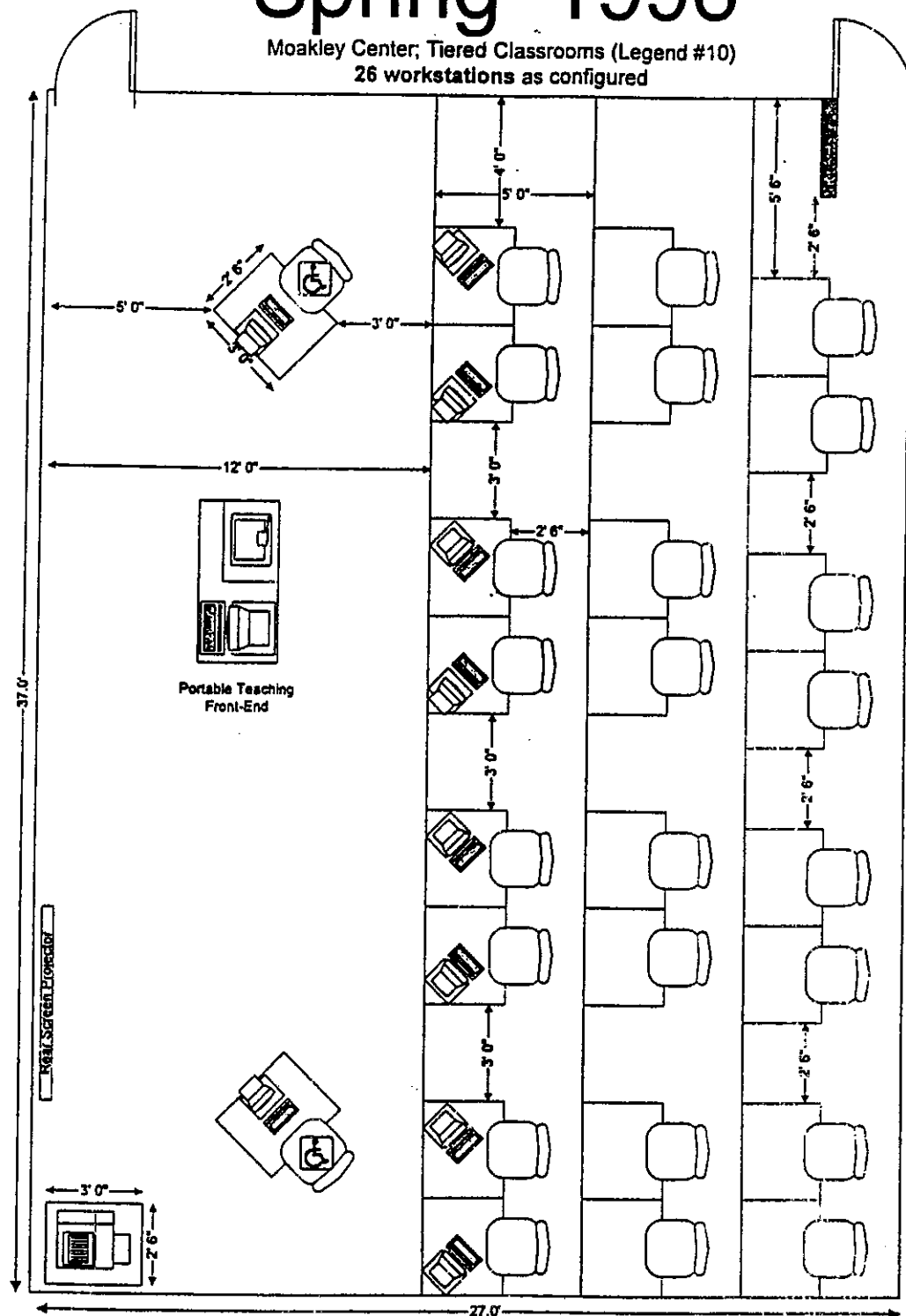


Computers in Chemical Education Newsletter Spring 1996



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Committee On Computers in Chemical Education
Don Rosenthal Chair

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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. Email submissions are frequently lost, and formatting and special characters are changed.
Submission deadlines: Fall issue - Sept. 25; Spring issue - March 15.

ALL NEW AND RENEWAL SUBSCRIPTIONS: PLEASE SEND REMITTANCE TO CCE Newsletter, c/o Donald Rosenthal, Department of Chemistry, Clarkson University, Potsdam, NY 13699-5810.

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FROM THE CHAIR

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The CCCE seeks to promote and publicize the use of computers in chemical education. Some of the activities of the Committee are: A. Organizing Symposia at National Meetings B. Organizing On-Line Meetings and Symposia C. Organizing On-Line Intercollegiate Courses D. Organizing National Computer Workshops E. Publishing this Newsletter F. Holding open meetings at the biennial BCCE meetings. These activities will be described in this message and elsewhere in this Newsletter.

A. SYMPOSIA AT NATIONAL MEETINGS

A symposium on "The Use of Computers in Introductory Chemistry" is being organized by Harry Pence (SUNY at Oneonta, pencehe@snyoneva.cc.oneonta.edu). Harry Pence is organizing a symposium on the use of simulation in teaching chemistry for the fall 1996 ACS meeting in Orlando, FL (August 18 to 22). Yuzhuo Li (Clarkson University, yuzholi@cadvax.clarkson.edu) will organize a symposium on the "Use of Research Grade Computational Chemistry Packages in Undergraduate Chemistry Courses" for the fall 1997 ACS meeting in Las Vegas, NV.

If you have suggestions for symposium topics or chairs for future ACS symposia, please send them to me.

B. ON-LINE MEETINGS AND SYMPOSIA

The CCCE sponsored an on-line conference (CHEMCONF) on "Applications of Technology in Teaching Chemistry" in 1993. (see <http://www.wam.umd.edu/~toh/Chemistry.html>)

Donald E. Jones (a past chair of the Division of Chemical Education Executive Committee, djones@nsf.gov) organized EXECCOMM an On-Line Information/Discussion with the Division of Chemical Education Executive Committee during the spring of 1994 and 1995. An on-line symposium entitled "Faculty Rewards: Can We Implement the Scholarship of Teaching?" was organized by Michael Pavelich (Colorado School of Mines, MPavelic@Mines.Colorado.edu) and Arlene Russell (UCLA, Russell@chem.ucla.edu) was held in October 1995. (see <http://www.wam.umd.edu/~toh/Chemistry.html>)

An on-line symposium entitled "New Initiatives in Chemi-

cal Education" will be held June 1 to July 19, 1996 (see the announcement elsewhere in this issue).

A symposium entitled "General Papers in Chemical Education" is planned for the summer and fall of 1997 and during the winter and spring of 1998. (see the article in this Newsletter). Marco Molinaro (UC at Berkley, molinaro@cchem.berkley.edu) and Charles B. Adams (McGill University, Abrams@omc.lan.mcgill.ca) will organize a symposium on "Computer-Aided Immersive Learning Experiences" for the fall 1997 ACS meeting at Las Vegas, NV.

Other on-line conferences and symposia are in early stages of planning. Suggestions may be sent to me.

C. ON-LINE INTERCOLLEGIATE COURSES

An on-line chemistry course entitled "Environmental and Industrial Chemistry" for upperclass chemistry students was held during the spring semester of 1996. (See the article in this issue.)

D. CCCE NATIONAL COMPUTER WORKSHOPS AT CLEMSON

The CCCE is sponsoring Workshops just before the BCCE at Clemson. Further details are provided in an announcement elsewhere in this Newsletter.

E. CCE NEWSLETTER

This Newsletter is currently being published twice a year. Articles which are submitted and accepted will appear in a timely manner. We are anxious to receive articles from readers.

F. OPEN MEETING AT THE BCCE

An open meeting of the CCCE is planned for the BCCE at Clemson. This will provide an opportunity for you to meet members of the committee -to learn what we are doing - to provide ideas and suggestions and to ask questions. Future symposia, on-line meetings and courses will be discussed. If you plan to attend the BCCE, please attend our meeting.

G. COMMITTEE ON COMPUTERS IN CHEMICAL EDUCATION (CCCE) MEMBERS - 1996

The names and affiliations of the twenty-two members of the CCCE are provided below.

Charles B. Abrams - McGill University, Montreal, Canada
James M. Beard - Catawba College, Salisbury NC
James W. Beatty - Ripon College, Ripon WI
Joseph Casanova - California State University, Los Angeles CA

Wilmon B. Chipman - Bridgewater State College,
Bridgewater MA

Nancy S. Gettys - University of Wisconsin, Madison WI

William P. Halpern - University of Western Florida,
Pensacola FL

Carolyn Sweeney Judd - Houston Community College,
Houston TX

Alfred J. Lata - University of Kansas, Lawrence KS

Yuzhuo Li - Clarkson University, Potsdam NY

Robert Megargle - Cleveland State University, Cleve-
land OH

Marco Molinaro - University of California, Berkeley CA

Thomas C. O'Haver - University of Maryland, College
Park MD

Brian J. Pankuch - Union County College, Cranford NJ

Harry E. Pence - SUNY College, Oneonta NY

Donald Rosenthal - Clarkson University, Potsdam NY

Gwen Sibert - Roanoke Valley Governor's School,
Roanoke VA

Stanley G. Smith - University of Illinois, Urbana IL

Carl H. Snyder - University of Miami, Coral Gables FL

Brian Tissue - V. P. I. and State University, Blacksburg
VA

David M. Whisnant - Wofford College, Spartanburg SC

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We've been wrestling with what to require or recommend to our students when it comes to preparation for using computer hardware and software. Given no time or room left in an average course, about a negative 20% it seemed this last semester, and a curriculum which is bursting, we wonder. . . I decided to read a number of books-several reviewed below, and of course read widely in the computer area to help decide.

I selected authors who use computers and have innovated in this and closely associated areas. I've come to the conclusion that learning to use a variety of software and in particular to be able to use scripting as a way of personalizing software is of more benefit for most than programming ability in C++. Some interesting trends and ideas also surfaced as related below.

Several points come across loud and clear from the books reviewed. Teleconferencing, encryption and increased recording of your life will be important. Teleconferencing because of the acceleration of hardware technology which will greatly accelerate the downward spiral in cost and make it much easier to use.

Encryption will be important if you want to safely make

financial transactions over the Net. The authors seem satisfied with new schemes, but a little nervous. I recently read an article in Discover which looked at some unlikely breakthroughs in computers which would allow breaking of current encryption schemes in seconds. The authors are nervous for good reason.

Having a card the size of a credit card (and some small additions) with the ability to video record everything you say and your surroundings might be useful for police and others in potentially dangerous, litigious situations. With Net support it might be useful if it could scan individuals you are talking with at a meeting and prompt your memory of your last meeting with them. But to be on candid camera every waking hour, since you don't know when someone else is recording-no thanks.

Perhaps more useful for those of us teaching large numbers of students would be to have a system built into our glasses which will prompt us with the students' name, academic interests and background, score on the last test, etc. Of course if we could be prompted with student info why couldn't a student be prompted with subject area material as on a test.

While looking into what is now possible or will soon be, I thought of a few things that would be handy. For instance I'd find it useful to have a single Internet address where I could go and browse software I'd be interested in for myself and my students. Samples of programs, of commercial products, shareware and freeware. Might be a neat place to exchange ideas for use of specific packages and the results of using them. Another idea occurred to me when I got a email from the Union of Concerned Scientists (I'm a member of UCS). I volunteered to be one of a group who is willing to respond to inaccuracies in the press or to comment to elected representatives, editors, etc., on nuclear, environmental population, etc., topics. I get an email package containing the article in question, a usually rational analysis of the weaknesses of the article backed with facts. In one case this was an article in Time which concerned catastrophic climate change. Suggestions were made on how to respond and the email address of the Time editors included.

After reading the enclosed documentation and writing up a short comment I emailed it to Time and a few hours later had received a pleasant response from the Time editors (probably an office machine programmed to respond in a general way). A similar methodology is followed for contacting Representatives or the President. I mention this first because you may want to take part as an individual. You simply respond when you have sufficient expertise, interest, time and inclination, it's up to you.

Secondly this seems like a good thing to get students involved with-there is a lot of critical thinking involved in reading an article, its rebuttal and thinking through any comments you might want to make. Topics being very current is a big advantage.

