Chemistry 4021/8021 **Computational Chemistry** 3/4 Credits
Spring Semester 2010

FINAL EXAM

This exam is due May 13th at 3:00 PM. Please email an electronic version (preferably as a pdf file) to me at cramer@umn.edu or ensure that a hard copy is in my mailbox at that time.

Some might say that science is all about seeing important details in an otherwise enormous sea of data. Your task is to exercise your abilities in this regard using the data collected by the class over the final two problem sets and available at

http://pollux.chem.umn.edu/8021/PES/

You may work alone or as part of a group of people. You are limited to 500 words if you are working alone (exclusive of references, tables, or figures). If you are part of a group, the group is limited to 500 words per member (e.g., a six-person group can write an exam of up to 3000 words, although you need not feel compelled to hit the maximum).

Find one or more interesting things in the data and present them in the form of a scientific paper. We've read a lot of papers this semester, and I've offered editorial comments from time to time about what constitutes a good paper. Do your best to follow those guidelines. Try to structure your discourse according to Intro/Results/Discussion/Conclusions.

The subject(s) you choose to address are entirely up to you. You can talk about theoretical issues (how does DFT compare to HF for various things? How does solvation behave as a function of structure? How might you resolve discrepancies in the computations? etc.) You can compare data for one or several molecules to experiment or other calculations for the same compounds or analogs (Are there compounds related to known tautomeric equilibria? Can you associate connected reactants and transition states for particular unimolecular reactions and would predicted rate constants from, say, transition state theory compare well to experiment? Are relative energies, enthalpies, or free energies consistent with experimental values in the NIST database, if such values are available? What chemical trends are apparent for related compounds and how do they compare with known

experimental data, if any?). You can look at trends in bond lengths for different molecules, trends in energies—you can do *whatever you want*.

References, where provided, should be in *ACS* format. Note that if you find obvious errors in the data, these should be reported to me for repair. They are not fitting subjects for analysis, unless there is some interesting technical reason that errors might have been expected (a doubtful prospect here).

If you want to do additional calculations as a part of your analysis, you are welcome to do so using your class account(s). However, this is simply an option, not a requirement. It should be possible to submit an outstanding exam without having to generate any new data.

Grading will be based on clarity (30%), depth of analysis (40%), creativity (20%), and style (10%). The exam is worth 150 points total.