

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 stations

stations

Canon RE-650 MH IIN Video visualizer

visualizer

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

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#### A Web Page in Chemical Education

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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.

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**Review of Gaussian 94W**  
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**G**aussian has long been the premier ab initio quantum chemistry program. Recently, another ab initio program, Mullikan, 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.