sequence of a fairly small protein. First the student used the protein secondary structure prediction program, PROTYLZE (Scientific & Educational Software, P. O. Box 440, State Line, PA 17263-0440), to predict the presence of alpha helices and beta pleated sheets in the protein. PROTYLZE uses both the Chou-Fasman and Garnier-Osguthorpe-Robson algorithms to predict secondary structure. Then the Brookhaven Protein Data Bank x-ray crystallography data file of the same protein was used with MOBY to examine the actual structure and look for alpha helices and beta pleated sheets. The fact that MOBY can represent the structure of a protein in terms of a line drawing connecting the alpha carbon atoms makes it very easy for students to recognize the two types of secondary structure. Students can selectively color helices and sheets and rotate the molecule to get a better view of them. Comparing the predicted secondary structure with the actual allows students to get some feeling for the accuracy of the predictions.

Students can then represent the same molecule with increasing degrees of complexity

- Backbone only (line drawing)
- Complete structure (line drawing)
- Ball and stick model
- van der Waals radii.

It has been our experience that students have extreme difficulty in recognizing features of secondary structure in any of the latter three representations.

The software used runs on IBM PCs and compatibles and the total software cost is less than $1000. An 80X87 math coprocessor, 640 K ROM, VGA and a hard disk are essential; a 386 or 486 cpu and a mouse are strongly recommended. If you have a SUPER VGA card, such as the Paradise, MOBY supports both HIGH (800x600) and SUPER (1024x768) VGA. We have been using a NEC Multisync 3D monitor, but any system which supports VGA graphics is acceptable. MOBY uses over 500K of memory to run and requires 1MB of hard disk space.

A tutorial for students on the use of MOBY to visualize protein structures has been prepared and tested. Copies of the tutorial and a list of small proteins by their Protein Data Bank identifier are available by writing to one of the authors (WBC). We have used PROTYLZE, MOBY and the CD-ROM on one computer which was reserved for biochemistry students.

We are planning to use MOBY to allow students to investigate the active sites of enzymes and to study how restriction endonucleases interact with DNA, using files from the Protein Data Bank. MOBY uses the AMBER force field to do force field calculations on molecules of up to 150 centers in the presence of another larger molecule of up to 2000 centers. The structure predicted for the small molecule reflects all interactions, including those with the large molecule. For this reason, MOBY can be used to predict the conformation of substrates in the vicinity of the active site of an enzyme. We are investigating the use of an inexpensive reflecting stereoscope (Aldrich, Z15,675-2) to view the stereo representations that can be produced with MOBY. MOBY can do molecular dynamics simulations like the denaturation of a short protein alpha helix, and it can simulate the rotation of the side chain of an amino acid like tyrosine in a protein.

MOBY will do both MNDO and AM1 quantum mechanical calculations for molecules as large as glucose. The resulting charge distributions can be represented in user-selected colors. MOBY can read and write files that are compatible with many other molecular modeling and quantum mechanics programs and also supports a user-definable format. The next version of MOBY, now in beta testing, will be able to display the molecular vibrations that correspond to the peaks in the IR spectrum of a molecule. (Access to a version of MOPAC on a minicomputer or workstation is necessary to calculate the nature of the vibrations.) The new version will also have extended capabilities for doing very rapid rotations of molecules under control of the mouse.

Structure Drawing and Molecular Mechanics Programs.

Jim Beatty

Programs to draw structures and manipulate them are many. This listing includes only those I have literature for. There are more on the market. Upgrades are constantly being made. Prices quoted are for single academic copies. Most suppliers will send you a demonstration disk for a small charge or no charge. Some suppliers will send you programs on an approval basis. Some include minimization programs such as MM2, while for others you must purchase the program separately.

I consider these programs as word processing programs for chemical structures and more. I believe that one or more should be available to undergraduate chemistry students.

I. Tripos Associates, 1699 South Hanley Road, Suite 303, St. Louis, MO 63144-2913. Phone 800-323-2960.

Alchemey III, a powerful molecular modeling program for IBM compatibles or Macintosh computers. Prices start at about $500. MM2 available for IBM machines for $200.

LabVision, an advanced molecular modeling program for computer workstations. $2500. 30 day free evaluation available.

II. Serena Software P.O. Box 3076, Bloomington, IN 47402-3076, Phone 812-333-08232.

PCMODEL Molecular modeling for all worlds. Prices start at $200 and go up to about $4000 for programs for the fastest workstations.

III. Trinity Software P.O. Box 960, Campton, NH 03223, Phone 800-352-1282.

CHEMWINDOW, CHEMINTOSH and CHEMDRAFT III are basically structure drawing progams. CHEMDRAFT in version III has grown into a 3-D molecular modeling and presentation graphics program. Prices start at $99.

IV. Oxford University Press, 200 Madison Avenue, NY, NY 10016, Phone 212-679-7300.

Desktop Molecular Modeller for the IBM PS/2 55 compatible or above. A powerful and interesting moleular structures program which has a number of interesting options including a symmetry operator program for inorganic structures. Prices start at $495.

V. Springer-Velag New York, Inc., Electronic Media Department, 175 Fifth Avenue, New York, NY 10010, Phone 212-460-1653.

Moby is an interesting molecular modeling program for the IBM PC or compatible. Some very interesting options. Prices start at $498.

THE USE OF LINEAR LEAST SQUARES IN UNDERGRADUATE CHEMISTRY LABORATORY COURSES

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INTRODUCTION

The availability of microcomputers and appropriate software make the use of numerical and statistical methods by undergraduates readily feasible. The important question is how useful and meaningful is the use of such software by undergraduates? There is a risk that either too little or too much information about a numerical or statistical method is provided to the student. If too little information is provided, the student goes through a process which provides some computer output, but obtains no real understanding of what the information obtained means and how it is to be used. If too much information is provided, the student may become confused and frustrated. The level of instruction must be appropriate, considering the abilities and needs of the students.

Linear least squares is one of the most useful statistical methods for beginning students. In the pre-computer days it was common to include an experiment in the junior or senior level physical chemistry or instrumental analysis laboratory course which involved a linear least squares calculation. This exposed the student to the technique. Because of the amount of time required to do the calculations either by hand or calculator, it wasn't really feasible to have the student carry out more than one or a few least squares fits.

At Clarkson where every student has a computer (currently an IBM PS/2) in his (or her) own room and where there are computers in the laboratory and elsewhere on campus, I have asked students to use linear least squares software in a second semester freshman laboratory course and a second semester junior combined analytical - physical chemistry laboratory course.

In this article I will describe how linear least squares can be introduced at an elementary level. In my view it is not essential that

the least squares equations are derived by the instructor. What the student needs to understand is how the method is to be used and how the results of linear least squares calculations are to be interpreted.

Linear Equations

There are TWO different linear equations which the software must be able to fit:

$$Y = AX + B \quad (1), \text{ and}$$
$$Y = AX \quad (2)$$

Some software will only fit data to equation (1). Equation (1) is really not appropriate in some instances. For example, the dependence of absorbance upon the concentration of a single absorbing constituent is given by the Beer-Lambert Law (A = abc) which has the form of equation (2). In chromatography it is usually expected that peak height or peak area (Y) is related to concentration or amount (X) by equation (2). These are only a few examples of where equation (2) rather than equation (1) is appropriate. Very often equation (1) should be used to fit experimental data. If a substance R reacts to produce a product P and the reaction is first order in R, the integrated form of the rate expression is:

$$\ln[Rt] = \ln[R0] - kt \quad (3)$$

where [Rt] is the concentration of R at time t, and [R0] is the concentration initially (at t = 0). This is of the same form as equation (1) where Y = ln[Rt] and X = t.

Many students will use equation (1) indiscriminately because it gives a "better" fit to the data. If the purpose of the experiment is to test the validity of a theoretical or an accepted relationship which is like equation (2) (e.g. Beer's Law or chromatography equations), then equation (2) and not equation (1) should be fitted.

THE THEORY AND ASSUMPTIONS OF LINEAR LEAST SQUARES

In the least squares fitting of experimental data to equation (1) or (2), values of A and B (for equation (1)) are found such that the sum of the squares of the deviations (SSD) is a minimum.

SSD = Sum (Y(experimental) - (Y(calculated))**2 (4)

Y(calculated) is the value of Y calculated fron equation (1) (or (2)). Indeed, least squares means least sum of squares of deviations (SSD).

While students may not realize it, they are already familiar with a least squares calculation. The average of a series of measurements is a least squares value.

Implicit in the assumption that the least squares calculation gives a "best fit" to the data are the assumptions that there is little or no error in X and that the error in Y is independent of the value of Y and is normally distributed. (Normally distributed errors give rise to the typical bell-shaped curve. Small errors in Y are more likely than large errors and positive and negative errors are equally likely.) In discussing errors in Y we are considering random errors. Where equation (1) is being fitted, residual errors in Y will affect the Y intercept, B, but not the least squares value of the slope, A.

The assumption that the magnitude of the error in Y is independent of the value of Y is implicit in the method of unweighted least squares. Where this assumption is not valid, it is possible to use weighted least squares methods. While such calculations are relatively simple to perform, the topic and related techniques are too confusing to introduce at a beginning level.

INFORMATION WHICH SHOULD BE OBTAINED FROM THE LEAST SQUARES CALCULATIONS AND HOW THIS INFORMATION CAN BE USED

In addition to obtaining the least squares slope, A, and intercept, B (for equation (1)), there are a number of other statistics which a satisfactory least squares program should provide. Typical output obtained with the program used at Clarkson is shown below:

This is simulated kinetic data least squares fittedusing equation (3) where EXPT X is the time in seconds and EXPT Y is ln[Rt] obtained from experimental measurements. Ideally, more experimental points would be obtained. Only a few points are used in this calculation to conserve space and make it easier to check some of the calculations.

