General Chemistry Classes Held in the Computer Lab

by Carolyn Sweeney Judd, M.A., Chemistry Faculty
Britt Taylor-Burton, Student Computer Lab Specialist Central College
Houston Community College System
1300 Holman Houston TX 77004
email: cjudd@tenet.edu
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ABSTRACT: As a follow-up to a paper given at the 14th Biennial Conference on Chemical Education at Clemson University on August 5, 1996 (Creative Combinations: Chemi-Skill-Bildr and PowerMacs), we would like to detail a typical session in our computer lab. Our commitment is to be present with the students, making computer time an integral portion of the lecture - not simply an add-on, to be done by students on their own time. Our commitment grows out of two things: that students can do good group work, with one of the members of the group being the computer; and that very good tutorial and individualized homework programs are available for prices that make them accessible for our budget.

Envy started C. Judd on the path now followed. It started over 5 years ago with a visit to an introductory computer science lab, watching the intensity of the students, listening to their collaborations, and observing their reluctance to leave at the end of a 3- hour class. In contrast, at the end of the 3-hour general chemistry lecture, students appeared only too glad to stumble out of the room. C. Judd wanted some of that vitality for her classroom, and became determined to find a way to include computer time during the lecture time.

At first, when going to a computer environment for part of the lecture time, we looked for facilities that would allow one student per computer for an individualized homework program shared with Houston Community College System by the University of Texas at Austin (Project SHARE was underwritten by a Summer CATALYST Grant, May, 1993.) C. Judd was given a special section that was limited to 20 students, because that was the number of computers in the available computer lab. But then we noticed that the real learning was taking place when students leaned toward each other, sharing problems, questions, and solutions. We realized that the silence was not good — that a lot of noise meant that a lot of sharing was going on. And that the sharing was the best way for learning for beginning students. Our conclusion was that one computer per student is neither necessary nor desirable.

In the fall of 1995, we acquired our new physical science computer lab, with 12 PowerMac computers, equipped with DOS cards. We chose these particular computers because over the years, we had built up a reservoir of favorite software for both PC and Mac computers. In fact, we spend much effort trying to maximize the use of the computer lab while getting the most value from our computer budget. However, many faculty members, different classes, and various software packages all in the same lab are components for chaos. We have found that a well-versed student computer specialist is vital to the smooth operation of the physical science computer lab. Our computer lab has been running relatively trouble-free and virus-free.

One-third of the lecture time is now spent in the computer lab. We do not cover issues twice; the computer lab is not redundant. Computer tutorials cover concepts that are well done with available software. - e.g., nomenclature, gas laws, stoichiometry, and drawing Lewis structures. We use several programs: "Introduction to General Chemistry" by Stanley G. Smith and Ruth Chabay (Falcon Software); "Chemical Bonding" by Gordon Galloway and Paul Hunter (Falcon Software) , and "SIRs" by John Martin (JCE:Software.) At the same time as we opened our new computer lab, we began to use the individualized homework program, "Chemi-Skill-Bildr" by Jim Spain, furnished to each student on a floppy disk. Students are responsible for their own homework, but we encourage collaboration by having students work together on one student's disk during the computer lab time. Because "Chemi-Skill-Bildr" also includes short tutorials as well as the homework problems, we often use this program.

Both the instructor and the student computer specialist are always with the students during the computer time, re-enforcing that this is not an add-on to the course, but an integral part of the lecture. Moving from one student group to another, we are able to address questions that are pertinent to that group. The result is that we focus our time on actual student problems. When we find that several groups do not comprehend a concept, we

computer specialist addresses any computer issues, and also serves as a student tutor for chemistry.

The result is that we have students who talk about chemistry, discuss and even argue about chemistry, and become active learners. For classes which include many foreign-born students, this vocalization and activity would not occur if recitations before the class were demanded. C. Judd is no longer envious of that computer science class, for her classes are now places of visible learning also.

Our method could be easily modified for other colleges. Because several students can use one computer, hardware costs need not be large. The advent of excellent tutorial programs over the Internet lowers the costs of software acquisition. Also very good software is commercially available at modest costs. For many institutions, group work with a computer as a member of the group can be an excellent way to engage students' minds in active learning.

HyperChem in the Physical Chemistry Laboratory

David Whisnant
Wofford College, Spartanburg, SC 29307

HyperChem is a molecular modeling program that runs on a variety of platforms, including a Windows 3.1 or Windows 95 based PC. The version we use at Wofford (HyperChem, Release 3) includes several molecular mechanics and semi-empirical molecular orbital methods. A more recent version also includes ab initio calculations. We have three copies of HyperChem available, two on 66 MHz 80486 machines and one on a 75 MHz Pentium, which we use in our general chemistry and physical chemistry laboratories.

In physical chemistry, my students use molecular modeling in two experiments. The first is an addition to a traditional experiment in which the students record the visible spectra of three conjugated cyanine dyes (e.g., Shoemaker, Garland and Nibler, 5th Ed., pp 440 - 446). They obtain the wavelengths of maximum absorbance from the spectra and calculate the photon energies corresponding to the transitions. These energies can be fitted to a particle-in-a-box model and used to estimate average bond lengths for the molecules (Moog. R. S. J. Chem. Educ. 1991, *68*, 506). At the end of this experiment, my students use the MM+ molecular mechanics option in HyperChem to calculate an alternate model of the smallest dye molecule. They then use the ChemPlus extensions for HyperChem to vary the torsion angle between the two ring systems in the dye. The molecular modeling calculations add around an hour to the experiment when the program is run on the 75 MHZ Pentium and somewhat longer on a 486 machine, mainly because of the time required for the torsion angle search. The bond lengths obtained from molecular mechanics and the average value estimated from the particle-in-a-box model differ by less than 1%. They also are within 4% of the bond length in benzene.

Small carbon clusters have been of considerable interest in the last decade, due to their relevance to interstellar and combustion chemistry, and because of the synthesis of the fullerenes. Our second physical chemistry experiment involving molecular modeling is a semi-empirical MO study of the C_5 molecule, based on the description of such calculations in Weltner and van Zee, Chemical Reviews 1989, 89, 1713-1747. The students begin by using MINDO/3 to calculate heats of formation for several possible C_5 isomers — linear, pentagonal, trigonal bipyramidal, square pyramidal, trapezium, and tetrahedral. They then use the heat of formation values to predict that the linear structure is the most stable.

Having decided that the linear structure is the most stable form of C_5, the students then use PM3 calculations to make predicions about this isomer. They find that the calculated bond lengths are around 1.28 Å, consistent with the model :C=C=C=C=C:. They calculate the energies of the molecular orbitals and use contour plots to draw pictures of the orbitals, to which they assign , , and inversion symmetry labels. They also calculate the wavelengths and oscillator strengths of the three most intense visible-UV peaks, as well as the wavelengths of peaks in the IR spectrum. These predictions can be compared with theoretical and experimental results in the literature.

The C_5 computational chemistry experiment, on which the students work in pairs near the end of the second semester, is useful because it ties together several topics which we have discussed in lecture throughout the year. First, it gives the students experience with a practical application of molecular orbital theory, which I find it difficult to cover effectively in lecture. The students also make a brief return to thermodynamics (which they have learned in the first semester) when they use heats of formation to predict the most stable isomer. They use group theory to identify the point groups of the six C_5 isomers and apply symmetry to label the different molecular orbitals. The predicted oscillator strengths of the visible-UV peaks lead them to discuss allowed, symmetry-forbidden, and spin-forbidden transitions. Finally, HyperChem shows animated pictures of the vibrations corresponding to the infrared