INSTRUCTIONS FOR MOLECULAR MECHANICS
PROBLEM SETS, SEPTEMBER 11, 2004

Many years ago, Dr. Bartmess prepared a set of about ten problems that could be solved by the molecular mechanics program MMX. In subsequent years, I prepared many additional problem sets, based on interesting molecules that had appeared in the literature (or in my fevered imagination). You can find all of these problem sets at the URL for Chem. 550: http://web.utk.edu/~rmagid/index3.html

In past years, I would photocopy all of these more than 400 problems and distribute hard copies to students at the MMX training session. Upon reflection, I decided that this was a monumental waste of paper.

Last year (and again this year), I decided to do something different. I have available for you hard copies of the newest set of problems (Nos. 393-403) and an "addendum" that lists newer references and updated information if you decide to do a problem from one of the earlier sets. You should select a problem (either from this latest set or from any earlier set on the web site) and sign up for it - FIRST COME, FIRST SERVED!!

The individual projects are explained in the problem sets. Most often, they consist of doing calculations on the structure, energy, structural parameters, etc. for some four or five related molecules and answering questions that are posed; most of these questions ask you to compare your results with those in the literature reference that is cited. You are not restricted to answer only the specific questions posed in the problem set - in other words, if your interest is piqued by what you've done, do calculations on some other related compounds. Be creative! Be imaginative!!

Four weeks from today (October 9) is the deadline for you to turn in your report. As described at our first class meeting, you can earn up to 20 points (of the 450 total points for the semester) for a well-done project. Dr. Bartmess and I will grade these independently. Your report should be a relatively brief discussion (say 3-4 pages, preferably typed) of what you found and how it compares with what is in the literature. Make use of tables for a clear presentation of results. As part of your report, you should turn in printouts of all of the structures that you calculated and the floppy disk on which you saved your calculations. Because I've already done the calculations on every problem that's listed at the course web site, you should compare your results with mine before you write up the final report.

If you'd like to do a project of your own invention (rather than one from the Chem. 550 web page), fine! What you should do, however, is check with Dr. Bartmess or me for some advice on whether it is suitable for MMX treatment. The calculation program works best for hydrocarbons and for molecules with not too many functional groups; it fails when it encounters "exotic" functional groups that are not in its memory.

Ron Magid