(If the data had been fitted to equation (2), which is obviously inappropriate, the SLOPE would be -2.80E-03, S.D. SLOPE is 5.41E-04 and S.D. REG is 2.963.)

One of the most important statistics obtained is the standard deviation from regression (S.D. REG). The standard deviation from regression is the square root of the sum of the squares of the deviations

EXPT X	EXPT Y	CALCD Y	DIFFERENCE
1000	-6.990	-6.992	2.0E-03
2000	-7.710	-7.699	-1.1E-02
3000	-8.390	-8.406	1.6E-02
4000	-9.120	-9.113	-7.0E-03

LEAST SQUARES SUMMARY

SLOPE = -7.07E-04 S.D. SLOPE = 6.56E-06

INTERCEPT = -6.285 S.D. INTERCEPT = 0.0180

S.D. REG = 1.47E-02

(SSD) divided by the number of degrees of freedom and can be represented by the equation:

S.D. REG = SQR (SSD/(N - NLSP) (5)

where N is the number of data points, and NLSP is the number of least squares parameters (constants), which would be 2 (A and B) for equation (1) and 1 (A) for equation (2). For the data given above SSD is 4.30E-04 and S.D. REG is the square root of 4.30E-04 divided by 2 which is 1.47E-02.

The standard deviation from regression is to be understood as the "average" difference between the experimental and calculated value of Y. Perhaps the most important question to be answered from the results of any linear least squares calculation is: "Is there really a linear relationship between Y and X?". Is the reaction really first order? Is absorbance linearly related to concentration? Is peak height linear related to the amount of a particular constituent present? One means of deciding whether the results of the least squares calculation are consistent with the hypothesis that the reaction is first order is to compare the standard deviation from regression with an estimate of the random error in Y (ln (Rt)). If the standard deviation from regression is comparable to the estimated random error in Y, this is consistent with the hypothesis there is a linear relationship. If SD(reg) is much larger than the estimated error in Y, the data do not support the idea of a linear relationship. (The F test (reference (1)) can be used to provide probabilities but this is unnecessarily complicating at an elementary level.)

A linear least squares program can be used to fit a straight line to ANY set of data. The fact that a least squares fit is obtained does not prove there is a linear relationship. The standard deviation from regression provides some information. Another source of information is the deviation pattern. Suppose the relationship between y and x is really logarithmic and the data is fitted to a straight line. There will be positive (or negative) deviations at small and large values of X and negative (or positive) deviations in the middle. The presence of such a pattern suggests that there really isn't a linear relationship. Thus, looking at the signs and magnitudes of the deviations may suggest a non-linear relationship. Conclusions based upon the deviation pattern are generally only possible when many points are available.

Students should be asked to plot the data and least squares line in addition to performing least squares calculations. Such plots should initially be done by hand. Students have a lot to learn about the proper plotting of data (scaling, labelling, representing experimental points and least squares lines). The plots help to identify points which are far removed from the "best" line or curve. Systematic deviations or curvature may be revealed by such plots. At a later stage students should learn to use appropriate plotting programs. In the junior level course students were required to use a plotting program. Such programs save time and computer generated plots are generally used in the real world.

If it has been determined that the data are adequately fitted by a linear equation, the least squares constants and their standard deviations are then examined. For the kinetic data, once it has been established the reaction is first order in R, the slope gives the first order rate constant and has a value for the sample data of 7.07E-04 1/sec. S.D. SLOPE can be used to estimate the random error. At the 90% level of certainty, the random error in the rate constant is 0.19E-04 1/sec (2.92 X 6.56E-06 t-test (reference (1)). (The half life is 980 + 26 sec.) The Y intercept is - 6.285 ([R0] = 1.86E-03 M). S.D. = 0.0180. The random error in Y is 0.053 at the 90% level.

Sometimes it is the slope and sometimes it is the Y intercept which is the more important result of the least squares calculation. Generally, when equation (3) is used, it is the rate constant (or slope) which is of most interest.

In the junior level course at Clarkson students prepare Nylon 66. The viscosity of several different Nylon 66 solutions is measured. A functions of the measured viscosity is plotted versus concentration (reference (2)). Extrapolation to zero concentration (the Y intercept) gives the intrinsic viscosity. In the experiment, the extrapolation and determination of the Y intercept (intrinsic viscosity) was determined from two different least squares calculations. The average molecular weight of the polymer is calculated from the intrinsic viscosity. S.D. INTERCEPT can be used to estimate the random error in the molecular weight.

As explained above, S.D. REG is used to decide whether the data are satisfactorily fitted by the expected linear equation. If S.D REG is much larger than the estimated error in Y, it is concluded either that the data is not adequately fitted by the linear equation or that the estimated error in Y is incorrect. Perhaps some other equation is appropriate and/or some of the assumptions leading to the expectation of a linear relationship are not valid. For example, in the kinetics experiment the forward reaction might not be first order, there may be a back reaction, the temperature may not have been maintained constant, there may be unsuspected errors in the estimation of [Rt]. It may not be appropriate to consider too many complications, particularly when students are at an elementary level.

For one kinetics experiment performed at Clarkson, students are asked to determine whether a reaction is zeroth order, first order or second order in R. A different linear equation can be written for each case and a least squares calculation performed. Students are asked to draw conclusions using the results of each least squares calcula-

tion.

SUMMARY - SOME IMPORTANT QUESTIONS

Some questions which need to be considered by students in performing and analyzing the results of experiments:

(1).What is the expected or theoretical relationship between the variables (X and Y)?

(2) Are there other variables or equations which need to be considered? For example, the temperature may need to be measured and kept constant in a kinetics experiment. Absorbance may be used to monitor concentration and it must be confirmed (or assumed) that the system conforms to Beer's law.

(3) What are the values of the least squares constants and their standard deviations? What is the standard deviation from regression?

(4) What are the assumptions made in performing the least squares calculations? Are these assumptions correct?

(5) What is the estimate of the random error in Y? Have all important sources of random error been considered in estimating the random error in Y?

(6) Is the theoretical or expected equation consistent with the results of the least squares fit?

(7) If the answer to (6) is yes, what can be concluded from the results? For example, the reaction is first order in R. The numerical value of the rate constant is --- and the random error in the rate constant is ---.

(8) If the answer to (6) is no, what conclusions can be drawn? This is usually a more difficult question to answer.

(9) What additional experiments might be useful?

THE LINEAR LEAST SQUARES PROGRAM

Any least squares program which will fit either of the two equations and provides the other statistics is satisfactory. The linear least squares program used at Clarkson was developed over a period of years. It was originally written in FORTRAN for a main frame computer. The current version is available in BASIC and runs on a microcomputer. For anyone interested in the program, a source listing will be available on the Chemistry Education Discussion List (CHEMED-L) on June 1 and September 1, 1992. (For information on CHEMED-L look elsewhere in this Newsletter.) Those without access to CHEMED-L may obtain a listing of the program and an ASCII source file on either a 5 1/4 inch or a 3 1/2 inch disk (if desired) by sending $ 3 to me.

REFERENCES

(1) G. W. Snedecor and W. G. Cochran "Statistical Methods", 8th edition;Iowa State University Press, Ames IA, 1989.

(2) D. P. Shoemaker, C. W. Garland, and J. W. Nibler, "Experiments in Physical Chemistry", 5th edition, p. 370-380; McGraw Hill, New York, 1989.

Call for Papers:

COMPUTER DEMONSTRATIONS IN THE CLASSROOM AND LABORATORY

Users of computers in the classroom and laboratory continue to explore avenues for expanding the learning environment of students. The computer provides visual communication of ideas which heretofore required the use of expensive equipment, editing and production facilities and a considerable amount of time and effort. With the speed and graphic capabilities of today's desktop computer it is possible to write, edit and produce a computer/video demonstration with limited financial resources.

The Division of Chemical Education's Committee on Computers in Chemical Education is soliciting such computer demonstrations to be presented at the National ACS meeting in Denver, CO., Wednesday evening, March 31, 1993. This session will publicize the uses and capabilites of commercial and locally developed software and hardware. These interactive "poster-like" sessions will consist of a "show and tell" type environment on PC or Macintosh platforms. Other platforms or PC/Mac platforms requiring specialized hardware are invited with the presenter providing the required hardware.

Anyone interested in participating in the session should send their name, address and phone number together with a tentative title and platform type to one of the addresses listed below:

M. Lynn James, Dept. of Chemistry and Biochemistry, University of Northern Colorado, Greeley, CO 80639 (303) 351-1285; or Henry R. Derr, Dept. of Chemistry, Laramie County Community College,1400 E. College Drive, Cheyenne, WY 82007-3299,

(307) 778-5222; Internet: HDERR@CORRAL.UWYO.EDU

Software we use

Tom O'Haver, Department of Chemistry and Biochemistry, Univ. of Maryland, College Park, MD 20742. toh@umd2.umd.edu

In the last few years we have reviewed quite a lot of microcomputer software that is either aimed specifically at chemistry instruction or might be adapted to that purpose. Not everything we have bought has actually been used by our instructors, however. Here is a brief pictorial survey of some software that has turned out to be useful in our teaching program over the last two or three years. Lack of inclusion in this survey does not mean that a program is not good or useful, but only that it has not yet been "discovered" by our instructors. (Macintosh versions of the the programs are illustrated here, but IBM-PC versions of most of these programs are also available).