Thirdly with all the prejudice, misinformation and errors in reporting anything involving chemistry maybe ACS should think about setting up something similar to correct these errors. For more information you can email to abaptista@ucsusa.org, or go directly to the UCS homepage at <http://www.ucsusa.org>.

Bill Chipman wrote me that he also had a problem losing a modem to lightning this summer. Apparently the surge followed the phone line in. I related my surge problems last issue. My solution has been to use American Power Conversion surge protectors, you can get them at various levels of voltage ratings. They can also have phone line protection. I called them at 800-800-4APC with a list of equipment I wanted to protect- they gave me their suggestions. I then called around for the best prices from my favorite mail order houses. The surge protector itself is guaranteed for as long as you own it. Equipment attached is covered depending on the cost of the surge protector-with 4 pages of caveats. Perhaps most important if the surge protector catches a surge it will trip its internal circuit breaker, you then have to reset it. Many of the cheaper surge protectors fail in a way which allows the next surge to come right on through. Perhaps my biggest protection has been getting the culprit who left the system plugged in on her own system.

Book Review-by Brian Pankuch

"The Road Ahead," by Bill Gates (Chairman Microsoft), Nathan Myhrvold (Ph.D. Theoretical/mathematical physics, Princeton), Peter Rinearson (Pulitzer Prize-winning journalist) 1995, Viking-Penguin Group, ISBN 0-670-77289-5, 266 pp, \$29.95. Includes a CD which is not reviewed.

Given the team listed above I was somewhat disappointed by the lack of flow and enthusiasm this book generated for me. Not that Gates doesn't cover a lot he does-his examples are easy to understand and probably correct since most of them have already been written up in many magazines. His attention to detail is impressive and perhaps it is this detail which makes the flow somewhat slower than I like. The attention to detail may also be why he is one of the richest people in the world.

He was in our area and gave the keynote speech almost a decade ago and I had a chance to listen further and talk after the address. Some of the things he predicted are just now starting to show up in my software and some are still in the planning stage. He's worth listening to.

I suggest minimally that you read chapter 9, 'Education: The Best Investment (pp 184-204). You'll be treated to..."We've all had teachers who made a difference. I had a great chemistry teacher in high school who made his subject immensely interesting, Chemistry seemed enthralling compared to biology.... My chemistry teacher sensationalized his subject a bit and promised that it would help us understand the world....It seems amazing to me now that one great teacher made chemistry endlessly fascinating while I found biology totally boring."

Further ..."There is an often -expressed fear that technology will replace teachers. I can say emphatically and unequivocally, IT WON'T.... However, technology will be pivotal in the future role of teachers." Gates foresees the future of teaching as extremely bright, but not without changes. The information highway will presumably make the work of excellent teachers more available for us to use, misuse or emulate. We'll have easy to use tools available to find, change, and combine material much as we do now with word-processing. Simulations and virtual-reality that are geared to interactivity and exploration will get more realistic. Great courses from great teachers will be available for all of us. Continuing Ed and lifelong learning should be easier. So should inviting knowledgeable guests to join a class discussion from their office or home.

He also gives a bit of a tour through his home (pp 205-226) being built with advanced communications capability throughout. Most of it I would rather not have and certainly wouldn't pay extra for. A few capabilities such as turning off lights and appliances in unoccupied rooms appeals. Also having a considerable library (over a million in Gates' case) of high resolution images of great art and views which could be projected on whole walls. Others such as having my choice of music or video follow me through the house are not desired, but each of us will have wide individual choices. Each individual would be able to select their desired interaction with the system. It will be interesting to see how a system will decide to adjust when one family member wants quiet to read journals, another a rock station, and another their favorite TV program all in the family room. Perhaps we should call the system Solomon. The April, 1996 issue of Scientific American, pp. 68-76, has an interesting article on Smart Rooms.

The current Internet isn't the information highway though the primary difference is the immediate and easy access to information. We will have a series of experiments to see what works with groups of people. Perhaps more important what are people willing to spend on these services. Gates makes a strong, logical and self serving argument for no regulation—let the market decide how to finance and how to use these new systems. Servers holding and distributing all this information may be anything from super computers to linked PC's.

He believes that future change will be both destroying jobs and creating more. He doesn't know what the new jobs will be but he is confident there will be many. One of the chief keys will be learning new skills. What we do best is to teach our students not just chemistry, but how to learn. Learning how to learn and being comfortable around computers will allow many to be more comfortable with change in the future. Creating the physical resources of great private schools in each poor inner city would be very expensive, connecting them as equals to the information highway-relatively inexpensive. An intriguing possibility.

E-mail is increasingly connecting us to many areas. It is easier to connect electronically to our federal government representatives than to go to a public meeting or send a letter. Getting real time opinions from constituents has interesting implications.

In fact see my editorial for a use of this idea and increasing student critical thinking about headline stories (global warming, federal funding for research, etc.) of the day.

Gates includes a brief history of computing and software development and the technological revolution supporting and driving it.

"You'll know the information highway has become part of your life when you begin to resent it if information is not available via the network. One day you'll be hunting for the repair manual for your bicycle and you'll be annoyed that the manual is a paper document that you could misplace. You'll wish it were an interactive electronic document with animated illustrations and a video tutorial, always available on the network."

Maybe, but I'm well organized and can find those instructions which have a bit of oil and grease on them. They survive having tools dropped on them, grease smears, being stepped on, etc. I can still access them during power outages, without hardware or software glitches.

Of course I teach at a college whose infrastructure has

yet been able to provide a working overhead projector even half the time it is requested. For me the number of systems needed to provide Gates' future is not going to happen without commitment of substantial resources.

Book Review-by Brian Pankuch

"Harmony," by Arno Penzias. 1995, Harper Collins Publishers ISBN 0-88730-724-8, 178 pp, \$23.

Arno Penzias is a Nobel Prize winner in physics, and until recently, director of research at Bell Labs. Many of his individual examples are quite interesting, but the point of the book wanders with broad generalizations such as, we are responsible for how we use this new 'computer' power.

Penzias sees an increase in the storage of basic RAM memory chips by a factor of a thousand. "...in practical terms? Picture the largest consumer electronics store you've seen or heard about, with row upon row of TV sets, stereos, personal computers, electronic games, VCRs, camcorders, and the like. In the four gigabit era, all the electronic circuits in every appliance in sight will fit into barely enough silicon to make a noticeable bulge in a shirt pocket."

The idea of harmony is based on this predictable increase in computer power. It is the possibility of increasing connections, decreasing discord, and bridging gaps within human society.

This increase in capability will make many innovations possible. One might think that software development might be moving off to software engineers in China, India and the like where salaries are a fraction of ours. "...Software manufacture consists of a sequence of processes, of which the actual writing of the code itself represents less than one-third of the total task. Most of the job consists of finding out what the customer wants and making sure that the program performs as required. ...a computer can even generate the desired program from specificationssoftware production shows little sign of moving to low wage countries."

He sees the development of hardware continuing to move around the globe, but less exporting of jobs where a human interface is needed. "As managers look to computer-based information sources for help in making decisions they risk facing the proverbial drunk's dilemma: Should he search for his lost coin on the dark roadway where he lost it or under a distant streetlight where he can see so much more clearly? Given computing's power to illuminate numerical problems,

many managers seem tempted to conduct their search for answers in that arena alone, even though the real questions lie elsewhere."

Although many of his examples are based on his research and business experience, looking at the numbers is an increasing part of higher education. The ability to look behind the numbers and grasp the real people and changes and the implication for the future requires us to be aware of the limitations of the systems being used.

Intelligent agents take action on the basis of inferences drawn from their users' behavior. Extend toward using environmental sensors to control the area around the user. A home assistant would be able to learn enough about your needs and desires to take over meal planning and support for the many details of keeping a house and all the equipment in it up and running. Keep complete record and take care of all tax forms, warranties, medical insurance forms, etc. (I can't wait.) You'll be able to talk with your assistant and choose its' voice and physical appearance (this could be fun).

One of his favorite areas of speculation is the medical field. Currently many hospitals use computerized testing equipment, but the results from different areas are often on paper and stored and collated that way. If you've not done much programming you may wonder why integrating these systems isn't done routinely. One of the answers is that of course it has been done, but the updating, adding features which were not in the original system, is fraught with problems. Mostly as you add these software patches over the years the reliability of the system decreases. Not a good thing in most applications, but particularly bad when peoples health or wealth are concerned.

One of the solutions is object oriented programming which cuts down on this type of problem (pp 116-118). Most professional programmers are using C++. Current languages such as C++ and the subset Java which has been designed to facilitate communication on the Internet are the ones I'm somewhat familiar with. They may help but the given the number of programs that take much longer to develop than planned and still have many flaws we have quite a way to go yet.

A potentially better solution would be an Apple Newton which communicates with Macs or PC's and can put handwriting with error checking into specific forms which are readable by the computer. This is being used in a number of areas such as pharmacy and medicine.

I liked his idea of solving some of the commuting problems we share in my home state of NJ, which has added 300,000 vehicles with no appreciable addition of

roads. He sees a fleet of limo vans -very comfortable, keeping a door to door service for a large number of people. This would require 'instantaneous and complete knowledge of every vehicles location, the individual destination of all passengers, and traffic conditions-together with all the internals of the business itself.' With additional incentives for electronic commuting and political pressure to limit commutes by single driver cars it's an interesting idea.

Penzias spends little time on education. He cites our National Labs as an example of needed reemployment of the scientists and engineers. He is skeptical about finding large national problems which could be tackled by the experts at these Labs. One possibility is to purchase individual videoconferencing equipment for each scientist. They could then share their expertise with students around the country. I'm rather skeptical about this.

Some interesting ideas, but it never really flies.

Computers in the Classroom - What Works and What Doesn't

Joseph Casanova

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In a frenetic effort to introduce the latest technology into the classroom, we sometimes behave like lemmings guided unerringly by a mysterious force toward an uncertain destiny. We try to do what we judge best for our students, and to make the most effective use of limited class time. In the process we try to assure that students capture and retain the most important concepts in chemistry. Yet we are collectively investing an inordinate amount of time inventing new approaches to the presentation of material. This time investment, on the part of many faculty across the country, reflects the pressure on all of us to do something new, anything new, to improve the retention of students in our programs, and of chemistry by these students.

The plethora of new technological devices and computer applications that pour across our desk every day stimulates our instinct to innovate and to deliver knowledge and understanding to students in the best way we can. Much of this new effort comes at the expense of time which we formerly spent in "one-on-one" course discussions, and in benchtop research efforts with students, activities which in themselves have an important salutary effect on students' professional development. It is easy to understand why this change in emphasis has occurred. Laboratory research is diffi-

cult, often frustrating or tedious, usually expensive, and requires the availability of increasingly expensive and less readily available instrumentation. It is very time consuming for both the student and the professor. In contrast, development of new software, or of the lecture/laboratory applications of new software presents a simpler challenge, with a much greater apparent return/investment ratio. We can work with a few students to develop computer material, or we can work alone, in the quiet of our offices or home, uninterrupted. Colleagues and administrators alike see that we are advancing the cause of innovative teaching. Following the modest investment for purchase of a microcomputer, technological innovations using that computer are certainly less expensive, safer, and much cleaner than conducting bench chemistry. A significant number of colleagues share a concern that we are moving too far and too fast in technology. J. Lagowski has expressed the concern well [J. J. Lagowski, Editorially Speaking, "The Impact of Technology on Education", J. Chem. Ed. (1995) 72, 669.]

In the interest of productive investment of our intellectual "free time", it is increasingly important that each of us critically examine the manner in which we apportion that time among extra-classroom student oriented activities. To that end, we should carefully evaluate our own efforts to develop and utilize new technology-based teaching strategies, to assure that they are likely to produce the most significant teaching impact possible in our own specific circumstances, and represent the best investment of our limited time. The foregoing admonition notwithstanding, in the next paragraphs this writer will review a few of the technology-based activities that are most familiar to him, and comment on their efficacy. This article is not intended to be a comprehensive examination of the use of computers in chemistry, focusing instead on the experiences of the writer.

(1) Massive and passive use of the computer in lecture.

