screen. As they work on their new compound we ask them to think about the structures of known sunscreens, the general rules they have learned for constructing organic structures, and the relationship between polarity and water solubility.

One of the objectives of this project is to have students write individual formal reports based on their own experiments and on information accumulated by the class as a whole. This information is shared by posting it on a Sunscreen and Ultraviolet Radiation Web site that I maintain (http://www.wofford.edu/~whisnantdm/sun_uv98.htm). At the end of the second week's laboratory, the groups turn in their experimental spectra and the structures of their proposed sunscreens, which I incorporate into pages on the project Web site. During the third week, in lieu of their regularly scheduled laboratory, individual students search the Web for information on sunscreens, ultraviolet radiation, stratospheric ozone depletion, and related topics. Most students have had experience with the WWW, but few have used search engines with a Boolean search structure. To help students who haven't had experience with advanced searches, we distribute a handout describing how to use HotBot and Alta Vista. Because Web sites are not peer-reviewed, the quality of information on the Web is variable, to say the least. This handout also suggests strategies that students can use to help evaluate information from the Web for credibility and reliability[2] http://www.sccu.edu/faculty/R_Harris/evalu8it.htm. Each student is asked to turn in the titles and URLs of three good web sites by the end of the week. After testing, links to these URLs are posted to the project Web site.

During the final week of the project, the students use Quantum CAChe, running on 266 MHz Pentium II computers, to model their compound. They optimize the structures of their proposed sunscreens using molecular mechanics and then predict the electronic spectra using ZINDO. Each group copies their predicted spectrum to a paint program and then saves it as a .jpg file suitable for posting on the WWW. I add the spectra to the project Web pages that already contain names of the students in the groups and the structures of their proposed sunscreen. I also post ZINDO spectra from CAChe calculations for four common components of sunscreens along with wavelengths of peaks from experimental spectra [1]. These can be compared to give the students an idea of the reliability of the ZINDO predictions.

At the end of the project the students write formal laboratory reports. To put the experiments in a larger context, the students are asked to include a discussion of ultraviolet radiation, health effects, the ozone layer, and classes of sunscreen in their introduction. Other then some leading questions in the project handout, we give the class no written information on these topics. The URLs found by the class and linked to the project Web page furnish more than enough information to write this introduction. In their report the students also discuss their experimental work, the expected quality of the CAChe UV spectrum predictions, how good a sunscreen their proposed compound would appear to be based on the molecular modeling results, and which of the compounds proposed by the class they would expect to be the best sunscreen.

[1]C. Walters, A. Keeney, C. T. Wigal, C. R. Johnson, and R. D. Cornelius, *J. Chem. Educ.* **1997**, *74*, 99.
[2]Harris, R. (1997). *Evaluating Internet Research Sources*, [Online]. Available:

Integrating Computational Chemistry and Molecular Modeling into the Undergraduate Chemistry Curriculum.

A Symposium Report

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At the spring, 1998 meeting of the American Chemical Society in Dallas, Texas, the Committee on Computers in Chemical Education sponsored a symposium entitled, "Integrating Computational Chemistry and Molecular Modeling into the Undergraduate Chemistry Curriculum." The following description is intended to briefly review that symposium(with apologies to the various presenters for compressing their papers so much).

Molecular modeling and computational chemistry have become standard tools for many industrial and synthetic chemists. The decrease in the price of computer hardware and software has made it increasingly possible to include this type of material in the undergraduate program, but it is not yet clear how this material can best be integrated into an already crowded curriculum. Thus, it was not surprising that a wide variety of different approaches are in use by the institutions represented at this symposium.

Many of the papers described efforts to introduce molecular modeling into existing courses. For example, both the University of Northern Colorado (Greeley, CO) and Clarke College (Dubuque, IA) use molecular modeling in the general chemistry course. Texas A & M University (College Station, TX) teaches molecular modeling in the introductory organic labs, and the University of Hartford (West Hartford, CT) teaches this material in an upper-level synthesis course. On the other hand, Lebanon Valley College (Annville, PA) incorporates molecular modeling into all levels of the curriculum through the laboratory work.

The same diversity was found among the schools that are introducing computational chemistry. The University of Michigan (Ann Arbor, MI) has added computational chemistry into several courses in its curriculum, but especially the Structured Study Groups, that are the basis of the Honors section of the undergraduate Structure and Reactivity course. Michigan State University also has been merging computational chemistry into existing courses and is developing an undergraduate specialization in computational chemistry.

The University of St. Thomas (Houston, TX) introduces computational techniques to students in the physical chemistry course, by doing normal mode analysis. Rather than attempting to integrate computational chemistry into existing courses, Valdosta State University (Valdosta, GA)is developing a new required course.

The symposium also included some industrial representatives. The Wavefunction Corp. (Irving, CA), well known for its modeling software, has developed a workbook with experiments and demonstrations for use inorganic courses, and a speaker from SUNY Oswego demonstrated a new, inexpensive molecular modeling program.

Many of the questions during the discussion concerned what level of the curriculum was best for introducing these sophisticated topics. Some speakers felt it was better to delay until students had enough background to fully understand what they were doing, whereas others proposed to introduce the material early in the curriculum, so that students would become familiar with these methods early in their chemical careers.

These symposia papers, and the discussion that accompanied them, raise some fundamental questions about the way that we teach chemistry. The argument that we should not teach advanced techniques, like computational chemistry and molecular modeling, until students have the mathematical background and maturity to better understand them, is both reasonable and attractive. The opposing arguments are, however, also very compelling.

It has become traditional to teach chemistry in a recursive manner, that is, to return to the same topic at different levels of the curriculum in increasing levels of detail. Perhaps the best example here is atomic structure. Very few students really understand the orbital diagrams in general chemistry, but these experiences lay the groundwork for a more in-depth treatment in physical chemistry and other advanced courses. Should a similar approach be used with molecular modeling?

General chemistry, and even organic, are mainly service courses, where students majoring in other sciences pick up enough modern chemistry to serve as a basis for their majors. Since these students don't normally take advanced chemistry courses, can we overlook the possibility to introduce them to molecular modeling, one of the most powerful tools of modern chemistry?

The discussion in this symposium clearly has ramifications far beyond a single scientific meeting. These opposing viewpoints will continue to be expanded and debated. This symposium represents a early step in what will surely become a more extensive dialogue in the years ahead.

Why Use Presentation Software?

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Over the past several months, Brian Pankuch and I have exchanged several e-mails about the ways to use presentation software, such as PowerPoint, more effectively. Growing out of those conversations, this is the first of what may become a series of short articles, intended to share the results of my own efforts to find better ways to utilize this technology. Of course, it should be read with the usual disclaimers that the opinions expressed are solely my own and that alterna-