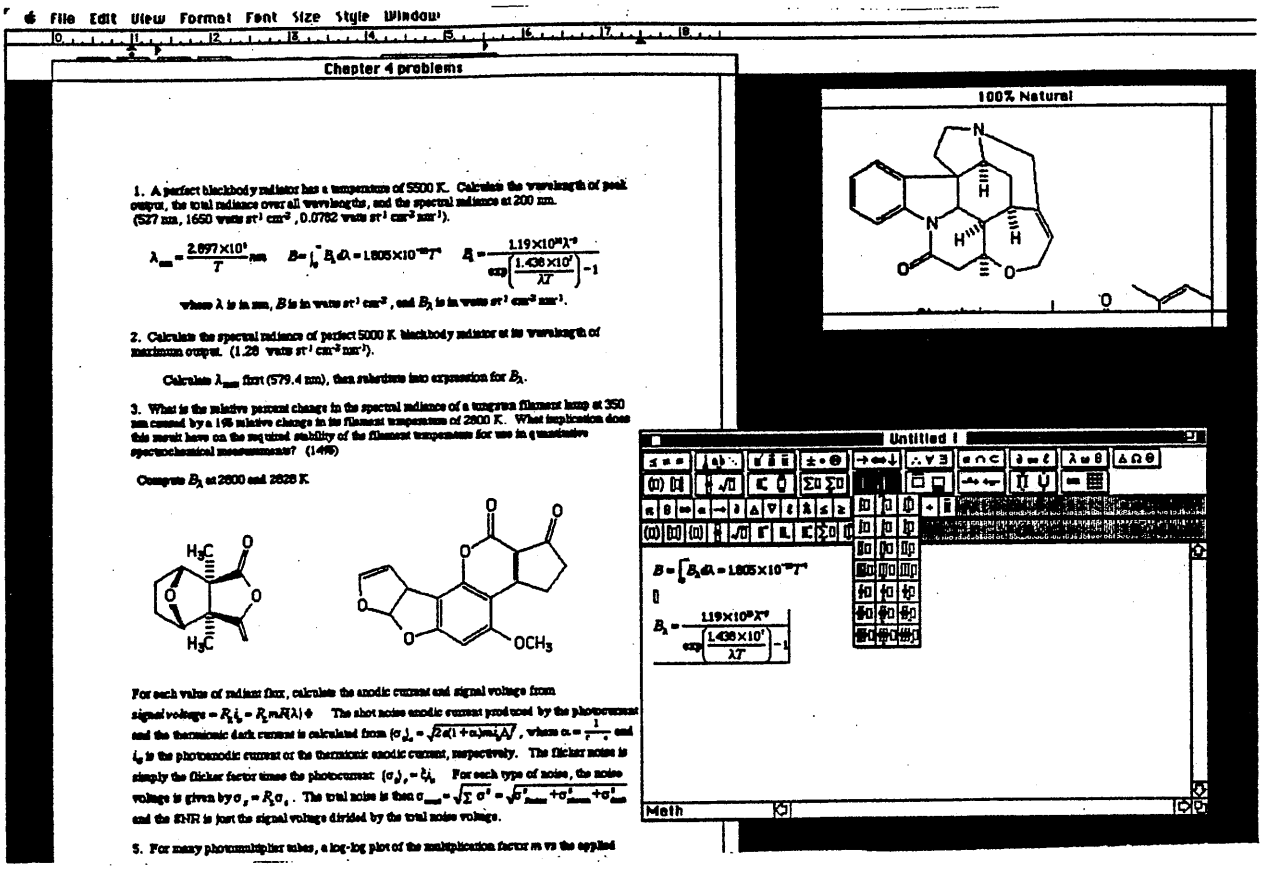

Figure 1: Word Processor with *MathType*

Most people probably spend more time doing document preparation than any other single computer application. For a chemist this means not only word processing, but also structure drawing and equation formatting. Although there are a few specialized word processors for chemists, we have elected to use popular general-purpose word processors (e.g. *WordPerfect*, Microsoft *Word*) in conjunction with a separate chemical drawing program for structure drawing, such as the popular *ChemDraw* (Cambridge Scientific Computing, Box 2123, Cambridge, MA 02238. 617-491-6862) and an equation editor for math expressions. The topmost window in this screen shot is *MathType* (Design Science, Inc., 6475-B E. Pacific Coast Hwy, Ste. 392, Long Beach, CA 90803), a very easy to use pop-up math equation editor available for Windows and Macintosh. In a window environment, copy and paste operations are used to integrate these parts into the document. Although we neither require nor provide instruction in these applications, they have now become easy enough that most students pick them up by watching other students or by going through the publishers' tutorials. By the time they are juniors, almost all students routinely use computers to prepare their lab reports and writing assignments.

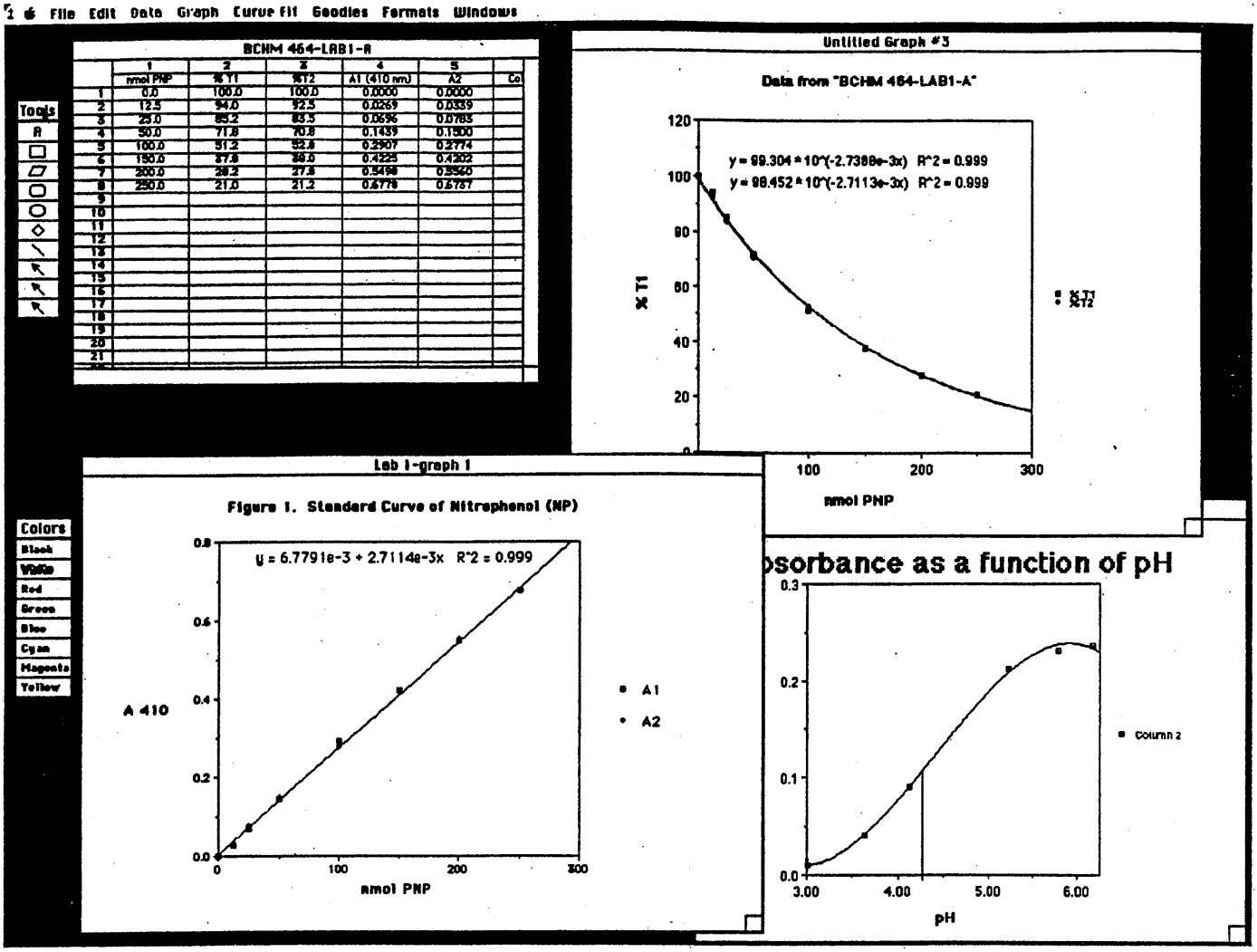

Figure 2: ***CA-Cricket Graph***

Our first actual assignments that require computer use are based on plotting and curve fitting of laboratory data. Such assignments are made in the sophomore organic lab (an Arrhenius plot/activation energy experiment), in the biochemistry lab (an enzyme kinetics experiment), and in several other courses. There are of course lots of data plotting programs, including many powerful ones. The particular program we use most often is *CA-Cricket Graph* (Computer Associates International, 10505 Sorrento Valley Rd., San Diego, CA 92121, 800-531-5236) available for Windows and Macintosh). It is probably the easiest to use of all the data plotting programs, yet it provides the essentials for basic scientific plotting (log axes, error bars, curve fitting, arrows and labels, etc). The program is very popular with students at all levels, although more advanced users eventually move on to more sophisticated programs.

