

multiple documents, allowing an author to create and maintain a consistent interface throughout a set of Web pages by editing only one file. More tools and information about cascading style sheets are available on the following Web sites:

CSS draft specifications: <http://www.w3.org/Style/css/>
HTML Help by The Web Design Group: <http://www.htmlhelp.com/>

DYNAMIC HTML

The cascading style sheets provide the tools to control style and layout on a Web page. Combining style sheets and scripting languages allows delivery of dynamic and interactive elements on a Web page. A useful feature for interactive tutorials is the ability for a text block or image to change based on the position of the pointer or on a mouse click in a certain area. Other examples include drop down menu boxes, text boxes, and animated text or image overlays.

Unfortunately, these dynamic features are where Netscape Navigator and Microsoft Explorer diverge in their implementation of DHTML. DHTML pages on the Web currently, are either browser-specific, or they incorporate browser testing and two sets of DHTML code. The more sophisticated DHTML development tools have the capability to produce browser-independent code. The following development tools support CSS and DHTML to varying extents.

HomeSite 3.0, Allaire Corp., <http://www.allaire.com/>
HoTMetaL PRO 4.0, SoftQuad Inc., <http://www.softquad.com/products/hotmetal/>
Interactor 1.1, mBED Software, <http://www.mbed.com/>
NetObjects Fusion 3.0, NetObjects Inc., <http://www.netobjects.com/>
Dreamweaver 1.0, Macromedia Inc., <http://www.macromedia.com/software/dreamweaver/>

More tools and information on DHTML are available on the following Web sites.

WebReference.com (sm) - The Webmaster's Reference Library: <http://www.webreference.com/>
ZDNet InternetUser / Garage / Dynamic HTML: <http://www.zdnet.com/products/garage/dhtml.html>

Collaborative Intercollegiate Physical Chemistry Projects

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In Spartanburg, South Carolina, there are three relatively small colleges - Wofford College (1100 students), Converse College (1000 students), and the University of South Carolina - Spartanburg (3300 students). Our departments all are faced with the problem of small enrollments in our physical chemistry classes, which makes it difficult to justify the purchase of expensive equipment to update laboratories or to regularly use research-style collaborative projects. For the last four years, with support from two NSF ILI grants and Oxford Molecular Modeling (1) the three physical chemists from these colleges have cooperated by sharing equipment and collaborating on experiments in which all our students participate. The collaborative experiments have been particularly valuable because they have converted our sometimes small classes, in which there are only a limited number of students with whom to interact, into effectively larger classes.

Our first venture into collaborative experiments was during the 1996-97 academic year. Conversations with Theresa Zielinski of Niagara University had introduced one of us (Whisnant) to the potential of the Internet for promoting the interaction of students from different schools (2). For the two previous years we had struggled with problems involving a laser system designed to measure heat capacities by thermal lens calorimetry (3). Last year we decided to involve our students in a research-like project intended to narrow down the sources of error in the experiment. Groups from two of the colleges studied the effect of variable changes (e.g., cell positions, concentrations, or solvents) on the results of the experiment. They statistically analyzed their data and submitted the results to one of us who posted the results on the project Web page (4). When the students wrote their reports on the project, they were responsible not only for discussing

their own results, but also for drawing conclusions from the entire set. All three colleges continued this project this year, although experimental difficulties led to fewer results than we were able to obtain the year before. A recent communication from Ben DeGraff (5) has suggested changes in the experiment that may help us extend this project in the future.

This year, we have expanded our cooperation by adding two collaborative projects involving computational chemistry. In the first project, which was done during the first semester, the students played the role of R&D chemists working on hair dyes. They were told that the ready availability of benzene makes the project manager think that benzene derivatives might be a good place to start. Benzene compounds also are attractive because they are small and can penetrate hair fibers more readily than larger compounds such as azo dyes. The students were asked to do some preliminary work using semiempirical calculations to predict what types of benzene derivatives were more likely to give colored compounds.

