ments and finding "break-proof' ways of moving the equipment around was time-consuming. The multi week collaborative projects also require a lot time, both for planning and for managing the e-mail discussions and Web pages. We have been happy to have colleagues with whom to share the load.

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Spartan in Organic Chemistry

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During the second semester of the last academic year, I used MacSpartan with students who had completed about two thirds of the usual first year organic course (chemistry and biology majors). I also used it in a first year graduate course in Organic Chemistry for chemistry master's degree students. Using the program at two different levels at the same time started me thinking about the best place(s) in the curriculum to teach molecular modeling and computational chemistry.

I was impressed with the way that Spartan helped students visualize molecules in three dimensions. A certain number of students seem to be able to get through the first semester of organic chemistry without making a good connection between three dimensional physical models and two dimensional formulas. Years ago, students were often exposed to mechanical drawing and solid geometry before they took organic chemistry. This suggested that, if you consider the percentage of chemistry majors in introductory and organic chemistry, it might be important to teach three dimensional visualization to students in freshman chemistry, particularly if the growing importance of this concept in biology and biochemistry is factored in. The molecular modeling capabilities of a program like Spartan are very useful in teaching students to visualize molecules in three dimensions. The ability to rotate the representation of a molecule under mouse or keyboard control helps students build a mental model of a molecule. It also helps students to move between models and three dimensional structures. These skills are useful to any student who will go on into biochemistry.

Chemistry majors need to learn to think like organic chemists. An important part of a chemist's mental picture of a molecule is an idea of the distribution of charge over the molecule. A **calculated** distribution of charge, clearly identified as such, can become an important part of a student's mental picture of a molecule. Both a mental picture of charge distribution and a calculated distribution of charge can be used to predict reactivity. The idea that computational chemistry is most valuable when it is used to predict an observable result is important. It gives students some idea of the validity, or lack thereof, of their computations. Spartan is a very fast computational package on current microcomputers; this suggests that the program can be very useful in the introductory organic course. The idea of making Spartan available to laboratory students who are waiting for one reason or another is an attractive one. Computations can be set up, submitted, and the results examined at separate times. Since computations run in the background, other students can use the program while computations are running.

I found the tutorials in the MacSpartan manual to be superb. After a brief demonstration of the capabilities of Spartan, organic students at either level quickly learned how to use Spartan as a computational package, with very little effort on my part. They were able to make the jump to applying the package to molecules that they were interested in with little or no hesitation. The ability to compute geometry, electron distribution, and even transition state geometry, allows students to ask all kinds of questions relevant to the understanding of organic chemistry. In fact, Spartan proved to be a very useful tool to get students to think like organic chemists.

Due to an institutional decision to phase out Macintosh computers, we are using PCSpartan this year. Wavefunction allowed us to upgrade our copies of MacSpartan to PCSpartan at a very reasonable fee (after return of the Macintosh hardware lock). We are running PCSpartan under Windows 95, on a TCP-IP network with a Windows NT server. So far, we have had no problems with the PC hardware lock.

CCCE National Workshops

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