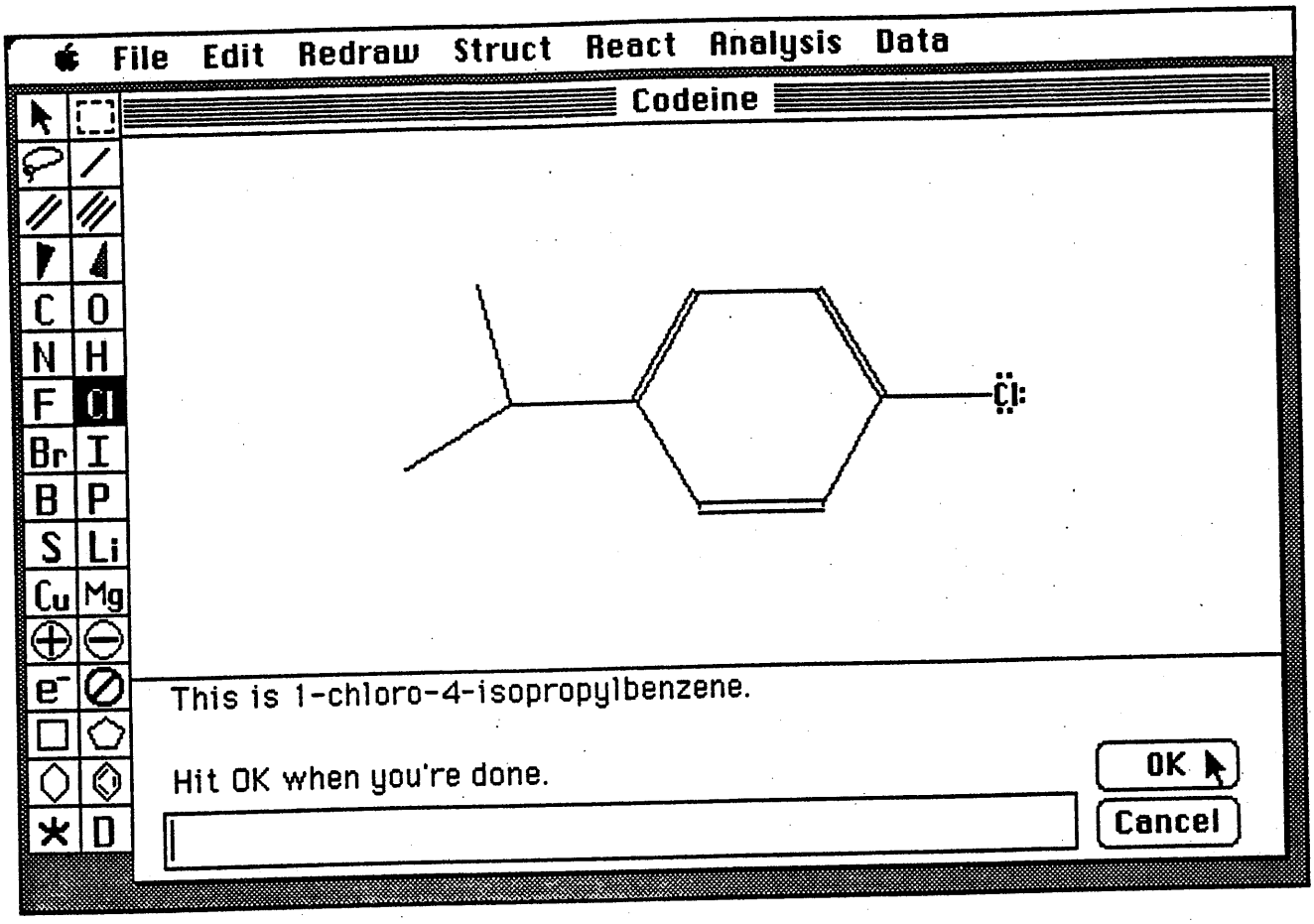

Figure 3: *Beaker*

For elementary organic chemistry, some of our instructors have used *Beaker 2.0* (Brooks/Cole Publishing Co., 511 Forest Lodge Rd., Pacific Grove, CA 93950, 408-373-0728), a kind of rule-based expert system for organic chemistry students. This a remarkable program; it can, for example, draw a 2D structure of any molecule whose IUPAC name is typed in by the student. Conversely it can give the IUPAC name of a structure drawn by the student, using this set of drawing tools. It can draw resonance structures, Lewis dot structures, Newmann projections and calculate the distribution of rotamers, and much more. Beaker also allows one to perform reactions with some of the standard reagents, showing and explaining the mechanisms, even allowing reactants to be isotopically labeled. However, my organic colleagues tell me that the rule set is not sufficiently comprehensive, with the result that the program makes too many "mistakes" and tends to confuse students. Therefore we do not use this particular part of the program. There is also no way for the instructor to add to the knowledge base of the program (a common complaint about much commercial software). Nevertheless, Beaker is a very innovative program that challenges our conceptions of what chemistry educational software can be. It is also worth pointing out that Beaker is extremely inexpensive, costing less that many textbooks, and low-cost network license make it affordable to the largest networks.

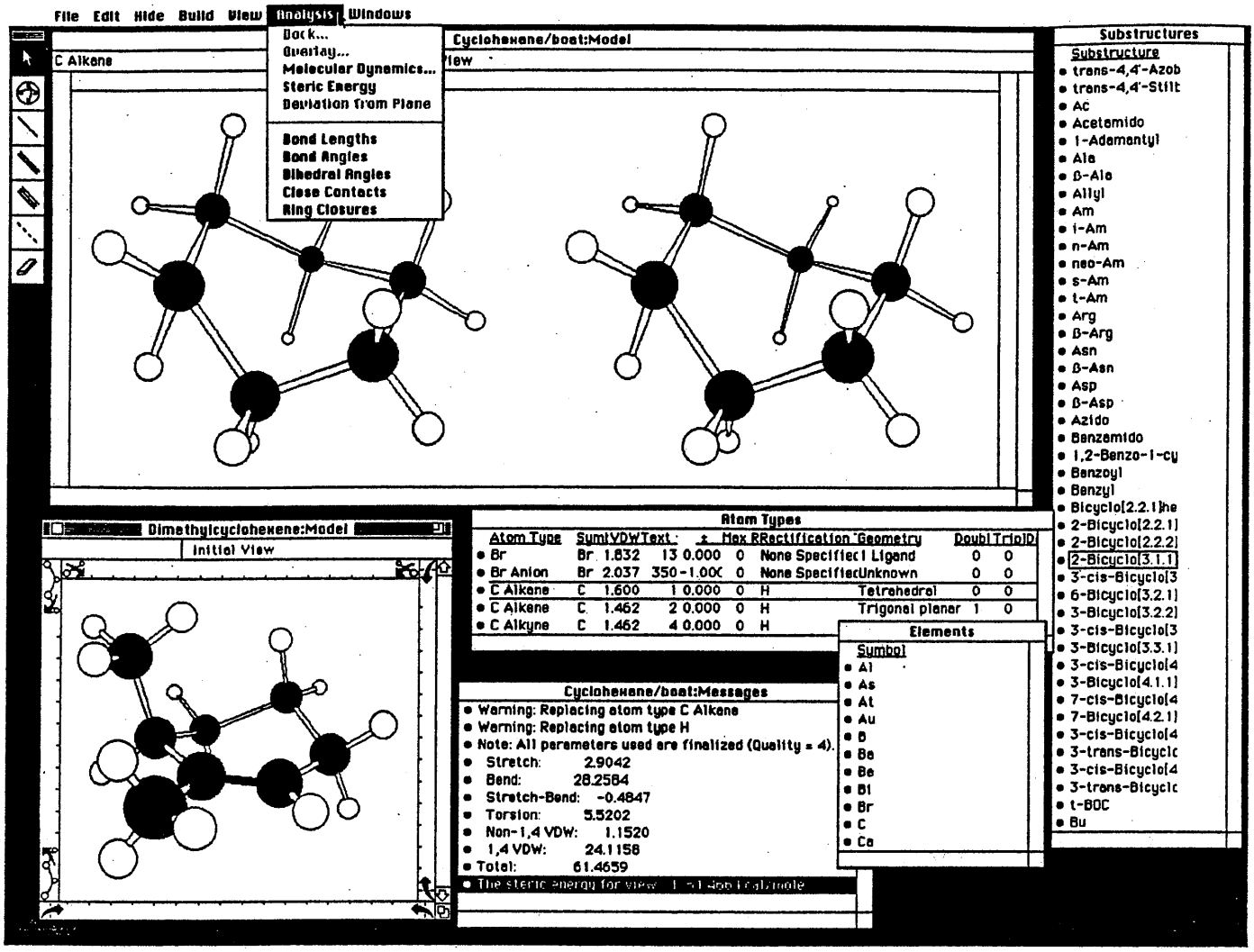

Figure 4: ***Chem 3D Plus***

Molecular modeling is introduced in our sophomore organic chemistry course. Students use *Chem 3D Plus*, a molecular mechanics package that supports point-and-click model construction, a library of pre-built substructures, rotation, display of wire frame, ball-and-stick, or space filling models, stereo pairs, and energy minimization with a simple MM2 force-field (Cambridge Scientific Computing, Box 2123, Cambridge, MA 02238. 617-491-6862). Using this program, students observe the effect of structure and substitution on molecular conformation, compare steric energies of different conformations, explore the conformational space available to a molecule, and discover preferred (lowest-energy) conformations. The program can also compute molecular mechanics trajectories – animating the molecular motion on a femptosecond time scale as a molecule is "heated" and "cooled".

Microcomputer-based molecular modeling software is easy to learn and use but is naturally limited in power compared to professional workstation-based software. Nevertheless, these programs are satisfactory for an introduction to molecular modeling, particularly with medium size molecules. Even faculty and graduate students who have access to more sophisticated molecular modeling workstations still use such program as a convenient way to obtain attractive black-and-white molecular graphics for publications and for slide and overhead presentations.