The Hair Dye project lasted several weeks. The first student groups guessed a few derivatives to try, optimized geometries using Quantum CAChe MOPAC PM3 calculations (6), and predicted visible-UV spectra using ZINDO CI. After each group had completed their calculations, the structures and corresponding predicted spectra were added to the project Web page (7). We also encouraged an e-mail discussion of ideas about the experiment, with all messages being sent to one of the instructors, who forwarded the messages to a distribution list of all the students. Subsequent groups used the accumulated experience of the previous groups to make a more informed choice of derivatives. The compounds, such as 2,4-dinitroaniline, studied by some of the final groups were similar to compounds used as hair dyes (8).

The e-mail distribution list also gave the instructors the opportunity to ask questions of the group as a whole. For instance, toward the end of the first phase of the project when the students had homed in on likely compounds, we asked them how they could test the reliability of the spectra predictions. The students decided that they should record the spectra of some similar compounds and compare the experimental spectra with CAChe predictions (which do appear to be fairly reliable for these types of compounds). As part of this discussion, we were able to bring up solvent effects and the fact that the computational model was of gas-phase molecules. We also encouraged the students to make literature searches about compounds that are used in hair dyes and about potential health and environmental problems that might arise from use of these chemicals. Some of the students contributed information on these

topics from the World Wide Web and Chemical Abstracts Online.

At the end of the Hair Dye project we asked each of the students to decide on the compound they thought was most likely to be a good hair dye, and to use their knowledge of organic chemistry to devise a synthesis of the compound. We had reached the end of the semester by this time and were not able to have an online discussion of the proposed syntheses. This was unfortunate because many of the syntheses that students proposed in their final reports would have profited from such a discussion.

This semester we are in the middle of a third collaborative project, again involving computational chemistry. In 1989 scientists from the Kitt Peak National Observatory observed the absorption spectrum of the carbon star IRC+10216 and found a series of infrared absorption lines in the region of 2164 cm^{-1} (9). We have told the students that there is the possibility that these lines are due to a transition in a small carbon cluster molecule - probably C_3 , C_4 , or C_5 . We want to use computational chemistry to help identify the molecule that is being observed, and to infer some of its molecular properties from the spectra and computational results. We started the project by asking the students to list all the possible isomers of C_3 , C_4 , or C_5 . We then posted the combined lists to the project Web site (10) and assigned different isomers to groups of students from all the colleges for further work. During the next week the students optimized the geometries and predicted the heats of formation of their assigned isomers using CAChe PM3 semiempirical MO calculations. The PM3 calculations were not wholly successful, which did not come as a surprise to the instructors because the PM3 computational model is not always reliable for small carbon clusters (11). The calculated heats of formation did clearly favor linear isomers for all three carbon molecules, though.

We are in the third week of the project as this article is being written. As part of the e-mail discussion we have asked the students if the linear isomers make sense, given what they know about the bonding characteristics of carbon. We supplied the hint that they might check tables of covalent radii for carbon, which can be compared with the predicted bond lengths to help them draw Lewis structures for the molecules. The predicted bond lengths all turn out to be closest to double bonds, which does make sense. Double bonds give most of the carbon atoms four bonds and the 180° bond angles in the linear molecules correspond to those expected from VSEPR arguments. At the end of this week, we supply them the information that recent experiments (12) indicate the possible existence of a low energy cyclic C_4 isomer, and discuss what we can do to obtain more

reliable computational results. We also have asked them to recall the context of the project (identifying the source of IR lines in a carbon star), because conversations with some of the students had suggested that they were losing track of the project's purpose in the midst of all the calculations and e-mail discussion.

