Assignment #3

Date Assigned: 1/25/06; Date Due: 1/30/06

1. We are nearly finished going over the basics of molecular mechanics and force fields and will next be turning to applications & actually doing some calculations ourselves. To help you consolidate the material to this point I’d like you to review the primary reading (not the Allinger and Jorgensen articles) and the worksheets to date and do the following:

(a) Come up with three (six if you are submitting solutions as a pair) questions concerning some of the central ideas in this material. Your questions should be suitable for a closed book exam that stresses basic understanding rather than memorization of details. Provide answers as well as questions. (I will share these questions with the class and, to the extent that I think they are appropriate, some will be used for the first midterm.)

(b) Identify at least two (four if you are submitting solutions as a pair) aspects of the reading that we either did not touch on or that you think require further clarification.

(c) (Optional) I would appreciate any feedback you can offer concerning whether the way the course is going and any suggestions you might have for changes that would help you learn the material more effectively.

2. The next assignment, which I will hand out on Monday, will require the use of the program HyperChem. There will be time on Monday for a short demonstration and for you to work with the program together. However, I encourage you to start going through the tutorials in the “Getting Started” manual, Lessons 1-5, so that you can actually make some progress on Monday.

As of this moment HyperChem is available in the Chemistry Resource area (207 Whitmore), the labs in Life Science Building, and 111 Boucke.