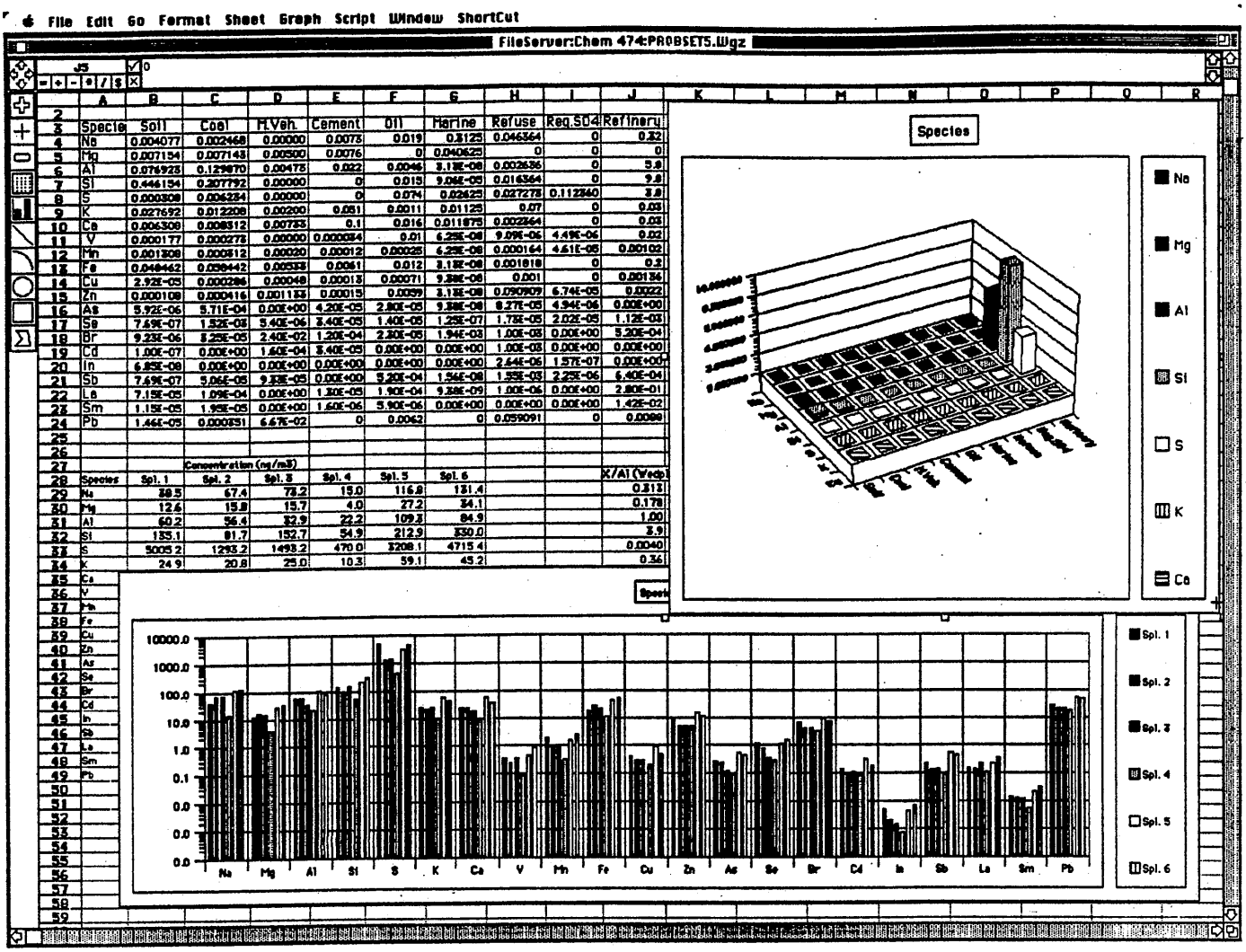

Figure 5: *WingZ*

In our environmental chemistry course, students use a spreadsheet (*Wingz*, available for Windows, OS-2, Macintosh, Unix; Informix Software, Box 15998, Lenexa, KS 66219, 913-492-3800) to work with large atmospheric pollution data sets provided by the instructor. Their objective is to use elemental analytical data on suspended particulates to determine the relative contributions of several pollution sources, such as soil, coal- and oil-fired power plants, motor vehicles, etc. Modern spreadsheet programs are excellent tools for performing basic data processing calculations and for viewing large data sets graphically that would otherwise be hard to interpret.

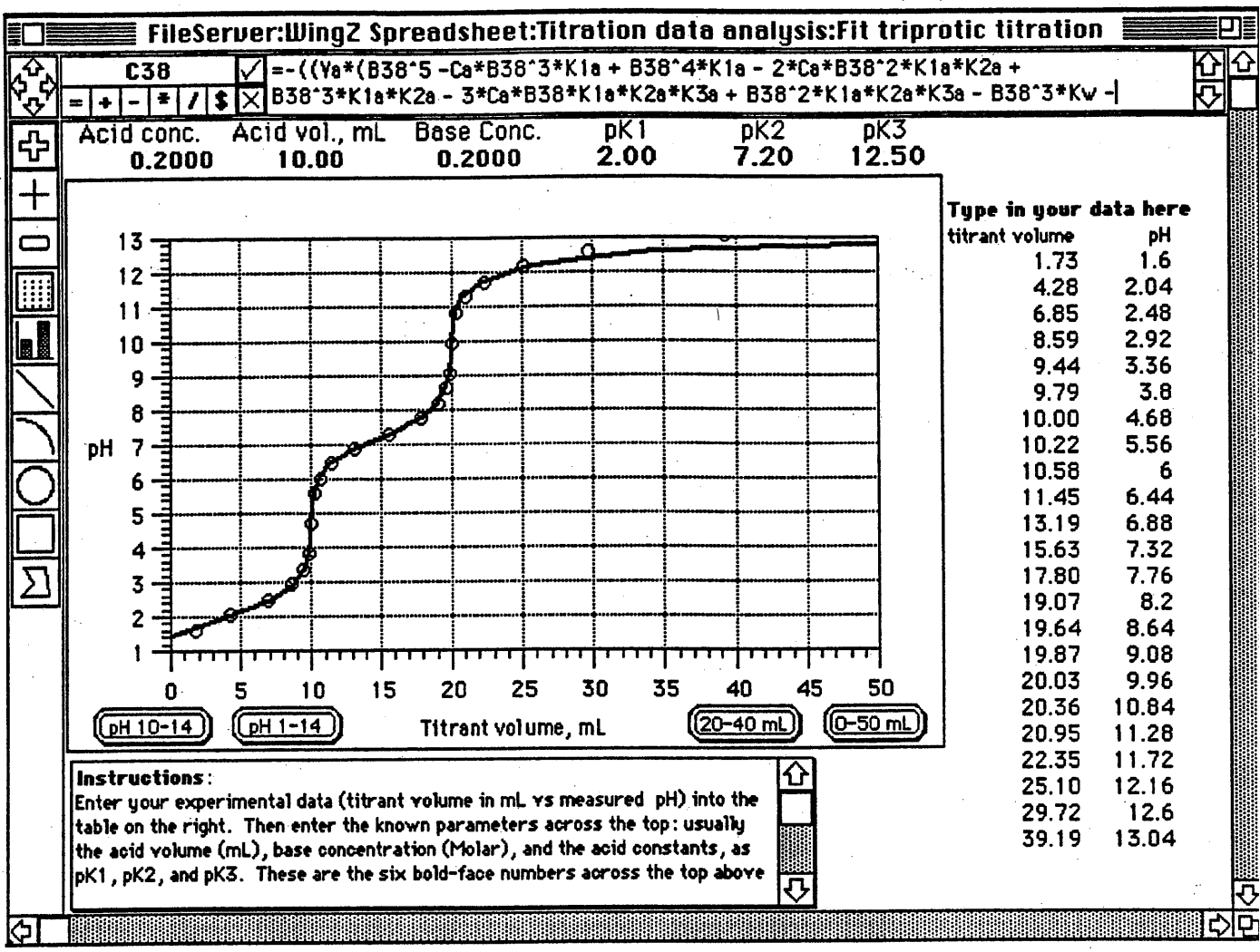

Figure 6: Titration data analysis in *WingZ*

Students in an undergraduate analytical course use a spreadsheet as a modern alternative to the traditional methods of analyzing titration curves. After performing a pH titration of a weak polyprotic acid, they type their pH/titrant volume data into a spreadsheet that contains an exact algebraic model of the titration curve (ref JCE article by Adon Gordus). For a triprotic acid, that is a quintic equation — too complex to evaluate by hand but easy for a spreadsheet to handle. By adjusting the parameters of the model and observing graphically the fit between the experimental data (circles) and the calculated model (line) they can estimate the unknown parameters, such as the pKs of the acid. A dynamic model like this allows interactive investigation of such questions as: "What is the weakest acid that gives a discernible inflection at the endpoint?", or "Can titration be used at trace concentration levels by using a very dilute titrant?", or "Is the inflection point always exactly at the equivalence point?"