We conducted a year long experiment to substitute the microcomputer for both the blackboard and the handheld molecular model, using the microcomputer, in the words of MIT's Project Athena, as an "electronic blackboard." [J. Casanova, S. L. Casanova, "Computer as Electronic Blackboard: Remodeling the Organic Chemistry Lecture", *Educom Review* (1991) 26 31.] Nearly all of the lecture material was contained in the microcomputer. Lecture material that would normally be written on the blackboard was developed in lecture fashion projected on a screen. We sought to make the computer itself as unobtrusive as possible.

Students took very few notes, but listened and watched intently. Class participation (questions, comments, discussion) was high, of good quality, and stimulating. Students were very favorably impressed and asserted

that they had a good understanding of the subject, particularly the visual representations of molecular structure. However, very poor performance on conventional examinations did not support this assertion. A control section (taught by Professor Stanley H. Pine) took all the same examinations on the same days as did the experimental section. There was a striking difference in result between the experimental section and the control section, with the experimental section performing more poorly in all categories of test items. The overall average in the course for students in the experimental section was 44%, contrasted with 63% for the control section.

We considered the following issues to rationalize our results. The electronic blackboard allows for the presentation of substantially more information in a given period of time than does the conventional blackboard but students may have trouble absorbing the added information. There is ample evidence that only a fraction of the information conveyed in any typical lecture is in fact retained by the student [R. Menges, "Instructional Methods" in *The Modern American College*. Arthur W. Chikering and Associates, Eds. San Francisco: Jossey-Bass. (1981).]. The presentation of more information does not ensure the retention of more information.

The electronic blackboard allows for the simultaneous presentation of graphic, pictorial, written, and spoken information. We do not know if simultaneous presentation enhances learning or makes assimilation, integration, and recall more difficult. Research in artificial intelligence has renewed interest in attentional selection, filtering, and reconstructive retrieval. [A., Allport, "Visual Attention" in *Foundations of Cognitive Science*. M. A. Posner, Ed. Cambridge, Mass: MIT Press. (1989); S. Yantis, and J. C. Johnston, "On the Locus of Visual Selection: Evidence from Focused Attention Tasks." *Journal of Experimental Psychology: Human Perception and Performance*. Vol. 16, No. 1. (1990). pp. 135-149; D. E. Rumelhart, "The Architecture of the Mind: A Connectionist Approach." in *Foundations of Cognitive Science*. M. A. Posner, Ed. Cambridge, Mass: MIT Press. (1989).] In the electronic organic chemistry lecture, the combination of words and images presented concurrently on the screen may have been a problem.

The electronic blackboard encourages greater reliance by the instructor on metaphor, illustration, and imaging, but the instructional effectiveness of these techniques is unclear. Metaphor, illustration, and modeling are important tools of teaching, but are often filtered and interpreted by unique individual experiences [R. W. Kleinman, *J. Chem. Educ.* (1987) 64, 766]. The capacity of the computer to illustrate in real time what will

happen in an experiment when variables are altered, and to portray, rotate, and alter complex molecular structures, is what makes it so exciting for incorporation into the lecture. The fact that this enriching capacity did not translate into higher test scores we called the "Feynman effect." Richard Feynman's legendary physics lectures were amply illustrated with mental images and analogies. Examples, rich in visual imagery, punctuated his lectures, which were delivered with remarkable organization and clarity. Students left the lectures believing they understood physics, later to discover that they understood only the illustrations. Students at the introductory level need to be carefully guided to link chemical imagery with chemical theory. The profound implications of providing to undergraduate chemistry students the pictures and movements of models that were at one time envisioned and manipulated only in the imagination need to be mentioned. The photographic reality of current computer models makes it harder than ever to persuade students that these images are not real.

Finally, in changing the lecture priority from words and theory to graphics and visualization, the electronic blackboard conveys to students a different set of priorities within the discipline which may or may not be tested in traditional examinations.

(2) Computer response system - active involvement of students in the process. In a resurrection of ancient history, we revisit a 25 year old experiment that, in retrospect, was more successful than we appreciated at the time. [J. Casanova, "An Instructional Experiment in Organic Chemistry", J. Chem. Ed. (1971) 48, 453.] We utilized a classroom response device which permitted students to respond individually to questions raised by the instructor after presentation of each concept (15-20 minutes). Responses were recorded individually and collectively, and were part of the final grade. The lecture could be modified on the fly to ameliorate any widespread misconceptions. Experimental and control sections (control sections taught by Professor Stanley H. Pine) were conducted and students in all sections took all the same examinations. The nature of the curriculum experiment was not advertised in advance to avoid student self-selection. While the performance of students was nearly the same in all sections, the retention of students whose performance was marginal was nearly twice as good in the experimental section (10% drop) as was retention in the control sections (17 and 20% drop). The latter drop rate was comparable to drop rates in most other sections at that time. The positive effect of more active student engagement was considered even in 1970: "The greater the passivity of the student, the less benefit he is likely to derive from the lecture." [see also J. J. Lagowski, Editorially Speaking, "Teaching is More Than Lecturing", J. Chem. Ed. (1990)

67, 811.]

(3) Commercial packages for computational chemistry with student exercises. The capacity of the computer to mimic what chemists had done mentally—to model and manipulate images - was recognized early by most chemists, and computer modeling and computation have rapidly become indispensable tools of the discipline. We have used several modeling and structure display applications in the organic lecture. PC Model [Serena Software, P.O. Box 3076, Bloomington, IN 47402-3076] and Molecular Editor (This latter display application is now dated). Most recent we have used the display application Rasmol. Rasmol is an excellent new display program, recently modified and improved by M. Molinaro, and is available for the Macintosh as RasMac v.2.5-ucb1.3

[<http://hydrogen.cchem.berkeley.edu:8080/Rasmol/>]. In general, [see <http://www.ch.ic.ac.uk/infobahn/boc.html>] for the most widely used chemistry software. Although this is a very important application of computers in teaching, little more will be said here. The reader is referred to detailed publications [J. P. Bays, J. Chem. Ed. 1992, 69, 209; J. Casanova, "Computer-Based Molecular Modeling in the Curriculum", J. Chem. Ed., 1993, 70, 904].

We are currently integrating computational chemistry into several laboratory exercises in our basic organic laboratory course, with the idea of asking students to test a stereochemical result on the computer, predict the result, then conduct the experiment and compare theory and practice. This activity is being conducted under an NSF ILI award.

Semi-empirical calculations permit examination of electronic structure as well as molecular geometry, hence analysis of reactivity and chemical behavior. It is now possible for students to compute and view important electronic features of molecules qualitatively using even ab initio methods. Orbital energy levels, electron distributions and charges, dipole moments, vibrational frequencies and heats of formation are readily available for classroom use. Several applications suitable for the computation of electronic structure are available: CAChe [CAChe Scientific, P. O. Box 500 M/S 13-400, Beaverton, Oregon 97077] system is an integrated seamless application that works best with a higher-end Macintosh. It offers unique stereo visualization, and can be used for semi-empirical calculations. HyperChem [Autodesk, Inc., Scientific Modeling Division, 2320 Marinship Way, Sausalito, CA. 94965.] operates on a relatively inexpensive pentium or Power PC platform, and will permit semi-empirical calculational methods. Spartan software of WaveFunction [WaveFunction, Inc., 18401 Von Karman, Suite 310, Irvine, CA 92715.] is a third. Spartan is the first fully integrated package for semi-empiri-

cal and ab initio calculations. Spartan will calculate and display conformations, electron density surfaces, as well as HOMO and LUMO representations, in vivid color images. These capabilities make the teaching of both structural chemistry and chemical reactivity an attractive possibility. Faculty are already beginning to explore the use of Spartan in the classroom [Shusterman, A. J. "Advanced Computation at Predominantly Undergraduate Institutions: Using Spartan on the IBM RISC System 6000 Workstation", A Series on Molecular Modeling, N. S. Mills, Ed, Council on Undergraduate Education Newsletter, XII, No. 3, 60, (1992); W. J. Hehre and W. W. Huang, "Chemistry with Computation. An Introduction to Spartan", WaveFunction, Inc. (1995)].

The inexorable development of faster hardware and of fully integrated visually sophisticated molecular modeling software makes inevitable rapid change for the use of 'molecular modeling' in chemistry. Molecular modeling will soon extend to 'reaction modeling', and students will understand earlier and perhaps more intuitively what we have been asserting at the chalkboard for so long. Imagine students in the beginning organic course discovering resonance and hybridization, visualizing the reactivity of the carbonyl group, and calculating transition states for reactions. The accelerating trend toward more powerful desktop machines to make such calculations rapid and inexpensive shows no sign of abating. The time is right for dedicated classroom lecturers to review and revise the formal lecture approach to introduce these new techniques.

(4) Courses in the use of computers for chemistry. We have taught a course called "Microcomputers in Chemistry". It is the objective of this course to introduce the student to the use of the microcomputer, so that microcomputers could be used as an integral and routine part of the educational experience of a chemistry/biochemistry degree program. It was aimed at the individual who has little or no prior experience with microcomputers, and is designed to familiarize the student with the use of a microcomputer as a productivity tool - that is, for word processing, graphing and interpreting data, drawing, presentation graphics; for computations, structural computation and display; for data collection and instrument control; communication with a server, electronic mail, literature search via Chemical Abstracts. It is intended that students take this course as early in their undergraduate experience as possible so that they can exploit fully the benefits of the microcomputer in their programs. Students who took this course evaluated it very highly, and apparently learned a great deal from it. Once again we believe that the key to success was that this was a laboratory course in which every student sat at a computer actively engaged during and following every class.

(5) Drill and practice. We have had modest success using a variety of drill and practice programs in general and organic chemistry. We particularly have found Paul Schatz's spectroscopy tools (ir and nmr simulators, and spectra interpretation software [Trinity Software, Campton, NH 03223] very useful. Several versions of nomenclature drill software have been used, as has Beaker [J. Brockwell and collaborators, Brooks/Cole Publishing Company, Pacific Grove, CA 93950]. But all these exercises are only as useful as we were successful in getting students to use the computer. We have often seen that when, for example, we conduct review sessions in advance of major exams, it is the better students who participate in such voluntary enrichment activities. It is no different with the use of software. Students who avail themselves of drill and practice learn from it. Active student engagement is the key. Active student participation is once more the centerpiece of success in this mode of computer use. It is imperative to acknowledge here the enormous contributions of John Moore and his collaborators in developing and organizing software for the Division of Chemical Education.

(6) Electronic communications among students, with the instructor, and to the world beyond. "Oh what a tangled web we weave, when first we practice to deceive" [W. Scott, (1808)]. Without question the most rapidly expanding use of computer in teaching is in the introduction of materials for teaching on the WorldWide Web. This topic is addressed elsewhere in this publication [C. H. Snyder, "A Web Page in Chemical Education"]. A veritable explosion is occurring at this time, with each day bringing a score of new projects and activities on the Web. With no review or filtering to intercept marginal material, the quality of what can be found is highly variable, from spectacular to abysmal. Among the better starts that we have seen in this approach, we note that many faculty are already heavily immersed in Web use in their daily class activities [see for example B. Luceigh: http://web.chem.ucla.edu/~luceigh/BAL/BAL_exmcntr.html] and J. Charonnat: [http://www.csun.edu/~hcchm007/]. An excellent entry to some of the best Web activities in chemistry is available at [http://www.ch.ic.ac.uk/infobahn/boc.html]. It is premature to see how developments in this WWW use will best fit into our teaching, but the opportunity for active student engagement and interaction in class activities either via the Web or the internet is certainly available. One of the most attractive and advanced use of the WWW in undergraduate instruction can be seen at the MC² web site [M. Molinaro: <http://www.cchem.berkeley.edu/Education/index.html>, follow link to MC² or MultiCHEM].