In the next phase of the experiment, the students will do ab initio calculations using Gaussian 94W (13). Different groups of students will optimize the geometries and calculate the vibrational frequencies for the linear isomers of C_3 , C_4 , and C_5 , and the cyclic isomer of C_4 at the HF/6-31G(d) and MP2/6-31G(d) levels (unrestricted for the triplet linear C_4 molecule). Again, the computational results will be communicated within the group by e-mail and posted to the project Web page. From our experience with these calculations, we expect the students to find that, at this theoretical level, the cyclic C_4 isomer is of slightly lower energy than the linear C_4 isomer. The most intense IR-active frequencies predicted for the C_3 and C_5 molecules are 2054 cm^{-1} and 2220 cm^{-1} respectively [MP2/6-31G(d) values scaled by 0.9434 (14)], which agree with literature values calculated using the same theoretical model (11). Both frequencies are within 5% of the 2164 cm^{-1} experimental value, with the C_5 value being slightly closer. The linear and cyclic C_4 frequencies are clearly different from the experimental value.

The final phase of the project will take place in two weeks, following the spring breaks at two of the colleges. The students first will be asked questions about the most stable C_4 isomer and the molecule most likely to be responsible for the 2164 cm^{-1} lines. As the discussion develops, we will give them the information that for linear C_n molecules the rotational lines in the vibrational-rotational spectrum should be separated by around $4B$, where B is the rotational constant, and ask how this can help us choose between C_3 and C_5 . Although the lines are not equally spaced, even a rough average gives an approximate rotational constant of 0.086 cm^{-1} , or 2.6 GHz , which is much closer to the value predicted by Gaussian for C_5 (2.6 GHz) than for C_3 (12.9 GHz), supplying additional evidence that the C_5 molecule is responsible for the series of experimental lines from the carbon star. During this phase we also will ask the students why some transitions are only IR active and some only Raman active, and whether we could observe linear C_3 or C_5 by pure rotational microwave spectroscopy.

Given the time we have left in the semester, this probably will conclude the on-line discussion phase of the project. In the student reports we can ask them to answer a few more questions. One set of questions will be about the reaction, cyclic $C_4 \rightarrow$ linear C_4 . From our project's calculations, why would we expect JH to be

small for the isomerization reaction? Thinking about the structures of the cyclic and linear isomers, what can we say about the sign of JH ? Given the low JH and the sign of JH , which form of C_4 might we expect to be more important at high temperatures? We also can ask the students to use point groups to classify all the isomers of C_3 , C_4 , and C_5 in the original list assembled by the group.

We are enthusiastic about collaborative projects such as these and plan to continue them in the future. They convert our small classes into a group large enough to use research-style projects that put some of our laboratory experiments into the context of a larger problem. The online nature of the projects also gives the students practical experience using the Internet as a routine tool in their work, both for communication and gathering information. The two computational projects have not been easy for the students, because the projects introduce methods of building computational models before we have reached this topic in lecture. A major advantage of having several students collaborate is the increased effectiveness of a group in solving problems, especially when the students are in new territory. Even if individual students may be mistaken on a particular point, the group discussion (sometimes with hints from the instructors) usually points the way to the correct answer.

Even though at times the students probably have felt deluged by e-mail (one student remarked that he had 10-12 new messages every time he opened his e-mail account), most of the students seem to be enjoying the experience. For one thing, other instructors have told us that they have heard students talking favorably about the projects in their classes, which has not been our usual experience. Of the nineteen students in our three classes this semester, fifteen are regular participants in the e-mail discussions and everyone has contributed at one time or the other. In fact, a certain amount of camaraderie appears to have developed among the students, few of whom know each other personally. Some of the students have asked us about having a "Carbon Clusters Convention" at the end of the semester so that they could meet the students from the other schools, which we are planning on.

We also are enjoying the collaboration as instructors, because it has effectively expanded our small departments to include three physical chemists. As was remarked one day when we were discussing a project, there is no way we could have done this alone. At various phases in our collaboration, each one of us has taken the lead on a particular project. This is good because these projects do take a lot of time. None of us were very experienced with the use of lasers when we began our cooperation, so developing the experi-

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.