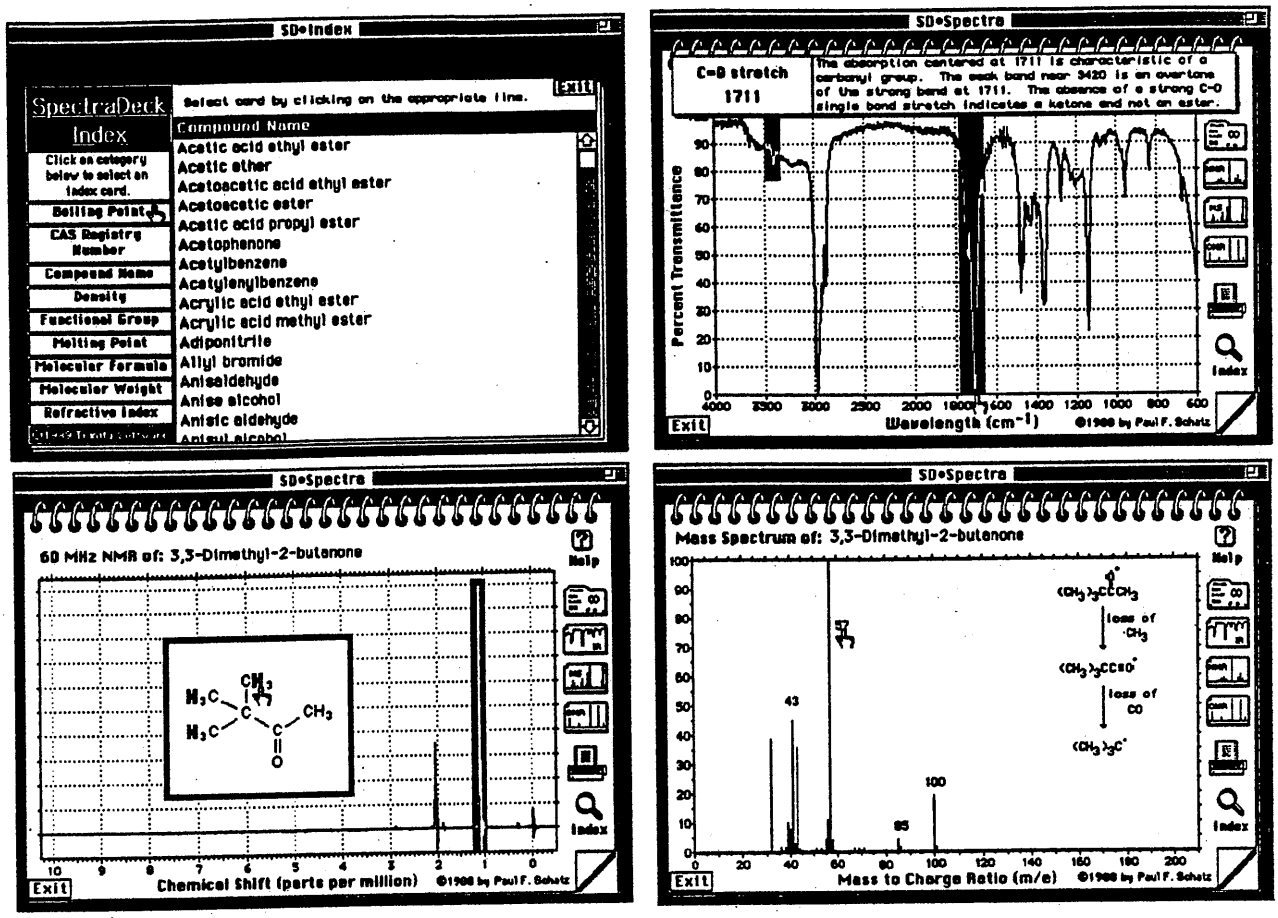

Figure 7: ***SpectraDeck***

Our organic chemists have found Paul Schatz' *SpectraBook/SpectraDeck* (Trinity Software, Box 960, Campton, NH 03223) to be very useful for teaching proton and carbon NMR, IR, and MS structure-spectra correlations to organic students. It comes with a database of compounds that are keyed to their physical properties (upper left) and their IR, proton NMR, carbon NMR, and mass spectra. The dynamic links between spectral features and the molecular structure provide a completely new and very dramatic way of interacting with this material. For example, clicking on any peak in the carbon NMR spectrum highlights the corresponding carbon in the molecular structure drawing. Conversely, clicking on a carbon in the molecular structure highlights the band generated by that carbon. Clicking on a peak in the mass spectrum displays the ion or fragmentation sequence that resulted in that peak (lower right).

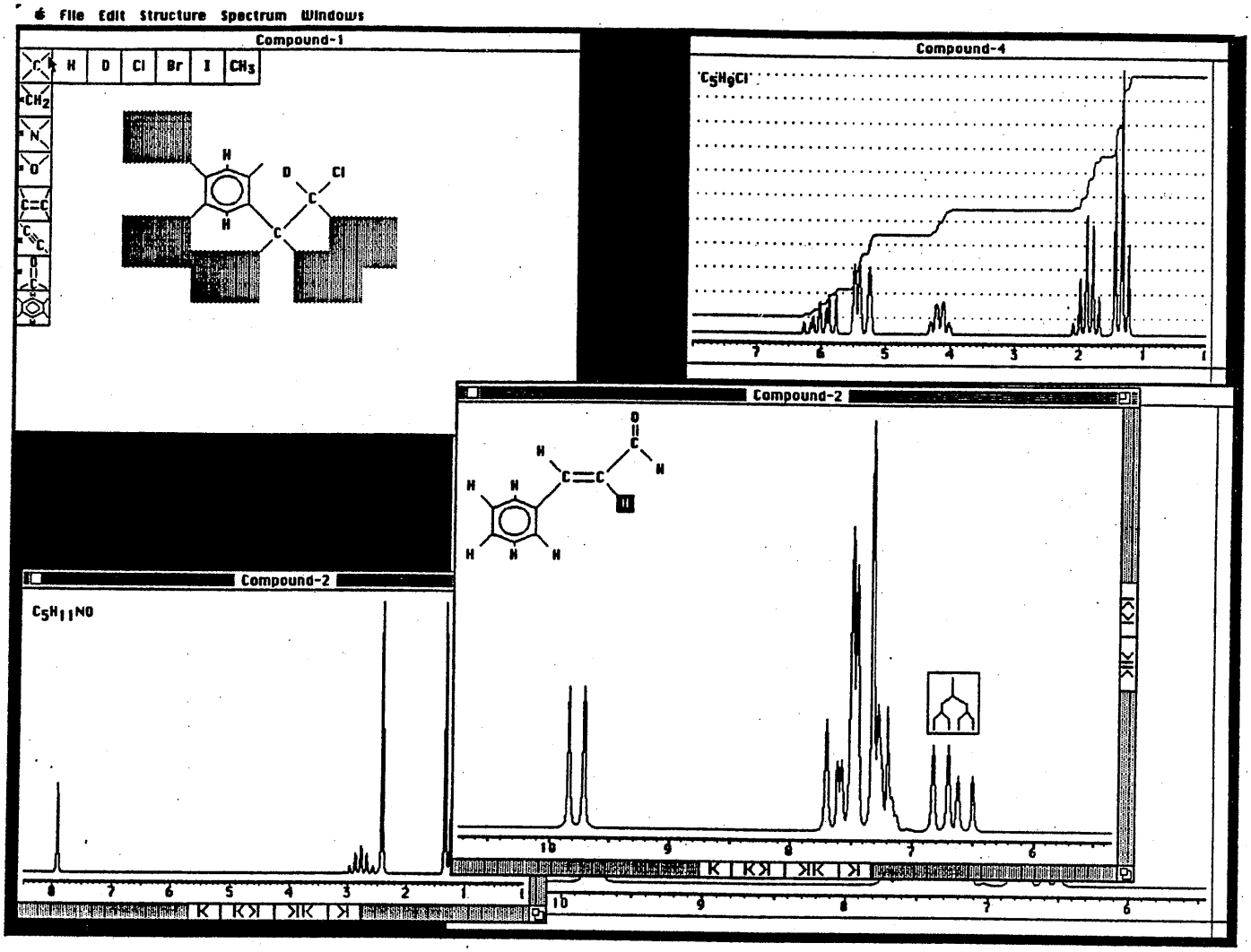

Figure 8: ***Proton NMR Simulator***

A more open-ended tool for teaching proton NMR structure-spectra correlations is Kersey Black's award-winning *NMR Simulator* published by JCE Software (Kersey Black, *Proton NMR Spectrum Simulator, JCE Software*, **1990** , Volume IIc, No. 1). The program provides a set of drawing tools (upper left) with which a student can draw a wide range of molecular structures, then calculates the proton NMR spectrum by means of a rule-based algorithm that estimates chemical shifts and coupling constants, taking into account the field strength of the spectrometer (which can be selected by the user). Spectra can be scale-expanded on the x and y axes, integrated (upper right), and annotated with a structural diagram of the molecule (lower right). Clicking on a hydrogen in the molecular structure indicates the multiplet generated by that hydrogen, and clicking on any peak in the spectrum highlights the corresponding hydrogen in the molecular structure drawing. The program also allows the instructor to prepare "unknowns" in the form of spectra (with or without the empirical formula) for students to identify.

