

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 predictions about this isomer. They find that the calculated bond lengths are around 1.28 Å, consistent with the model $:C=C=C=C:$. They calculate the energies of the molecular orbitals and use contour plots to draw pictures of the orbitals, to which they assign σ , π , 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

transitions. This gives the students the opportunity to think about vibrational modes and the relationship of changing dipole moment to the intensity of the transitions in the infrared.

8. Problems in Paradise: Expect the Best, Prepare for the Worst
- III. The Future
 9. New Directions
 10. Network Learning: A Paradigm for the Twenty-first Century
 11. Epilogue: Email from the Future

- Appendix A. Learning Network Resource List
- Appendix B. Commercial Services
- Appendix C. Vendors of Computer Conferencing Systems
- Appendix D. Lists of Free-Nets
- Appendix E. Nonformal Education and Online Services
- Appendix F. Sample Course Description and Letter to Online Students
- Appendix G. Annotated Excerpts from an Online Course

**"Learning Networks:
A Field Guide to Teaching and Learning Online"**
by Linda Harasim, Starr Roxanne Hiltz, Lucio Teles
and Murray Tuross
The MIT Press, Cambridge MA, 1995
ISBN 0-262-08236-5 \$ 35

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This book considers the use of computer networks for educational activity in primary, secondary, university, and adult education. It indicates how this new technology can strengthen and transform teaching and learning practices, opportunities, and outcomes. It describes some of the advantages and pitfalls of network-based learning compared to traditional classroom techniques. The four authors have been actively engaged in online learning and describe their personal experience as well as providing information from a variety of online and published sources.

The book is 329 pages in length and consists of three sections, eleven chapters and seven appendices as well as eleven pages of references, a table of contents and an index.

The sections, chapters and appendices are:

- I. The Field
 1. Learning Networks: An Introduction
 2. Networks for Schools: Exemplars and Experiences
 3. Networks for Higher Education, Training and Informal Learning: Exemplars and Experiences
- II. The Guide
 4. Designs for Learning Networks
 5. Getting Started: The Implementation Process
 6. Teaching Online
 7. Learning Online

Here are a few selected quotations from the book:

"The traditional face-to-face classroom learning situation is generally assumed to be the best to support learning, with other learning modes perhaps perceived as less effective. There is no evidence to support this assumption. In fact, quite the opposite is true: Online environments facilitate learning outcomes that are equal or superior to those generated in the face-to-face situation."

"The asynchrony of online interactions allows participants time to reflect on a topic before commenting or carrying out online tasks. ... "

"In research on online ... courses ..., students identified the following benefits ...:

Increased interaction: quantity and intensity
"... I've never been involved in a course in which I've learned so much from other students. This was because there was no competition for the floor and therefore everyone was able to have her say. Also, as remarks were all documented, they were subject to more in-depth consideration than in the normal classroom."

Better access to group knowledge and support
"The information exchange is more diverse in that input is coming from everyone rather than only from the instructor."

"I learned much more than in a regular three-hour course because of the interaction of all the students in the course. It is much more enriching this way. Through this medium we could tap the combined knowledge of the group."

More democratic environment
"In online discussions, I think that there is a