After all it will be seen that the most profound effect of successful innovations arises mostly from engaging the

students in an active learning environment [J. Katz, M. Henry, D. Johnson, "Turning Professors into Teachers", Macmillan (1988); S. Tobias, "They're Not Dumb, They're Different: Stalking the Second Tier", Research Corp., Tucson, AZ, (1990); C. K. Herman, J. Chem. Ed. (1995), 72, 157.] This condition, of course, does not necessarily require computers or advanced technology, but clearly the computer based communication explosion that is now underway provides an excellent base from which to induce better communication from students to the professor, often from the safety and anonymity of a remote connection. It is a continuing irony that students are often more comfortable when their academic shortcoming are witnessed by the inanimate computer rather than the human professor. Scores of projects are ongoing which are designed to engage students more actively that involve new technology and multimedia, but in an ancillary and complimentary way and not as the *raison d'être*. Student engagement and collaborative learning are the main features of these programs. A number of these funded by NSF are underway at this time. "Sweeping Change in Manageable Units: A Modular Approach to Chemistry Curriculum Reform" [Modular Chemistry Consortium, MC², <http://www.cchem.berkeley.edu:8080/>], "ChemLinks Coalition: Making Chemical Connections", [spencer@beloit.edu], and "Establishing New Traditions: Revitalizing the Curriculum" [jmoore@macc.wisc.edu] represent three efforts currently funded by NSF as an attempt to break out of the traditional lecture mold. Many other similar activities are ongoing.

Certainly, many aspects of teaching chemistry are and will continue to be profoundly influenced by computer technology. But one gets the clear impression that much of our current fascination with technology is faddish and will produce few memorable improvements in chemistry teaching. Perhaps it is the novelty of using computers actively in exercises that engages some students, but this engagement, much more than the computer, is the key to improving student performance.

Using MathCAD in High School and Freshman Chemistry

by M. Gwen Sibert, Roanoke Valley Governor's

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<http://www.chem.vt.edu/RVGS/RVGS-home.html>

The chemistry course at the Governor's School is taken primarily by juniors, and some of the sophomores who enter the school as ninth, rather than tenth graders. The course itself is not high school chemistry, nor is it AP chemistry, rather it is like freshman college chemistry. The textbook currently used is *General Chemistry, Third Edition*, by McQuarrie and Rock.

The calculus course at the Governor's school uses MathCAD for MacIntosh, and there is limited use of it in the precalculus course. Because most of the chemistry students are in precalculus or calculus it is only natural that MathCAD be used by students taking chemistry.

I decided that the best, and simplest way to introduce MathCAD in the chemistry course was to have the students first use it to solve an equation, and then a couple of weeks later progress to graphing Beer's Law and kinetics data. I decided that the Rydberg-Balmer equation would be a great place to start. The students had just finished an activity in which they had observed the line spectra for several elements using spectrum tubes and hand-held spectrometers. They used a spreadsheet to calculate the frequencies and energies of the lines they had seen, and until last year they had also used the spreadsheet to solve the Rydberg-Balmer equation for the initial energy level of the hydrogen electrons. Most of the students were eventually successful, but it took several attempts to get the equation entered correctly, because all the nested parentheses that were needed to get the operations grouped correctly.

It was at this point last year that I participated in a workshop on MathCAD for the science faculty which was presented by our math faculty. I used the Rydberg-Balmer equation to practice my newly learned skills and was very impressed with the software and the appearance of the final product. MathCAD allows you to type out the equation the way it appears on paper. It is easy to enter text to define variables and constants and any other descriptions that might be desired. All of the Greek symbols are also supported, a feature I think is very important.

The class meets in the computer lab the day I introduce the students to MathCAD so that each student can work

on a separate computer at their own speed. I use an overhead display panel to show them how to enter text and how to manage the math mode. Some of the commands are really not very intuitive, as they are unique to MathCAD. Here is an example of how one student carried out the assignment this year.

Sarah Airey
March 5, 1996

Purpose: To use the Rydberg-Balmer equation to calculate the initial energy level for the hydrogen spectra as determined in Experiment 13.

λ = wavelength
 x = Balmer Constant
 n = initial energy
 i = counter

$i := 1..3$

$x := 1.097 \cdot 10^7$

$\lambda_i :=$

$435 \cdot 10^{-9}$
$490 \cdot 10^{-9}$
$660 \cdot 10^{-9}$

$$n_i := \frac{1}{\sqrt{\frac{1}{4} - \frac{1}{\lambda_i \cdot x}}}$$

n_i

4.973
3.954
2.99

The graphing assignment is coming soon, but I have changed it from what was done last year. That assignment was for the students to set up templates to graph Conc. vs time, ln Conc. vs time, and 1/Conc vs time for five sets of kinetics data. Then for the equation that showed a straight line they were to determine the order, the rate, and the rate constant for each set. This year they will have only one of this type of problem. They will also be asked to graph $V/T = k$ and $PV = k$, where k is a constant, using a minimum of 5 points for each. In addition, they will be given in $P = A \cdot \Delta H_{\text{vap}}/RT$ and values for vapor pressure and temp and determine the

value of ΔH_{vap} . Lastly, they will be given solution concentrations in molality and boiling points and after graphing conc. vs b.p., determine the slope to obtain K_b . I had my classes do this assignment on Kaleidagraph for several years to help them learn that graphing software, but since almost all of them are quite proficient at it when they come into chemistry, this seems like an excellent way to provide experience in graphing with MathCAD.

The specific directions that are given out to the students pertaining to MathCAD itself and the assignment details can be viewed at the website given above. I want to acknowledge the help of the math faculty at the Governor's School who showed me how to use MathCAD and who developed the student directions for the various assignments. Thanks go to Julie Taibbi, Susan Kennedy, John Cannaday, and Ken Weddle.

ELECTRONIC CLASSROOMS

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You can't see atoms or molecules. Students have to establish a mental picture of atomic and molecular structure to understand chemistry. During the last year and a half we have been experimenting with the use of Pentium and Macintosh electronic classrooms in organic chemistry and biochemistry instruction. We find that the use of visualization software is an excellent tool to help students understand molecular structure.

Bridgewater State College has recently completed the John Joseph Moakley Center for the Application of Technology to Education. The building has two 26 seat Pentium electronic classrooms and one 24 seat Mac electronic classroom. Each classroom has two microcomputers set up for wheelchair access, and the building also houses an adaptive computing room where special software is provided. Each electronic classroom has a faculty station consisting of a cart equipped with a microcomputer with CD-ROM, a video visualizer, a VCR, a laser disc player and a network connection. All of these are connected to a Sony three-gun projection TV system through an audio/video switch, and an Exxtron converter box. The individual microcomputers also have 4X CD-ROM drives and network

connections.

In organic chemistry we have used software in two ways; as a lecture aid to help students understand the geometry of molecules and orbitals (PCMODEL) and as self-contained teaching modules (IR-TUTOR). We would be very happy to have more software of the same quality as IR-TUTOR to cover other areas of organic. The ability to rotate a computer visualization of a molecule in PCMODEL really seems to help students to conceive of molecules as three dimensional.

We have used MOBY and RASMOL in biochemistry to help students to understand protein and nucleic acid structure, and to understand how proteins can recognize large and small molecules. It is gratifying to see the improvement in student's understanding of three-dimensional structure that starts in organic chemistry make the transition to large biomolecules. The ready on-line access to biomolecular structure from the Brookhaven Protein Data Bank (FTP or FETCH) makes the display of proteins, nucleic acids, and the recognition of DNA by proteins easy. RNAFOLD and PROTYLZE can be used to predict RNA and protein structure, and the predictions can be compared with reality. This is important as the predictions are not always that good.

We have been using STN EXPRESS to teach students to access the chemical literature on-line. A Pentium electronic classroom is particularly well-suited to do this economically, as the instructor can demonstrate techniques useful to narrowing a search before the student goes on line. (You can also demonstrate how to narrow the search too much.) Counting "hits" shows the student the effect of operations like the logical AND. STN has run a seminar for faculty and students that was very valuable- I recommend it highly.

A plan of one of the tiered Pentium classrooms accompanies this article. We made a few minor mistakes- Rear Screen projection is a waste of time, space and money, and the lecturer's station should probably be a fixed podium, since by the time you get it connected to the projection TV, power, and the network it is essentially fixed in position. The omission of 35mm slide projectors was also a mistake, although presentation software can make up for some of this. But the projection TV system still has poorer resolution than the microcomputer screen or a 35mm projector. Partially for this reason, we are investigating the use of screen control systems and will be trying out software from ROBOTEL next year, in one of the Pentium classrooms that has been expanded to 35 microcomputers by ripping out the projection TV area.

Technology will never replace good teaching;

but visualization techniques and high quality instructional software can certainly improve undergraduate education. An investment of time and effort in these areas is most certainly worth the effort. I feel that the people who are "bashing" technology in the classroom need to use better software.

Hardware summary:

Macintosh Classroom

Powewmac 7100AV (80 mhz)
16 MB RAM
700 MB Hard drive
4X CD-ROM Drive
nubus AV card
System 7.5

Pentium Classroom

Compaq Pentium 90
16 MB RAM
420 MB Hard drive
4X CD-ROM
sound card
Windows NT 3.51 workstation

Lecturer Station ("front end")

same microcomputer as student sta-

tions

izer

Canon RE-650 MH IIN Video visual-

Pioneer LDV4400 Laser Disc player

Sharp two-head VCR

Audio/Video switch

Exxtron RGB 105 converter

Amplifier TCA Series 900, mono, NOT

stereo

Sony Multiscan VPH 1252Q three gun

projection TV

Custom designed cart from Anthrocart

A Web Page in Chemical Education

by Carl H. Snyder

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For several years I have been using e-mail in courses with the dual goals of adopting electronic communication as a pedagogical tool and inducing students to become familiar with e-mail for its

own sake. Here I describe briefly a minor disappointment in student response to e-mail, and an attempt at using Web quizzes to motivate students toward the use of the Web and electronic communication.

Undergraduates at the University of Miami can gain access to e-mail through two routes: 1) via individual, student accounts on a server dedicated exclusively to student use and 2) through class accounts on one of the University's mainframes. The individual, student accounts are private accounts, valid throughout a student's career at the University; the class accounts are class-based. They include all students registered for any given class and terminate at the end of the semester. The two are independent of each other; at any give time a student may have access to either, both or neither.

My own use of e-mail in classes has operated exclusively through class accounts. These have the advantage of providing easy construction of distribution lists, and liberal instructor privileges, including access to student directories and ease of determining the date of the latest student logon. In my initial foray into electronic communication I attempted to motivate students by awarding extra credit to students who submitted multiple-choice test questions electronically. Students created them and placed them in their own directories, and I used my own access to student directories to examine them. This work is described in "Applications of Networked Computers and Electronic Mail in a Chemistry Course for Nonscience Students," CHEMCONF '93: Applications of Technology in Teaching Chemistry, Summer, 1993, paper #11. Anonymous FTP: info.umd.edu Path:/inforM/EdRes/Faculty_Resources_and_Support/ChemConference. LISTSERV: CHEMCONF@umdd.umd.edu.

The results were disappointing. As noted in the reference, the higher-ranked students were generally "more likely [than lower-ranked students] to submit coursework electronically, perhaps because of differences in motivation and/or skills." Although I have discontinued this form of extra credit, I recently found the same trend appearing in logins taking place during the second semester of a nonmajors course that I currently teach. For those students who took the only examination given to date, the following data correlates the student's examination grade with the student's latest login date, as of 15 March 1996.

Grade	Login Date
94	never
89	08Mar
84	never
84	08Mar
82	never
80	07Mar
80	06Mar

79	never
76	07Feb
76	never
70	14Mar
68	12Mar
66	never
66	never
64	07Feb
62	07Feb
60	never
58	never
54	never
42	never

Paralleling the earlier, general correlation of class standing with electronic submission of extra-credit work, the examination grade appears to correlate roughly with the likelihood of a continuing interest in logging in. I find it disappointing to be unable to induce lower-achieving students to use electronic communication, even though I have tried a variety of inducements.

As a new form of motivation, I recently developed a rapid and easy method for converting multiple choice examinations into practice tests that can be placed on a Web page. Now students can not only gain access to file examinations posted on the Chemistry Web page, but they can take these examinations for practice at their convenience. (I have not yet worked out a satisfactory method to record a score or grade. Also, in what follows it's important to recognize that any student who wishes to and who knows the ways of the Web can read the html coding to uncover all the right answers quickly.)

Briefly, once the examination is at hand the process starts with a series of macros written for the word processing program I use. The general strategy involves:

1. Writing and using a macro that formats the multiple-choice answers for each question into a unnumbered list.
2. Applying a macro that produces a NO (wrong) html code for each one of the multiple choice answers.
3. Manually converting each correct answer from the NO into a YES (right) html code.
4. Using a macro to write an html NAME for each question.
5. Writing a small set of NO files, each of which states that an answer is wrong and allows return to the question.
6. Writing one YES file for each correct answer to provide a link to the next question (or, for the last question, to another portion of the Web page) via a NAME link.