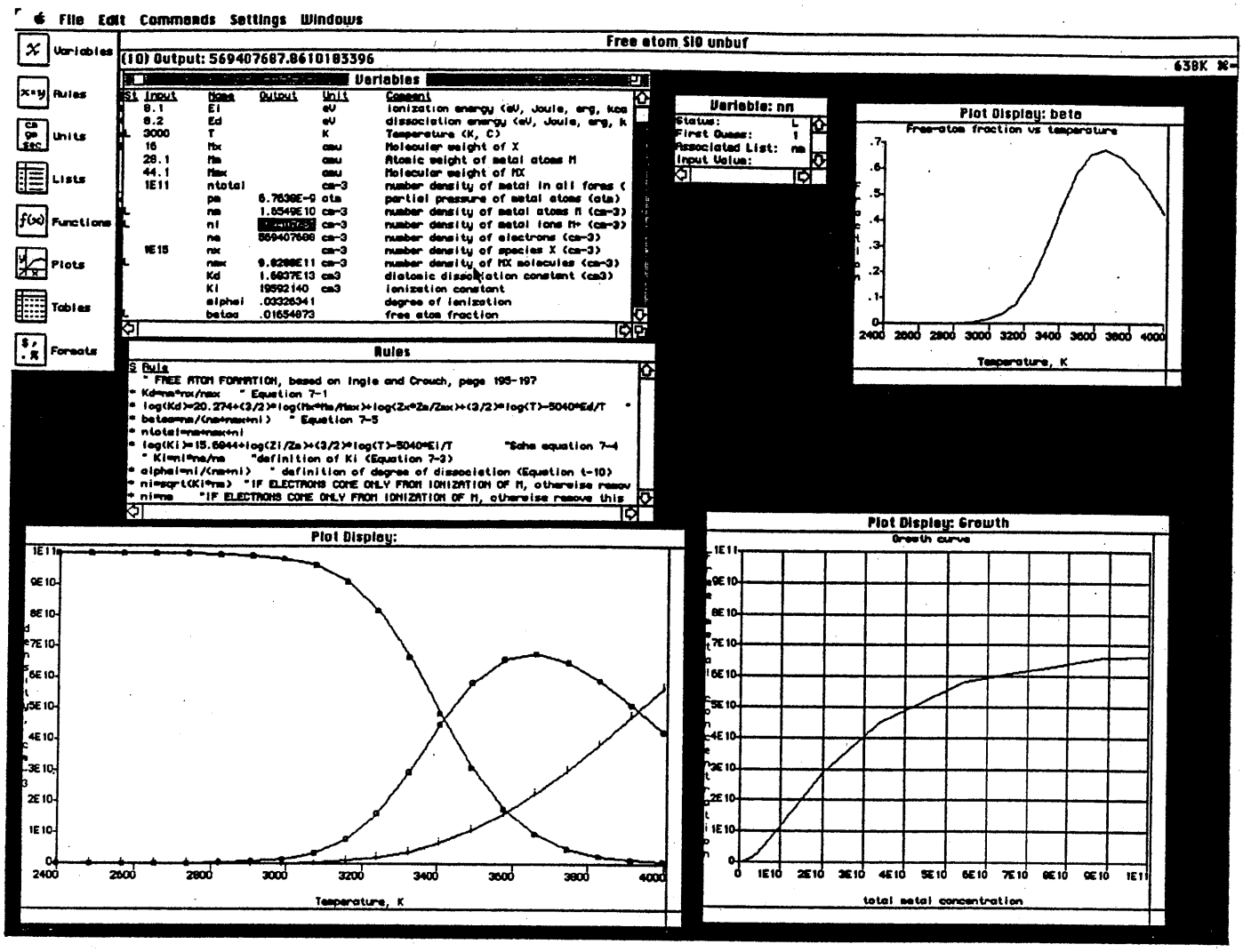

Figure 9: ***TK Solver Plus***

This is *TK Solver Plus*, a declarative numeric equation solver (available for the IBM-PC and Macintosh; Universal Technical Systems, Inc., 1220 Rock St., Rockford, IL 61101, (815) 963-2220). The difference between an equation solver and a spreadsheet is that an equation solver is capable of doing the algebraic substitutions needed to solve a problem without having an explicit algebraic expression for the unknowns. This example was constructed for a class in analytical spectroscopy. It models the gas-phase equilibrium behavior of silicon in high temperature flames and plasmas, where free Si atoms are in equilibrium with Si^+ ions and SiO diatomics. The objective is to determine the temperature at which the free Si atom density is greatest. To construct this model you need only type in the eight defining equations into the "Rules" window (left center). The variables in those equations are automatically extracted and listed in the "Variables" window (upper left). Then you enter all known parameters in the Input column of the Variables window. The program will then attempt to solve the model for the unknowns (those variables without values in the Input column) by substitution or by iteration. You can also create a list of temperatures and the program will solve the model for each temperature and plot the results (lower left). An equation solver allows the focus to be kept on the chemistry and not on the mathematical methods required for solution.

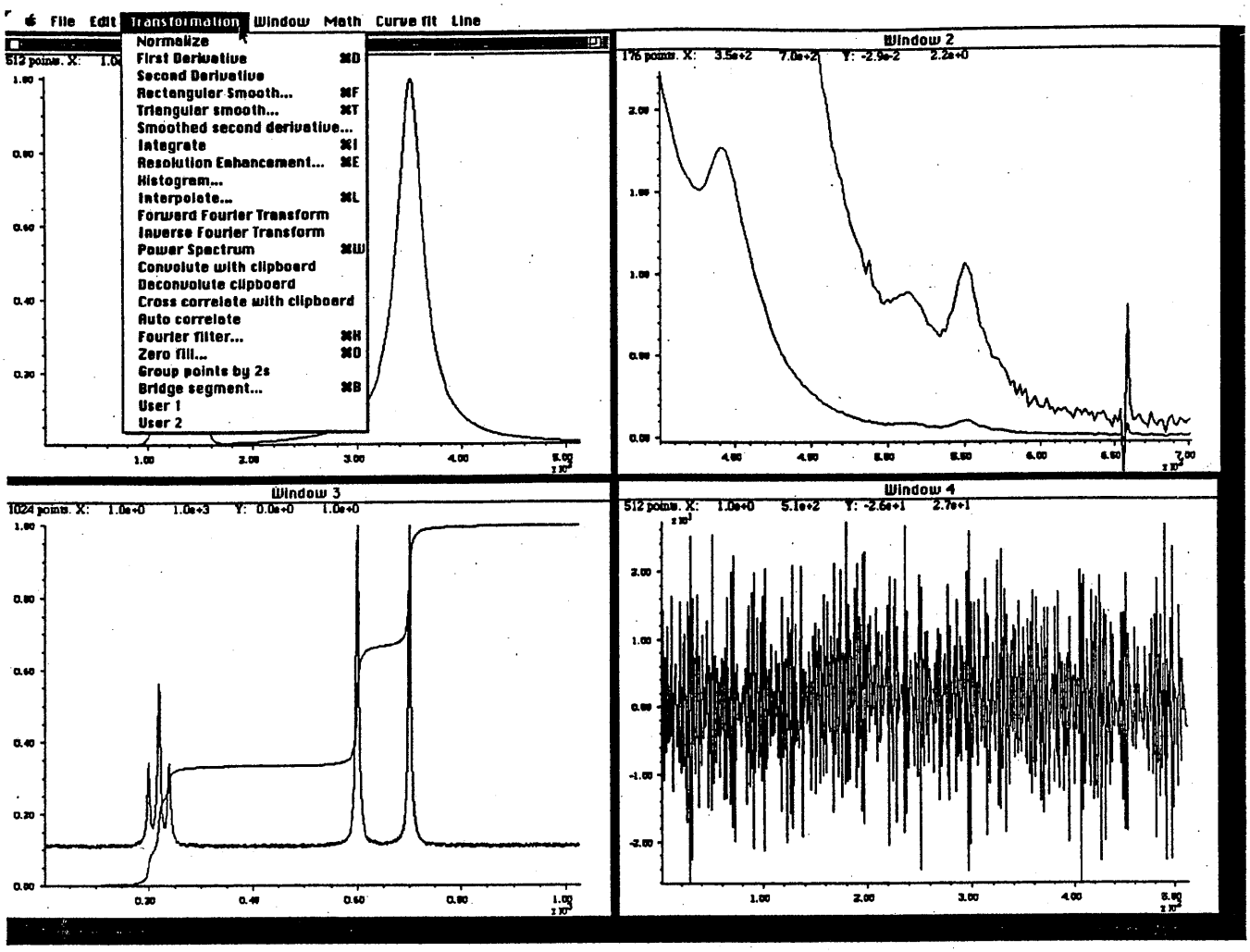

Figure 10: ***SPECTRUM***

Can electronic distribution of the UV, IR or NMR spectra of student unknowns be used as the modern tree-saving alternative to hard-copy distribution? If you have a text file containing the x and y values — of, for example, a spectrum or a chromatogram — there are lots of ways to use a computer to plot those data, using a spreadsheet or plotting program. Most ways require several steps, however....it's not as direct as opening a text file in a text editor. *SPECTRUM* (Office of Technology Liaison, Lee Bldg., Room 2114, University of Maryland, College Park, MD 20742, 301-405-4209, FAX 301-314-9569) requires only a single step to display a graph of a text data table (in single column y-only format or space- or tab-delimited two-column x-y format). The program provides a simple means of x- and y-axis scale expansion (zoom and scroll) for detailed inspection and mouse-controlled cursors for measuring peak positions, heights, and areas. There are additionally a large number of digital signal processing operations that can be conveniently applied.

