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Another Computer Conference will be held during the summer of 1995. It will be sponsored by the Division of Chemical Education. The theme of this conference has not yet been decided.

Anyone interested in helping to organize a future computer conference should contact Thomas O'Haver or myself.

NEWSLETTER

The Spring 1994 Newsletter will be distributed at the 13th Biennial Meeting at Bucknell University. Anyone wishing to submit an article for publication in this Newsletter should contact Brian J. Pankuch, editor.

EDITOR

A neophyte on Internet:

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I was fortunate this last year in that my college got on Internet in time for me to experience part of the first electronic Chemistry Conference on teaching chemistry. Part of the reason we got on Internet was because I kept explaining to two of our vice presidents how important it would be to be part of the first Conference. For the benefit of those of you who don't have electronic mail

or are in the process of bringing your faculty electronic mail let me give you my first impressions.

My situation was less than ideal since the only machine available with electronic mail was 2 buildings away and frequently not available due to other users, etc. The e-mail system in use was reminiscent of the first teletype I used in the late 60's. The only way to correct an error was to delete everything on the line to the error. The only way to check the mail was to go through piece by piece.

Innocently signing up for the conference I found myself getting hundreds of messages a week. With this primitive system this required reading or looking at each to find personal messages. If you ignored it for a while the system would fill over 430 messages on average, then start trashing anything that came in. Another problem with the old system was that I could only send 1 to 3 lines, and only about half of the messages got through. With no indication on my side of which were successful.

I could of course shut it off at any time, but it is fun seeing how many pearls you find in the downpour. I found the wide range of questions and opinions addictive. I found myself looking forward to certain individuals' comments and responses.

I serve as the chair of a college wide computer committee, and decided long before this that I would do my best to make computing as painless a way as possible. Learning to deal directly with a VAX is certainly possible, I used to program one. It is not something most faculty are going to enjoy. So I relentlessly applied pressure to get things simplified.

A real improvement came when our systems people finally relented and

put up a more modern system. If you are using a VAX as a server the latest version of DecNet and Mail for Macintosh is a vast improvement for e-mail. The new system allowed me to look at all my mail finding out who sent it and what the subject is. It is the difference between driving on a clear day able to see in all directions, versus traveling in a dense fog at night.

To illustrate the interesting way in which we each perceive reality I complemented our main systems engineer on the new mail system and he said it was the same system, just a different interface. Which is of course true, but the new interface allows a novice to learn how to use e-mail in about a minute and bring over their expertise from the word processor of their choice. This as opposed to spending hours or days learning VAX commands and editors. Not the same from the user standpoint by a mile.

About a week after the conference was over I got a Mac in my own lab, so I can play with e-mail anytime I have a few spare minutes.

Several programs were mentioned that make e-mail and navigating networks easier. Eudora apparently makes handling e-mail much easier. There is a free version and a \$25 commercial version, but you apparently need a NU Pop server on the Vax or other server to make it work. I haven't used either but the comments from those who have are very positive. You can get more information on the commercial version of Eudora from Eudora — sales@qualcomm.com. The free version is available at "ftp.acns.nwu.edu" in the /pub/nupop directory logging in as anonymous. NuPop is available from the same ftp address. Gopher allows you to find things on networks it was spoken of less but still positively.

Another Computer Conference is planned during the summer of 1995

(see above). I highly recommend signing up as a participant, and planning for 40-50 messages a day. I would strongly suggest planning some way of having your system automatically sort incoming mail — Eudora or its equivalent. If you don't have e-mail yet this may be a good opportunity to use this conference as I did to get connected to Internet. I've heard over a million new users are signing up every month. For those of us who usually can't make it to national meetings, this is an interesting way to be part of a conference. If you have any suggestions about topics you'd like to have covered, tell Don Rosenthal or Tom O'Haver.

SOFTWARE REVIEW: IR TUTOR, version 1.0 by Charles B. Abrams

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The Perkin-Elmer Corporation (Mail Station 12, 761 Main Ave., Norwalk, CT 06856-9966) has recently released a program called IR TUTOR as part of their 1600 Series FT-IR educational package. The entire package is listed at \$2,000 but the price is reduced to \$500 for purchasers of Perkin-Elmer IRs. I tested a pre-release copy of IR TUTOR the past summer in the second semester of introductory organic chemistry, and found the program to be a superb introduction to infrared spectroscopy. Not only did the students really enjoy using it, but what is more important, they learned how to interpret IR spectra. Twenty students had four unknowns each, and all of the IR spectra which they ran were interpreted correctly. The unknowns were taken from a much larger list of

unknowns of varying difficulty that we have been using for some time. The students received no other training on IR spectroscopy except that which they got during exams.

The most striking feature of IR TUTOR is the animations of the bond vibrations that cause peaks in the IR spectra. Once you see these, you will never be happy with any other way of teaching about bond vibrations. The other animations are outstanding, particularly the illustration of light as a wave and the graphics that combined a graph of the energy with the state of the molecular vibration. The animated diagrams of different types of IR instruments were also excellent. The best way I can describe the quality of the program is to state this is what CAI will be like ten years from now.

The most useful feature of IR TUTOR is the ability to overlay two spectra and compare them, which allows an easy correlation of peaks with functional groups. This is a very useful teaching tool, and the program takes advantage of it. The program allows the user to select a peak, like one which might be apparent from the difference between two overlaid spectra; when the peak is selected, the program will display the vibration responsible for that peak.

The only problem I found with the program was that you could not enter spectra into it. The author has informed me that the next version will allow the import of spectra from the P-E 1600 IR. The next version will also include an interactive, animated, correlation table and more theory, including a detailed explanation of the Fourier transform.

IR TUTOR could be used in the lecture part of a course, as a part of the lab, or as an independent assignment. Students seem to need from two to two and a half hours to finish the program. Students who have had no microcomputer experi-

ence are able to complete the program without help in running it. I am fortunate to have access to a lab with ten Mac Quadras, to which I assigned students in pairs; while I walked around the room commenting, teaching, or looking for students with problems running the program. (There weren't any.) IR TUTOR could be used with a single projection TV in a classroom. I did use it with an expensive LCD panel projector, but I wonder if it would work satisfactorily with the less expensive LCDs, because of problems in displaying the animated bond vibrations.

IR TUTOR comes in versions for both the Macintosh, (SE II Series, LC II, Powerbook 180, Quadra, Performa) and IBM PC or clone under Windows. A color monitor is desirable. The Mac and IBM versions look identical if the PC monitor is set to 256 colors. The author of the program used a very interesting way to produce the Mac and IBM versions essentially at the same time. (Macromind Director and Windows Player from Macromedia, 600 Townsend St., San Francisco, CA 94103). This system produces really superb CAI, with spectacular animations.

Rumor at the Chicago ACS Meeting was that Perkin-Elmer would accept the serial number of a Perkin-Elmer IR as sufficient evidence to get the discount.

An outline of the program follows:

- I. Introduction to Spectroscopy
 - A. Definition of Spectroscopy
 - B. Nature of Light
 - C. Measurement of an Infrared Spectrum
- II. Theory of Infrared Spectroscopy
 - A. Classical Model of a Molecule
 - B. Quantum Mechanical Model of