I have converted nine file examinations into three sets of three practice examinations each and have placed

them in a Web page:

<http://www.ir.miami.edu/CHM/LO/102unit2a/quiz.html>
... /102unit2b/quiz.html
... /102unit2c/quiz.html

Using Web utilities to examine these quizzes and the related set of YES and NO files will reveal the details of the strategy. I have only recently placed these quizzes on the Web page, and am about to announce their presence to the class. Whether the availability of these quizzes on the Web page will motivate weaker students to log in and to use electronic communication will be the subject of a future article. Meanwhile, they are available for general examination and might serve as models for more sophisticated programs.

Review of Gaussian 94W

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Gaussian has long been the premier ab initio quantum chemistry program. Recently, another ab initio program, Mulliken, has appeared. However, Gaussian is the only one that will run on a PC platform. The full implementation is available in the Windows 3.1 environment. Gaussian has powerful molecular modeling features and will calculate optimum geometry and energy, vibrational frequencies, excited states, thermochemical properties, and a wide range of other molecular properties. Transition states and solvent effects may be investigated. Gaussian is not a display program. The user may directly communicate with molecular modeling programs such as PC Model and HyperChem for visualization of structures.

We have been using Gaussian 94W for the past eight months for a senior student research project, and lately in the quantum chemistry part of our physical chemistry course on a Pentium 75 MHz computer. Previously, we used Gaussian 92 on a 486 computer. The combination of the jump to Gaussian 94W, the Pentium based computer, and our experience has made Gaussian 94W an interesting and useful addition to our program. We also have the CAChe molecular modeling program running on a Power Mac to complement the ab initio calculations of Gaussian 94W.

The minimum requirements to run Gaussian 94W is an

Intel 80486/DX or higher, 16MB or more of memory, 80 MB of disk storage, 100 MB of scratch disk space, and Windows 3.1 or higher. The price is \$750 for a single machine copy for educational use. The program comes with a user reference guide and a text, *Exploring Chemistry with Electronic Structure Methods*. The text contains chapters with sample calculations to run. The sample files in the chapters are included in the tutor subdirectory in the program. All that you need is time on the computer to run the sample calculations to learn how to use Gaussian 94. Recently I upgraded my machine from 16 MB to 24 MB of memory. This increased the speed of calculations significantly by decreasing the need to swap files. The only problem we have had is the linking of calculations and this may be due to not trying hard enough. We have transferred the small amount of needed data manually. I am using Windows 3.1 and plan to install Windows 95 to see how the performance changes. The interface is easy to use. An understanding of Fortran is helpful in setting up and understanding the data files. The interface to run calculations is user friendly.

Gaussian 94W is an appropriate addition to the physical chemistry laboratory program. A recent flyer on the forthcoming 6th edition of Shoemaker, Garland, and Nibler's *Experiments in Physical Chemistry* indicates that they are including experiments using Gaussian 94W. We have calculated bond energies, thermodynamic properties, vibrational frequencies, potential curves, and equilibrium structures. Our calculations have been for two to four atom molecules. Most calculations have been the order of minutes with potential energy surfaces running to hours. Basis sets have been investigated. The results are compared with literature values and infrared spectroscopy experiments. Students are impressed by the accuracy of the calculations which run from a few to about ten percent. The calculations fit well into a four hour laboratory with the same molecule being investigated on the CAChe semi empirical program on a Power Mac. The potential energy calculation is run over night.

The senior research student is using Gaussian 94W and CAChe for his senior research thesis project. CAChe is used for preliminary work, displaying structures, and for complementary semi empirical calculations. Gaussian based calculations are the major part of the effort. After performing the tutor calculations in *Exploring Chemistry with Electronic Structure Methods* he has expanded to molecules of his own selection. He has explored the capabilities of Gaussian on the PC platform and has given himself a senior-first year graduate course in quantum chemistry. I have been impressed by his progress and accomplishments. Again, calculations have been restricted to small molecules to keep computation times down.

In conclusion, Gaussian 94W is worth the cost. Students will have an understanding of the ultimate in quantum computational chemistry. They should view programs such as Gaussian as another experimental instrument available to all chemists. If you need more information on Gaussian, order a copy of Exploring Chemistry with Electronic Structure Methods. This text should be in every undergraduate library.

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DIVISION OF CHEMICAL EDUCATION WWW SITE
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A CCCE subcommittee is beginning development of a website for the Division of Chemical Education. Suggestions are welcome, especially concerning useful chemical education resources on the internet. Please send comments or questions to any of the subcommittee members:

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Brian Tissue (chair), tissue@vt.edu
Theresa Julia Zielinski, theresaz@chem.wisc.edu

At the Clemson BCCE some discussion of the Division's website will occur at an open meeting of the Committee on Computers in Chemical Education (CCCE) on Tuesday, August 6 beginning at 12:30 PM. Check the BCCE program for additional details.

A FEW SITES ON THE WORLD WIDE WEB

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Articles on the World Wide Web (WWW) and sites (URLs) have appeared in a number of recent CCE Newsletters. The Fall 1995 issue (p. 3) contained an article by Tom O'Haver entitled "Surfing the Net with Netscape", and recent issues of the CHED Newsletter have featured similar articles (e.g. see Theresa J. Zielinski's article (p. 44) of the Spring 1996 Newsletter). The World Wide Web is being used in courses and conferences. The ACS has a WWW site (<http://www.ACS.org>). The Division of Chemical Education is developing a WWW site. In this brief note I would like to identify a few additional sites which you may be interested in exploring.

<http://www.wam.umd.edu/~toh/Chemistry.html> This home page provides clickable links to many Internet materials which are of interest to chemical educators.
<http://owl.qut.edu.au/oz-teachernet/> Click on "Online Training" and examine "Internet Guides" and "Exploring the Internet Now". These provides valuable resources for exploring the Internet and help for developing your own World Wide Web materials.

ON-LINE CONFERENCE ON "NEW INITIATIVES IN CHEMICAL EDUCATION" **JUNE 1 TO JULY 19, 1996**

This summer an on-line conference will be held utilizing the World Wide Web for distribution of abstracts and papers (the URL is <http://www.wam.umd.edu/~toh/ChemConf96.html>). Questions and discussion will occur using Listserv. (To subscribe to the Listserv send the message:

SUBSCRIBE CHEMCONF your-first-and-last-name
To: LISTSERV@UMDD.UMD.EDU
or LISTSERV@UMDD.BITNET).

Thomas C. O'Haver will manage the World Wide Web and Listserv resources. Donald Rosenthal will chair the sessions.

The Conference schedule, list of speakers and titles of papers are presented below. Abstracts for each of the papers are presently available via the World Wide Web.

For additional information, contact:

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SCHEDULE:

April 8 to June 1 - Participants will register for the Symposium.

There is no registration fee.

June 1, 1996 - Papers will be made available for SESSION 1

June 3 - June 7 - Short Questions for Papers 1 to 5
Paper 1 on Monday, Paper 2 on Tuesday, etc.

June 10 and 11 - Discussion of Paper 1
Jerry A. Bell and Andrew Ahlgren
American Association for the Advancement of Science
"What is AAAS Project 2061? Why Should Chemists Care?"

June 12 and 13 - Discussion of Paper 2
George M. Bodner
Purdue University
"Mental Models: Implications of Differences Between Students and Their Instructors"

June 14 and 17 - Discussion of Paper 3 (LORETTA JONES)
Loretta L. Jones
University of Northern Colorado
"The Role of Molecular Structure and Modeling in General Chemistry"

June 18 and 19 - Discussion of Paper 4
Brian Tissue
VPI and State University
"Development and Delivery of Chemical Education Hypermedia Using the World-Wide Web"

June 20 and 21 - Discussion of Paper 5
John W. Moore, Jon L. Holmes, Elizabeth A. Moore,
Nancy S. Gettys and Lin W. Morris
University of Wisconsin - Madison
"What Should a Chemical Education Journal Be in an Age of Electronic Information?"

June 22 - Papers for Session 2 will be available

June 24 - June 28 - Short Questions for Papers 6 to 9

July 1 and 2 - Discussion of Paper 6
Henry Rzepa and Omer Casher
Imperial College - London
"Recent Applications of Hyperactive Chemistry and the World-Wide-Web"

July 3 and 8 - Discussion of Paper 7
Stanley Smith and Iris Stovall
University of Illinois - Urbana
"Networked Instructional Chemistry"

July 9 and 10 - Discussion of Paper 8
Paul Kelter and James D. Carr
University of Nebraska - Lincoln
"Personalizing the Large General Chemistry Lecture Experience"

July 11 and 12 - Discussion of Paper 9
Gary Wiggins
Indiana University
"Use of the Internet in Teaching Chemical Information Courses"

July 15 - July 19 - General Discussion and Evaluation
The papers and discussion will be archived and available at the World Wide Web site (<http://www.wam.umd.edu/~toh/ChemConf96.html>) after July 19.

FUTURE ON-LINE INTERCOLLEGIATE AND INTER-SCHOLASTIC COURSES

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I. INTRODUCTION

One recent initiative of the ACS Division of Chemical Education's Committee on Computers in Chemical Education (CCCE) is the development of intercollegiate and interscholastic on-line courses. Such courses are intended to be collaborative efforts with course instructors at each school. In planning such courses the Committee solicits ideas and needs volunteers to serve on organizing committees and as course instructors at participating school.

Discussion of on-line courses will occur at an open meeting of the CCCE to be held at the BCCE at Clemson on Tuesday, August 6, 1996. Those unable to attend the meeting may send ideas and suggestions or volunteer to participate by contacting me. In the follow-

ing paragraphs, I will outline some of the characteristics and possible scenarios for courses.

The first course sponsored by the CCCE was entitled "Environmental and Industrial Chemistry" and was offered during the Spring 1996 semester. An article on this course appears elsewhere in this Newsletter.

II. STUDENTS

A course could be offered for credit or not for credit to:

- A. A general audience of Students
- B. Pre-High School Students
- C. High School Students
- D. Two-Year College Students
- E. Underclass College and University Students
- F. Upperclass College and University Students
- G. Graduate Students
- H. Some combination of the above.

III. SCOPE OF THE ON-LINE SEGMENT

The on-line segment might constitute: A. a small part of a traditional course, B. a major part of the course, or C. most or almost all of the course.

An example of situation A - The trial session of the course on "Environmental and Industrial Chemistry" was part of physical chemistry courses and featured a paper on flames. Only a few weeks were devoted to this segment. (See discussion elsewhere in this Newsletter.)

Examples of situations B and C - In the course "Environmental and Industrial Chemistry" participating course instructors had considerable latitude in structuring their local course. Some course instructors required considerable off-line activities - class meetings, preparation of papers, etc. Other instructors required little other than participation in the on-line segment.

IV. NATURE OF THE ON-LINE AND OFF-LINE SEGMENTS

A. Listserv, Bulletin Board and/or World Wide Web available for distribution of:

1. Student papers
2. Expert papers
3. Student Questions
4. Questions from authors of papers
5. Answers to questions
6. Discussion
7. More or less formal debates on specific issues
8. Assignments
9. Other resource materials, e.g. graphics, film clips, audio, and links to WWW sites.
10. Computer Assisted Instruction materials

B. Off-Line:

1. Textbook
2. Class meetings
3. Assignments
4. Discussion
5. CD ROM and other materials

In many of the participating schools the course on "Environmental and Industrial Chemistry" included A-1 to 6 and B-2 to 4.

A course might include traditional components (B-1 to

4) and provide only discussion and the answering of questions on-line (A-3, 5 and 6).

V. COURSE PLANNING

Central to the development of a course is:

A. A course Chairperson B. A Course Organizing Committee - there may or may not be one. C. Course instructors at each participating school are essential in the model we propose.

In the "Environmental and Industrial Chemistry" course the Organizing Committee defined the nature of the on-line segment. Course instructors were responsible for off-line activities - class meetings and discussions, the assignment of student papers, examinations (if any) and course grades. In addition, each course instructor had the responsibility for familiarizing his students with the e-mail system, the Listserv and the World Wide Web.