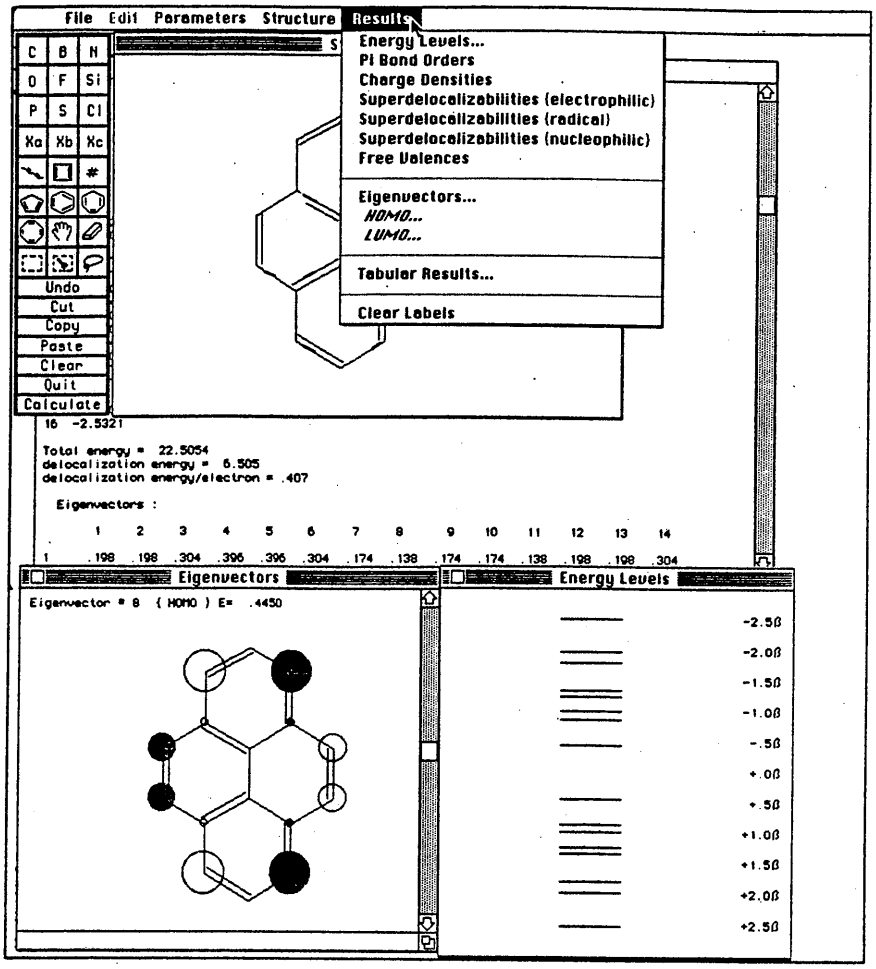

Figure 11: ***HMO 1.1***

The cost of commercial software is often a problem, particularly if one needs a number of copies for use by a large class or lab. Although some commercial software stands out as a real bargain (e.g. Brooks/Cole's *Beaker*), it's hard to beat public domain software and freeware, which costs nothing, and shareware, which costs very little. There is a huge amount of freeware and shareware, but only a tiny fraction of it deals with science. To help, I have put together a catalog of several hundred science/math/engineering public domain software and shareware programs for MS-DOS and Macintosh computers. These programs are available for the cost of downloading from commercial information services, such as Compuserve (800-848-8199), GEnie (800-638-9636) and America On Line (703-448-8700), and from several Internet archives. For those with Internet access, the list is available by anonymous FTP from ra.nrl.navy.mil (128.60.0.21) as MacSciTech/info/PD_Science.txt (and, for Mac users, in self-extracting compressed form as PD_Science.sea.hqx). For those with modems but no Internet access, it is available on GEnie in the IBM-PC libraries as PD_SCI.TXT (file number 24876) and on America OnLine in Computing & Software/Business/Special Interest Groups/Science, Engineering and Mfg. SIG/Science, Engineering and Mfg. library/ Science Public Domain Catalog.

The example shown here is HMO 1.1, a very nice public domain Hückel molecular orbital program for the Macintosh. It is available from GEnie (HMO1.1.SIT, file number 19659) and from ra.nrl.navy.mil in the MacSciTech/chem directory. Another useful program, this one for the IBM-PC, is teddemo.zip, an animated gas kinetics simulator available from meap.uta.edu in the /pub directory.

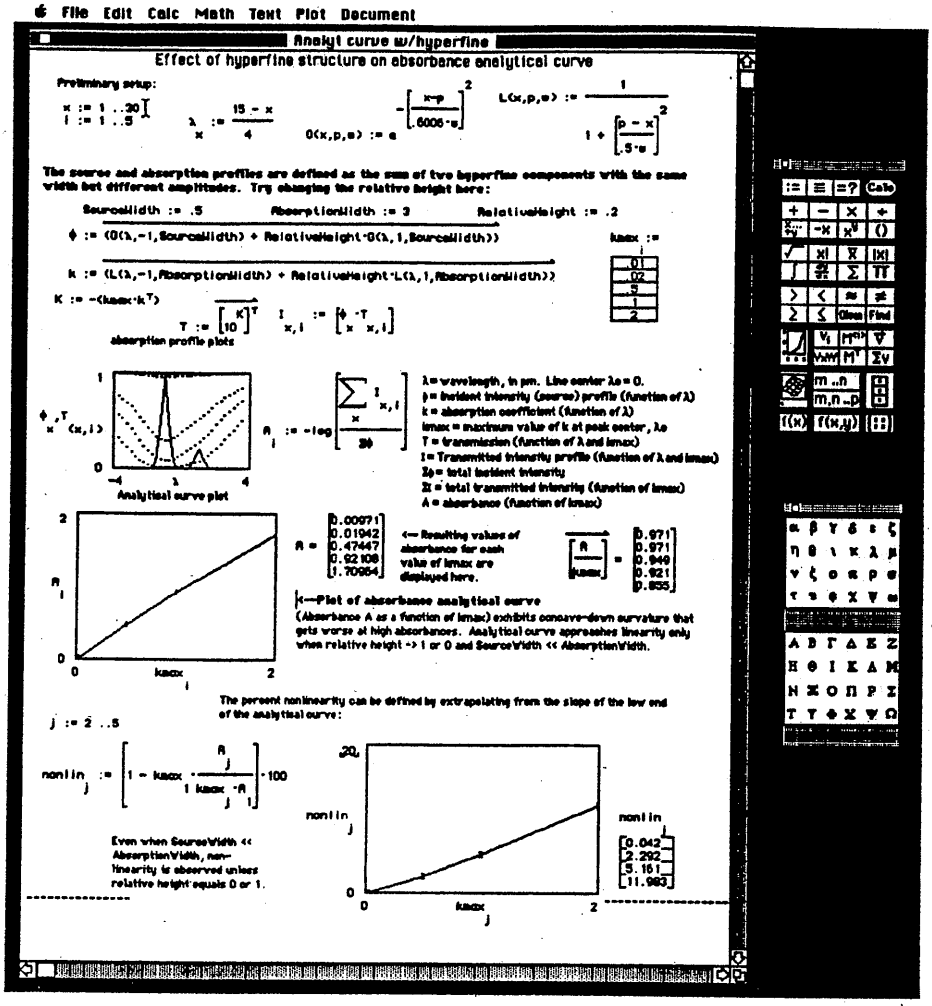

Figure 12: ***MathCAD***

MathCAD (MathSoft, Inc., 1 Kendall Sq., Cambridge, NA 02139) is an environment for developing and delivering on-screen documents that integrate text, mathematical equations, and graphics. MathCAD documents are presented in an interactive "live document" screen format that automatically recalculates and re-plots graphs when parameters are changed. MathCAD has been used widely for instructional purposes in engineering fields; sets of MathCAD documents in the areas of electrical, chemical, civil, and mechanical engineering, statistics, and numerical methods are sold separately. A low-cost student edition of this program is published by Addison-Wesley (Addison-Wesley Publishing Co., 1 Jacob Way, Reading, MA 01867). A example of an application to analytical spectroscopy is shown here. This screen shot shows a MathCAD document that implements a mathematical model of the effect of fine structure on analytical curves in atomic absorption spectrometry. The two small windows on the right are tool palettes for selecting operators and Greek letters. Unlike a spreadsheet model, a MathCAD document explicitly shows the underlying mathematical structure in a format very close to standard mathematical notation. Like a spreadsheet, the equations, tables, and graphics are linked so that changing anything causes all dependent results to change accordingly.

C. C. C. E.

Questionnaire

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OVER PLEASE

(5) Suggestions for a Symposium session theme:

_____

(6) Suggestions for a Symposium speaker (give name and address):

_____

(7) Consider the following workshop topics: Grade each workshop (A to F). **A** - most important. **F** - not important, probably should not be held. Also, rank these workshops from 1 to 12 (1 most important, 12 least important)

_____ Interfacing for the Laboratory

_____ Spreadsheets and Databases

_____ Chemometrics

_____ Minitab

_____ Mathematical Software

_____ Microcomputer Graphics

_____ Introduction to C

_____ Hypercard on the Macintosh

_____ Windows on the IBM

_____ Uses of Computers in Teaching High School Chemistry

_____ Uses of Computers in Teaching College Chemistr

_____ Computer Networking and Telecommunications

(8) ____ Yes ____ No Suggestions for additional National Workshop topics:

_____

(9) ____ Yes ____ No I would be interested in attending a National Computer Workshop on _____

(10) Additional suggestions and comments:

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_____

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Return to: Dr. Donald Rosenthal, Department of Chemistry, Clarkson University, Potsdam, NY 13699.

COMPUTERS IN CHEMICAL EDUCATION

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10. Other - please describe _____ ____

OVER PLEASE

11. Are you a member of the:

ACS?	____ Yes	____ No
Division of Chemical Education?	____ Yes	____ No
Division of Computers in Chemistry?	____ Yes	____ No

12. Areas of Computer Activity and Interest:
Leave the space provided below blank, if you have no present interest or activity. Insert a number from 1 to 4 depending on the amount of activity.
1 means with a consuming passion, 2 means considerable
3 means moderate, and 4 means a little.

	Activity	Interest	Description of Use
Word Processing	____	____	_____
Spreadsheets	____	____	_____
Data Bases	____	____	_____
Other Languages	____	____	_____
Simulation	____	____	_____
Numerical Methods and Statistics	____	____	_____
Graphics	____	____	_____
Interfacing	____	____	_____
Laboratory Automation	____	____	_____
Drill and Practice	____	____	_____
Other (specify	____	____	_____

13. Provide a brief description of the hardware you use.

_____

14. Other Comments or Suggestions:

CHEMED-L

ANNOUNCING A CHEMISTRY EDUCATION DISCUSSION LIST ON BITNET

A computer list has been established on **BITNET** for discussion of current problems, ideas, and questions in Chemistry Education. If you are a member of the list, you can submit notes through **INTERNET** or **BITNET** which will be read by all other subscribers. You will also receive all items sent to **CHEMED-L** by the others on the list.

CHEMED-L is a great place to find out information about experiments, teaching techniques, programs, and resources. The list also will give you a forum in which to share your ideas on the above topics.

To join **CHEMED-L**, send a note to **LISTSERV@UWF.BITNET**. The first line should read:

SUBSCRIBE CHEMED-L <your name>

If your computer has the **"TELL"** command, send:

TELL LISTSERV@UWF SUBSCRIBE CHEMED-L <your name>

Please note that you must send the subscription to **LISTSERV@UWF**, not **CHEMED-L**.

If you have any problems, let me know:

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Pensacola, Florida 32514
(904) 474-2741
<WHALPERN@UWF.BITNET>