

## Chemistry 478 — Molecular Modeling

Laboratory Report Format:

In order to complete this project, you should write a "lab report" with the sections outlined below. These should be turned in via email to Jay Ponder, preferably within about two weeks following the date of the lab period.

- (1) Introduction -- brief summary and reason for doing the project
- (2) Procedure -- what steps did you actually perform, and in what order
- (3) Methods -- kinds of calculations, programs used, level of theory, any assumptions or approximations such as quantities varied, restraints and constraints, special program options, *etc.*
- (4) Results -- data obtained, usually presented as both tables and plots
- (5) Analysis -- explain your results; why did things turn out as they did, what can you find in texts or published papers to support your interpretation of the data (*i.e.*, for this specific system or for analogous systems)
- (6) Conclusions -- what lessons were learned from this project, what kinds additional calculations could be done to further explore the topic
- (7) Questions -- answer specific questions provided as part of the project