D. Students may or may not participate in the planning process. One interesting possibility is that students help define the kind of course which is offered. The course is then developed with the assistance of V-A to V-C.

VI. COMPUTER SERVICES - THEIR NATURE AND ADMINISTRATION

A. A Listserv, Listservs and/or a Bulletin Board In the "Environmental and Industrial Chemistry" course two Listservs were established at Clarkson University. One (OLCC-FAC) was initially used by the Organizing Committee and at a later stage course instructors and expert authors were signed on. This was a private list. No one other than those I added was able to send or receive messages from the list. Besides being used by the organizing committee OLCC-FAC was used by course instructors and expert authors to exchange ideas, ask and answer questions and discuss various matters.

The other Listserv (OLCC-STU) was managed by George Long and me. It was a public Listserv (i.e. anyone could sign on, but the subscription had to be confirmed). Messages could only be sent or retrieved by subscribers. This list was intended for students and the authors of papers. Course instructors were asked to sign on but not participate in the on-line discussions. James Beard (the course chairperson and chair of the Organizing Committee) sent some announcements to this list. The list might have been moderated so that any message sent to the list was received by the list manager who then decided whether to distribute the message to the subscribers. Neither OLCC-STU nor OLCC-FAC was moderated.

B. A World Wide Web site (WWW)

In the "Environmental and Industrial Chemistry" course George Long managed the course website. The papers and much of the course information was distributed from this site. The papers and OLCC-STU discussion are archived at this site (<http://dirac.py.iup.edu/college/chemistry/chem-course/webpage.html>). While it is not essential that a WWW site be established, the presence of a site makes it easier to transmit papers, graphics and multimedia materials. The website manager controls information which is distributed via the site.

C. Access to e-mail and the WWW at each of the participating schools

Each student and course instructor needs to be able to access the appropriate Listserv and WWW.

VII. SOME ADVANTAGES OF ON-LINE COURSES

Offering a new or different course can be a formidable undertaking for an isolated teacher particularly if it involves the use of what may be new computer technologies. Few of us can afford to do this for one or a very few students. Bringing outside experts on campus may simply not be feasible.

Intercollegiate or interscholastic courses are collaborative efforts and can involve educators and outside experts assuming different individual responsibilities in producing a rich learning environment. Such courses provide a learning experience for teachers as well as students.

A. Some advantages for course instructors Provides an opportunity to: (1) collaborate with others in designing a course (2) interact with students, authors of papers and other instructors (3) involve experts (might be difficult because of geography, attracting experts to a course containing a very few students) (4) offer a course for a small number of students without having to devote an enormous amount of time (5) offer courses on topics which might otherwise not be possible.

B. For students Provides an opportunity to: (1) interact with other students, experts and other instructors (some from different parts of the country or world, some having very different points of view) (2) take a course on a topic which might not otherwise be available (3) collaborate with other students (perhaps even at different schools) in preparing papers or researching a topic.

VIII. WHAT NEXT?

The CCCE is prepared to ASSIST teachers in organizing on-line courses.

A course topic is needed - it could be General Chemis-

try, Environmental and Industrial Chemistry or anything else. One topic that was suggested at the BCCE meeting at Bucknell was "Careers in Chemistry". This seemed like a very good idea to me. As I visualize such a course, chemists in sales, management, research and development and teaching could talk about what they do and what opportunities exist in their fields. I believe upperclass chemistry students who are beginning to think about life after college would be interested in such a course.

Volunteers are needed to serve on an Organizing Committee and a Chair is needed. In the one course which has been offered, a Chair volunteered. We helped him to recruit a Committee. The course topic was selected by the committee after the committee was formed. (It does not have to be that way.)

The Organizing Committee will need to recruit course instructors at other schools. Authors of papers may be needed. Individuals are needed who are willing to manage the Listservs and Websites. The CCCE is prepared to assist in these recruiting efforts.

We are hoping to find a few good men and women who are willing to devote time and effort to organize courses. Please contact me (rosen@clvm.clarkson.edu) if you have ideas and wish to help OR come to the open meeting at the Clemson BCCE.

ENVIRONMENTAL AND INDUSTRIAL CHEMISTRY An On-Line Intercollegiate Course For Upperclass Chemistry Students Taught During the Spring 1996 Semester

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INTRODUCTION

During the summer of 1993 the Committee on Computers in Chemical Education (CCCE) sponsored the first on-line conference offered by the ACS Division of Chemical Education. At the conclusion of the Conference informal discussion of a number of topics continued. One suggestion which was made was that on-line intercollegiate courses be offered. Discussion of on-line courses (and conferences) occurred at an open meeting of the CCCE held at the 13th Biennial Conference on Chemical Education (BCCE) at Bucknell University during the summer of 1994. A number of useful suggestions were made. One

result of these discussions was that James M. Beard (Catawba College, Salisbury SC) agreed to recruit and chair an Organizing Committee which would plan and oversee an on-line course.

THE ORGANIZING COMMITTEE

The Organizing Committee consisted of James M. Beard (chair), Reed Howald (Faculty Coordinator and Trial Session Organizer - Montana State University, Bozeman MT), George R. Long (Technical Advisor and WWW Manager - Indiana University of Pennsylvania, Indiana PA), Maria D. Pacheco (Content Coordinator - SUNY College at Buffalo) and Carl H. Snyder (Publicity - University of Miami, Coral Gables FL). I served as chief kibitzer.

PRE-COURSE PLANNING AND ACTIVITIES

A private Listserv, OLCC-FAC, was established so that Committee members could readily communicate with each other. Any message sent to OLCC-FAC was distributed to all members of the Organizing Committee and archived in a Filelist. In the on-line discussions which occurred over several months decisions were made about the structure and nature of the course.

It was decided that the name of the course would be "Environmental and Industrial Chemistry". The course would consider what chemical industry and chemists are doing to solve environmental problems and reduce and minimize the effects of chemical manufacturing and chemical use upon the environment. Each instructor at a participating school would be asked to organize a course at his/her school. The exact nature of each course might be different, but there would be a formal on-line component extending from February 5 to April 19. During this on-line segment three papers would be presented by industrial chemistry experts and there would be two papers presented by students or groups of students from the participating schools.

The two student papers were to be selected from papers prepared by students who were taking the course. A list of some topics which might be used for student papers was prepared and distributed to participating faculty instructors.

The on-line segment would consist of discussion of five papers with two weeks being devoted to each paper. Students would download the papers from a course World Wide Web which was established and maintained by George Long using facilities provided by Indiana University of Pennsylvania (<http://dirac.py.iup.edu/college/chemistry/chem-course/webpage.html>). After reading the paper, there would be discussion in class of the paper. Questions and com-

ments would then be sent to the author and students using a Listserv, OLCC-STU. (George Long and Donald Rosenthal managed OLCC-STU using a Listserv and facilities provided by Clarkson University.) Only students, the authors of papers and Jim Beard as Chair of the Organizing Committee were to send messages to OLCC-STU. OLCC-STU was intended to serve as a vehicle for discussion between students and authors and between students. Course instructors were asked to subscribe to OLCC-STU and monitor the discussion. The above listed activities would occur during the first week. During the second week there would be another class meeting at each school and additional questions and answers and open discussion of the paper via OLCC-STU.

The CHED Newsletter, this Newsletter and the on-line Chemistry Discussion List, CHEMED-L, were used to publicize the course. Carl Snyder prepared an on-line course registration form and handled the registration process.

In recruiting the industrial chemists to serve as authors of papers, the Organizing Committee made suggestions, but Jim Beard and Maria Pacheco actively recruited the authors.

It was suggested that a trial session be held during the Fall 1995 semester. Reed Howald chaired this session and Theresa J. Zielinski (Niagara University) prepared a paper which was discussed by students at a number of different schools who were taking Physical Chemistry.

THE SPRING SEMESTER COURSE PARTICIPATING SCHOOLS

There were approximately 104 students from twenty-two schools registered for the course. Listed below are the schools which participated, the course instructors, followed in parentheses by the number of students who registered.

Bryn Mawr College, Bryn Mawr PA Dr. Michelle M. Franci (8) -- Buffalo State College, Buffalo NY Dr. Maria Pacheco (7) -- Catawba College, Salisbury SC Dr. James Beard (1) -- Concordia University, Austin TX Dr. James N. Stevenson (3) -- Indiana University of Pennsylvania, Indiana PA Dr. George Long (6) -- The King's University College, Edmonton AB, Canada Dr. Peter G. Mahaffy (2) -- Mississippi Valley State University, MS Dr. Mudligari Goli (1) -- Missouri Western State College, St. Joseph MO Dr. Leonard Archer (5) -- Montana State University, Bozeman MT Dr. Reed Howald (2) -- Nanyang Technological University, Singapore Dr. Thiam-Seng Koh (6) -- Niagara University, Niagara University NY Dr. Mary M. Schreiner (4) -- Pembroke State University Dr. Paul

Flowers (7)--Samford University Dr. James Fisk (7)--Southwestern Oklahoma State University, OK Dr. Sylvia Esjornson (13)-- University of Dallas, Dallas TX Dr. William H. Hendrickson (7) --University of Miami, Coral Gables FL Dr. Carl H. Snyder (1)-- University of Nebraska at Omaha, Omaha NB Dr. James A. Carroll and Dr. Frederic C. Laquer (2)-- University of Redlands, Dr. Barbara Murray (3) --University of Tennessee at Martin, Martin TN Dr. Michael Applequist (3)-- University of Wisconsin - Platteville, Platteville WI Dr. Charles E. Sundin (3) --Walla Walla College, Walla Walla WA Dr. Richard F. Daley (2)-- York College of Pennsylvania, York PA Dr. Lindy Harrison (12)

The number of students at each of the participating schools varied from one to thirteen. Obviously, on the local level a course with one student would be handled differently from a course having thirteen students. Nanyang Technological University in Singapore had computer problems and they were not able to fully participate.

FACULTY ON-LINE PARTICIPATION

The Listserv OLCC-FAC was used by course instructors, expert authors and the organizing committee to interact with each other. OLCC-FAC was configured as a private list. Initially the list was used exclusively by the organizing committee. At a later stage the course instructors and expert authors were added. Early drafts of the expert papers were distributed via OLCC-FAC and course instructors had an opportunity to send comments and suggestions to the authors. These comments resulted in revision of the papers. OLCC-FAC provided a forum in which questions could be asked and answered and information could be sent to instructors, authors and the organizing committee. Course instructors were added to OLCC-FAC at the beginning of 1996. From January 2 to March 21 (about the time this article was written), 258 different messages were sent via OLCC-FAC. (OLCC-FAC was managed by Donald Rosenthal using facilities provided by Clarkson University.)

THE EXPERT PAPERS, THEIR AUTHORS AND OLCC-STU DISCUSSION

The final versions of papers were made available via the World Wide Web. The first paper discussed was entitled "The Chemical Manufacturer's Association's Product Stewardship Program" and was submitted by Michael Trehy an analytical chemist at Monsanto Company. Dr. Trehy develops methods and provides analytical support for environmental testing as well as performing environmental risk assessment for new and existing products. His paper emphasizes the commitment of American industry to improvement and responsible care and describes present practices and future directions. The second paper entitled "The Effect of Ozone Depletion and Global Warming on the Cleaning Industry" was authored by Stanley S. Seelig, President of Seelig and Associates, Inc. a consulting group which helps users choose the best chemis-

try and equipment for their cleaning and drying operations. He is a Director on the Board of the Chicago ACS Section, Public Relations Chair of the Industrial and Engineering Chemistry (I&EC) Division of the ACS and Chair-Elect of the Practical Pollution Prevention subdivision of I&EC. In his paper he discusses ozone depletion, global warming, cleaning before and after ozone depletion and global warming regulations and future cleaning and drying methods.

John Armor presented the third paper entitled "Environmental Catalysis". Dr. Armor is at the Corporate Science and Technology Science Center of Air Products and Chemicals, Inc. His principal areas of research and development include catalysts and adsorbents synthesis, materials research and catalyst testing. His paper considers the nature of catalysis and catalysts, the ways catalysts can solve environmental problems, emission of greenhouse gases in the USA, selective catalytic reduction to abate greenhouse gases and future research and development needs in environmental catalysis. On-line discussion of these papers via OLCC-STU occurred between February 5 and March 23. By March 23 there had been 454 messages exchanged - questions, answers and discussion plus a few announcements.

