

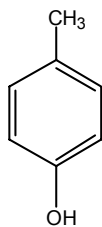
## Project I

Chemistry 5021/8021, Spring, 2005

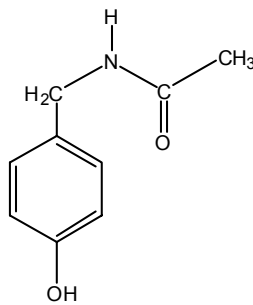
Assigned: February 2, 2005. Due: February 23, 2005

This project is learn the concepts of force fields, and energy minimization techniques. There are three problems in this project.

1. Often it is necessary to build an approximate force field for a new compound. Given the CHARMM force field for proteins and make use of analogous functionalities in the 20 amino acids, construct the “residue” topology and estimate the missing parameters in the appropriate places. Then, use the “topology” and “parameter” files that you have built to optimize the structure to obtain the minimum energy conformation. You may wish to try to use different optimization methods for your curiosity (and comparison). In your report, you should indicate key structural parameters (such as key – not all of them – bond lengths, angles and dihedral angles). It might also be helpful to include the topology file for the compound. Choose the compound according to your registration section.



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2. Use the minimized structure in problem 1 to perform a normal mode analysis. List vibrational frequencies in increasing order. Comment on the motions of the lowest vibrational mode.
3. Download the crystal structure of bovine pancreatic trypsin inhibitor (BPTI) (choose the one that has the highest resolution) from the protein databank (PDB). Build all hydrogen atoms that are missing from the X-ray structure (set all histidine residues to be protonated). Minimize BPTI structure using CHARMM. Calculate the root-mean-square deviation (RMSD) between the minimized and crystal structure for all backbone atoms. You should keep all crystal water molecules in your calculation. (CHEM 5021 students optional, but you will earn extra credits for doing this problem).