The papers and messages are archived at the World Wide Website: (<http://dirac.py.iup.edu/college/chemistry/chem-course/webpage.html>).

STUDENT PAPERS AND ON-LINE DISCUSSION OF TWO STUDENT PAPERS

It was suggested to course instructors that students be asked to write a paper for the course and that those papers deemed worthy of extended on-line discussion be forwarded to George Long for posting on the website.

The ten student papers which were posted on the WWW were: A. "Vitrification of High-Level Radioactive Waste at the West Valley Demonstration Project" by Mike D'Angelo, Jim Fox, Erik Ricker and Stacy Young of Niagara University. B. "Risk Assessment of Toxic Chemicals: The EPA Regulations and Procedures" by Teresa A. Hill of Catawba College. C. "Bhopal: The Disaster and the Aftermath" by Mitch Brantley, Lisa Kruse and Ryan Draiss of Samford University. D. "Love Canal: An Overview of the Toxic Waste Dump That Brought the Chemical Industry to Its Knees" by Bill Davidson, Kristie Hoek, Carrie Smith and Alline Peeler of Samford Uni-

versity. E. "Superfund - Expanding the Opportunities for Lawyers, Chemists and Bulldozers" by Christopher Archer, Kimberly Meier, Mark Stockmyer, Michael Wing and Phillip Zweerink of Missouri Western State College. F. "An Assessment of Reformulated Gasoline" by Brendan Lowrey and Benjamin Lasseter of the University of Dallas. G. "A Summary of The Clean Air Act as Amended in 1990" by Michael G. Montague and Kevin Lensing of the University of Dallas. H. "Study of Chemical Fire and Subsequent Chlorine Release" by Saadia Khan and James Kenny of the University of Dallas. I. "What Happens When You Harness the Atom: Evaluating current disposal and storage options as well as today's environment" by Stacy S. Blystone, Laura Markowski and Jeff Stiffler of Indiana University A and E for extended on-line discussion. Paper F received honorable mention. As this article is being written on-line discussion of Paper A has begun. All the above-listed student papers and discussion of Papers A and E are available on the course website.

AFTER THE ON-LINE DISCUSSION OF PAPERS

The on-line discussion of papers is scheduled to end on April 18. The authors of papers, course instructors, students and members of the organizing committee will be asked to evaluate the on-line course to indicate what worked well and what did not work very well. They will be asked to make suggestions which will be helpful in planning future courses. Also, information will be obtained about the off-line components of the courses. Some course instructors have asked that OLCC-STU be available for student use after April 18. Much less structured discussions are expected to occur.

OTHER RELATED ACTIVITIES

One or more additional articles will be written once the courses on "Environmental and Industrial Chemistry" have ended and the evaluation forms have been analyzed. Papers will be presented at the BCCE and Fall 1996 ACS Meeting in Orlando discussing the course. Members of the Organizing Committee and course instructors will be attending the BCCE at Clemson and discussion of this course and future courses will occur at an open meeting of the CCCE on Tuesday, August 6. See the article on future on-line courses elsewhere in this issue.

Advanced Molecular Modeling in Undergraduate Teaching at Clarkson University **Yuzhuo Li and James Peploski** **Department of Chemistry Clarkson University**

Advanced molecular visualization and simulation have been extensively used in the teaching of

undergraduate students at Clarkson. Clarkson University was the first university in the nation to issue a personal computer to each entering freshman. This practice will end this year as the campus network, linking dorm rooms to the university computer system, is completed. The chemistry department began to introduce students to the benefits of computers in organic chemistry using software developed at Clarkson called M6. Students could construct molecules by entering atomic coordinates and manipulate the molecules using a set of keywords. The three-dimensional nature of organic structure could be analyzed using the computer in addition to the traditional molecular modeling kits. A generous gift from IBM in 1989 allowed Clarkson to establish two advanced computer classrooms equipped with an array of state-of-the-art IBM RISC workstations. Each classroom allows up to 50 students (working in pairs) to explore the world of computational applications in science and engineering. In 1990, the modeling application PCModel (Serina Software of Indiana) was first used in organic chemistry lecture courses. Molecules could be constructed using a mouse driven interface and powerful computational features were available for molecular investigations. Students were introduced to the topics of molecular mechanics and semi-empirical energy and structure calculations. Students were able to determine molecular geometries, dipole moments, enthalpies of formation and other molecular properties which otherwise could only be determined by time consuming and advanced level laboratory studies. One of the first computational laboratory experiments performed in the classroom was an investigation of the nucleophilic substitution reactions of alkyl halides. By varying from methyl halides to t-butyl halides, the steric hindrance effect on the SN2 reactions was clearly illustrated. For SN1 reactions, the inability for a bridge halide to form a planar carbocation could easily be shown.

The rapid development of educationally oriented applications such as Hyperchem and Spartan, allowed for the incorporation of computational laboratory exploration in general chemistry. One of the RISC classrooms was equipped with specialized 3D graphics cards to allow for real time manipulation and motion of molecules. The ability of students to work separately on different molecular systems (extremely difficult in a conventional laboratory setting) and conduct independent investigations have lead to the development of a unique classroom experiment. Each group of students conducts a series of computational investigations on a different molecule. As the information is collected, it is reported to the entire class. As the investigations proceed, a database of information is collected for interpretation by the class. The large amount of information allows students to make broad conclusions about chemical properties and how these properties are

related to molecular structure. Currently, one third of freshman laboratories are conducted using computational investigations. Student interest and excitement have been high. The advantages of this type of approach are twofold. First, students benefit from a laboratory environment which more closely resembles a real work setting. Cooperation and communication between research groups are highlighted. Further, since the conclusions of an entire group are based upon individual results, the reliability of individual results is stressed. This type of laboratory greatly enhances the undergraduate chemistry experience. By working as a team, drawing conclusions from the results, and highlighting the connection between the molecular and macroscopic world, students will be able to see the importance and influence of chemistry regardless of their chosen fields of study. Secondly, a smaller group of science majors will fine tune their understanding of key concepts while gaining an understanding of the process involved in developing effective learning tools. In organic chemistry laboratory, students were asked to compute the electron densities on a benzene molecule with a range of substituted groups. Examination of the electron densities on the ring and the distribution of molecular orbitals allow students to investigate the seemingly contradictory behavior of electron withdrawing ability (through sigma bonds) and the electron donating effect (through p-pi conjugation). Students were surprised to find that electron density in the ring was greater for fluorobenzene than for chloro- or bromobenzene. The relative importance of the two effects changes when the bond length between the ring and the halogen atoms was varied. The relative importance of the p-pi conjugation effects could be clearly illustrated for nitrogen (amino), oxygen (hydroxyl), and halogen (chlorine). Investigation of these types of phenomena would have been virtually impossible in a conventional laboratory setting. Students tend to have a much better understanding of the concepts afterwards.

In computational chemistry courses students use research oriented computational packages. Gaussian (90, 92, and 94) is used in the investigation of both ground state and excited state molecules. The influence of solvents on the properties of both ground and excited states was examined. Students examine the computational resources required to achieve accurate results. For example students used various methods including density functional theory to investigate the acidity of excited phenols and aromatic carboxylic acids through calculation of Forster Cycles. The concept of pharmacophore and its potential applications in rational drug design also intrigued students.

While modeling is an important method for the determination of molecular properties, it is often difficult to

illustrate the relationship between these properties and the corresponding bulk system characteristics. Furthermore, since true molecular modeling is relatively new to chemical education, few laboratory procedures are available which illustrate fundamental chemical principles and are suitable for inclusion in the undergraduate curriculum. Thus, new investigatory procedures must be developed as the curriculum evolves. The amount of time necessary to develop an effective undergraduate laboratory is considerable, and in the case of classroom experiments where a large number of systems need to be investigated, the time investment can be prohibitory. We have recruited a group of highly motivated junior and senior chemistry majors interested in both computational applications and the development of educational tools. These students have the responsibility to identify those concepts which are most highly suited to computational investigation and develop a computational laboratory procedure which will clearly illustrate those principles. Students should be viewed as an outstanding source of new ideas and feedback which cannot be overlooked when developing new approaches to instruction.

After careful evaluation of various computational packages, the School of Science and the New York State Center for Advanced Materials Processing at Clarkson University (CAMP) have licensed one of the most advanced and comprehensive computational packages presently available. Biosym, which provides highly diverse molecular structure and property prediction features, is now being incorporated into the undergraduate curriculum. One of Biosym's greatest strength is its flexibility. Modules are designed to investigate key concepts in biochemistry, polymer chemistry, crystal structure, other areas of chemistry and related fields. Another strength of the Biosym package is the emphasis placed on arriving at macroscopic system properties. This allows for easier illustration of the connection between the microscopic and macroscopic worlds.

Biosym is currently being integrated into Dr. Linda Lucks's senior level biochemistry course. Crucial to this course is the visualization of proteins with solved structures and the production of three-dimensional models consistent with experimental data when structures are not known. Students investigate important structural characteristics of DNA and of proteins including secondary structure and features of the active site. Biosym has also been incorporated into Dr. Ramesh Patel's inorganic chemistry course. Students investigate molecular crystalline structures including zeolites. Students were able to construct the crystal lattice from unit cell data, display and examine Miller planes, and determine interatomic distances within the structures. Biosym was developed as a tool intended for research investigations. Students now have available to them, a tool

capable of producing high quality, publishable results. Undergraduates involved in independent study courses use these packages to conduct research on topics such as ozonolysis of excited state aromatic compounds or determination of the structure of metal oxides.

Students readily accept calculated or simulated results. It is a valid concern that they may be too receptive. It is our responsibility to help the students realize the limitation of molecular modeling and simulations. For example, computational results usually reproduce or predict some molecular properties such as dipole moment and charge density distribution for a molecule with good accuracy. However, the absolute energies calculated for the Foster cycle are far from reliable. In this case, the students are reminded that the trend of data is more trustworthy than their absolute values. Students should realize that computational methods do not always lead to valid conclusions.

Overall, using advanced molecular modeling and simulation packages in undergraduate teaching is both an exciting and rewarding experience. When they are systematically integrated into undergraduate courses, molecular modeling and simulations provide students much greater flexibility in learning and understanding key chemistry concepts. Our efforts reflect the increasing practice of using a computational approach to solving real world problems. In industry, the demand for qualified personnel, capable of solving problems using both computational and experimental approaches will only increase. As computational investigations become more common in the workplace, students will need hands-on experience using computational tools to be competitive in the job market and graduate schools.

On-Line Student Interaction for Learning Physical Chemistry.

by George Long, Reed Howald, Carol Ann Miderski and Theresa Julia Zielinski

During the Fall of 1995 students from three geographically separated chemistry departments participated in an on-line learning experience in physical chemistry. There were three reasons for this two week experiment. First, the segment would serve as a short test, i.e. a trial run, of the operating procedures for a longer full semester course entitled "Environmental and Industrial Chemistry" that was planned for the Spring 1996 semester (see the article by Don Rosenthal that also appears in this newsletter). Second, there was a need to assess

student response to this use of technology in teaching a chemistry topic. Third, the Web site manager, George Long, needed to test the structure and operation of the Web site prior to the start of the full semester on-line course. The three departments involved in the experiment were located at Niagara University (6 students), Indiana University of Pennsylvania (9 students) and Catawba College (5 students). The listserv manager for this on-line experiment was Don Rosenthal.

The scientific content for the trial run was a short paper that described the estimation of flame temperatures. The paper, a case study, was posted on the IUP chemistry department WWW page. Students obtained the paper at the start of the mini-session/conference and then proceeded to develop their expertise in the topic through interaction with each other in their own classes and with peers from the other the other participating campuses through the listserv at Clarkson University. The faculty involved in the project hoped to recreate a CHEMCONF experience for the students.

The flame case study paper used in the student mini-conference can be found at two WWW sites. The original paper and all accompanying documents are located at <http://www.py.iup.edu/college/chemistry/chem-course/trialrun.html>. A copy of the paper with corrections added along with other some associated files can be found at <http://www.niagara.edu/~tjz> under Case Studies. Interested readers are encouraged to check out these Web sites to access the original case and the accompanying files. The file containing the diary of the on-line discussions is especially interesting.

Overall the project was well received by the small set of faculty and students involved. Some important conclusions were drawn from this trial run. First, faculty involved in the process had very different expectations of what should be accomplished. These different expectations, as well as different teaching styles and course organization made bringing even this small group together a challenge. It was important to designate one individual to be the expert for a topic and the guide for the student interactions on the listserv. The expert in this case, TJZ, preferred a style in which the students would work among themselves to learn and resolve any problems in the case study, i.e. operate in a discovery/cooperative learning mode.

One difficulty encountered was the ease or lack of ease with which students could access the WWW and computer stations for using e-mail. One important observation was that the students had different levels of expertise in the use of e-mail and some were not used to and did not respond well to the use of it as a learning device. It was also apparent that the three different instructors fostered participation in the project to different degrees.

The class at IUP was the most involved in the project and entered the highest number of postings. They also completed the project with a very high degree of excellence. The IUP students prepared excellent reports and Mathcad documents. Some of these can be found at the IUP web site. It should be noted that for the IUP students participation in this project counted as 10% of their final grade for the course; this was a significant incentive. The NU students participated to a lesser degree. They and their instructor were content to use the mini-conference to study the problem posed in the case and to understand the process in the solution. Comprehension was assessed as part of their normal exam hour exam schedule; exam success on this topic was directly correlated with degree of participation in the on-line process. Closure for the NU students was adequate but not as well developed as that achieved by the IUP students. The students at Catawba College met serious network and computer access difficulties and their participation diminished as a consequence.

Student assessment of the on-line learning was collected. The result was that overall, the process was a moderate success. This is understandable in terms of network difficulties and student lack of experience in dealing with alternative learning environments. Nevertheless, this outcome is a concern for teachers of young scientists. Our students need to use the Internet and WWW to accelerate their own learning and enhance their access cutting edge information in any field of future study.

This small study may be important in that it provides a good example of how the Internet can be used as a non-traditional instructional tool. The WWW can surely be used to provide our students with the communication and research skills and tools that they will surely need in their careers. We can't let e-mail and Web use be just another after school activity; it will work best when it is an integral part of the of the educational experience. As a result of this study we have the following suggestions for all teachers. First, that we provide students with personalized help in starting to use e-mail and the WWW. Next, we suggest making time for this in the curriculum by using it in the classroom for original projects and learning experiences in addition to the delivery of information.

A paper with a more detailed description of the project and an analysis of faculty and student assessments is being prepared for submission to the new on-line chemical education journal, The Chemical Educator. TJZ thanks GL for putting the Flame manuscript in html format and getting her started with html. A copy of this newsletter article can be found at url: http://www.niagara.edu/~tjz/dpapers/flame_news.htm.

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**New Chemistry and Computers Book on the Horizon Theresa Julia Zielinski
Niagara University**

Publication of the book entitled "What Every Chemists Should Know About Computing" nears completion. The editors of this volume, Theresa Julia Zielinski of Niagara University and Mary L. Swift of Howard University, are collecting the final drafts of the 19 chapters included in the volume. Given the widespread use of computers in the practice of chemistry and the advances in commercially available software and hardware the editors and contributors are bringing their expertise to bear on the ways that changes in curriculum and pedagogy can lead to better training of the next generation of chemists.

The major goal of the effort in this volume is to provide chemistry faculty, graduate students, and others interested in science education with a resource for the development and implementation of effective and modern uses of computers for chemistry instruction. The contributing authors have developed chapters that are grounded in the realities of the current computing environment at a wide range of post-secondary institutions. The focus is on bringing modern computer usage into the classroom by providing the reader with a vision of what is done in research and industry and how that can be translated into real classroom experiences. The final manuscripts will be in the hands of the editors on or near April 15. The expected date of appearance of the volume is late Fall 1996 or Winter 1996. The publisher is ACS Books.

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SUMMER 1997 AND 1997-1998 SCHOOL YEAR ON-LINE CONFERENCE

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Information on the Summer 1996 On-Line Symposium appears elsewhere in this Newsletter.

Another on-line Conference featuring "General Papers in Chemical Education" will be held during the summer of 1997 and the 1997-1998 school year.

INTERNET COMPONENTS

All papers will be posted on a WWW site at the University of Maryland. Authors of papers may post their papers on their own local WWW site to which links will be established from the Conference site, or authors may provide papers to Tom O'Haver either with or without HTML mark-up.

CHEMCONF will be used as the Conference Listserv. Some announcements will be sent out prior to the beginning of each session. CHEMCONF will be used for discussion between authors and participants and for discussion between participants.

THE SUMMER 1997 SEGMENT

The format of the summer sessions will be similar to that of the summer 1996 symposium. Each session will be three weeks in length and will feature five papers. The papers will be available on the World Wide Web (WWW) at least a week before the beginning of each session. The first week of the session will be used for short questions directed by participants to the authors or other participants. During the second and third weeks, two days will be devoted to the answering of short questions and discussion of each paper. (For example, short questions relating to paper 1 will be sent via CHEMCONF during Monday of the first week. Answers to short questions and discussion of Paper 1 will occur on Monday and Tuesday of the second week.)

Depending upon the number of papers received there will be two (9 paper) or three (14 paper) sessions. The dates for the sessions will be June 2 to June 20 for Session 1, June 23 to July 11 for Session 2, and July 14 to August 1 for Session 3 (if needed). There will be one week for general discussion and evaluation at the end of the Summer segment.

THE 1997-1998 SCHOOL YEAR SEGMENT

The length of the school year segment will depend on the number of papers submitted. One week will be devoted to short questions and discussion of each paper. Short questions will be sent on Friday and discussion will extend from Monday through Thursday.

The first session will extend from September 5, 1997 to November 26, 1997 with room for a maximum of eleven papers. The second session will extend from January 30 to May 1, 1998 with room for a maximum of twelve papers. The last week of each session will be devoted to general discussion and evaluation. Secondary school and college students may wish to participate in discussion of some of the school year papers. It is even possible that some instructors may wish to incorporate some of the papers and related discussion into THEIR COURSES.

SOME INFORMATION FOR PROSPECTIVE AUTHORS

Papers are expected to be the equivalent to at least ten typewritten pages in length.

Authors are encouraged to contact Tom O'Haver or Donald Rosenthal as early as possible, preferably by e-mail. Please send your name and mailing address, title of your paper, e-mail address and phone numbers. Indicate in which session you prefer to present your paper. Papers which are likely to be of interest to students are best presented during the school year sessions. Since there are only a limited number of papers which can be presented, authors are asked to contact us as early as possible.

The deadlines are as follows:

Summer 1997 Sessions

January 1, 1997 - Deadline for title and abstract

March 3, 1997 - Summer Conference schedule will be established and sent to authors

April 1, 1997 - Deadline for receipt of paper

School year sessions

June 1, 1997 - Deadline for title and abstract

July 1, 1997 - School year session schedule will be established and sent to authors

August 1, 1997 - Deadline for receipt of papers for September to December session

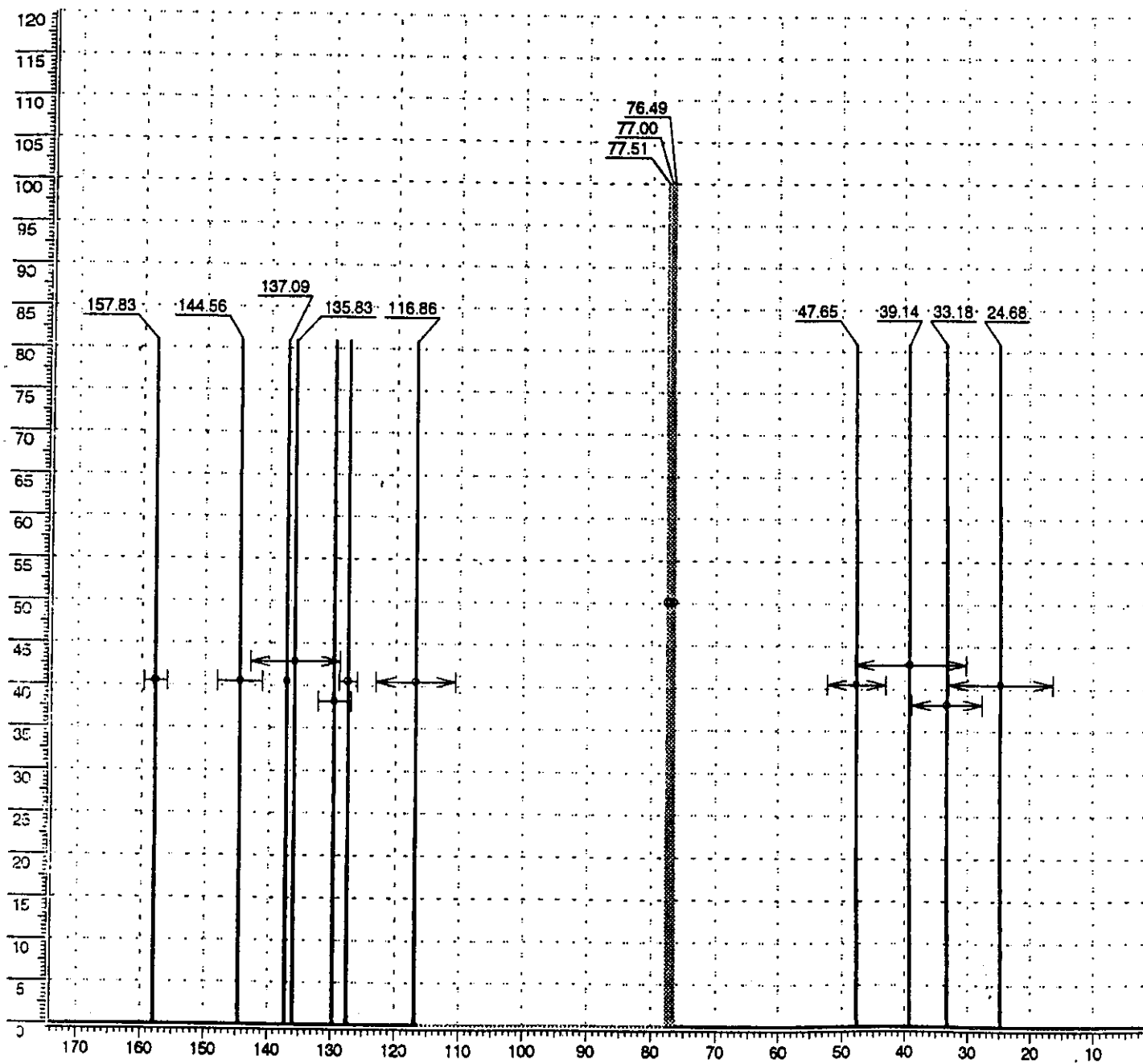
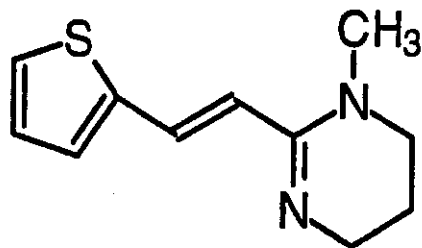
January 1, 1998 - Deadline for receipt of papers for February to May session

REGISTRATION AND PARTICIPATION

Anyone may register for and participate in this on-line conference. There is no registration fee. Since CHEMCONF is used for a number of on-line confer-

ences, it is suggested you register for the sessions you are interested in just a few months before the beginning of the session.

Figure 1: A ^{13}C NMR Simulated by the ACD/Labs Prediction Software



COMPUTERS IN CHEMICAL EDUCATION

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Types of articles you would like to see in future issues:
Rate on the following scale: 1 - Very important, 2 - Important,
3 - Average importance 4 - Not important

1. General articles on how teachers are using computers _____
2. Reviews of 'useful' software _____
3. Reviews of hardware _____
4. Brief "Who Done It" _____
5. Queries and Answers _____
6. Book Reviews _____
7. Programming tips _____
8. Calendar of Events of interest to computer users _____
9. Networking and networks _____
10. Other - please describe _____

OVER PLEASE

11. Are you a member of the:

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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 and Statistical Methods	_____	_____	_____
Graphics	_____	_____	_____
Interfacing	_____	_____	_____
Laboratory Automation	_____	_____	_____
Drill and Practice	_____	_____	_____
Other (specify)	_____	_____	_____

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

14. Other Comments or Suggestions:

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