

FINAL EXAM

This exam is due at 3:30 PM on Friday, May 14th. The completed exam should be turned in to me, Casey, or Sheryl Frankel (218 Smith), or it can be left in my mailbox if you feel confident about security.

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 last two problem sets and now available at

<http://pollux.chem.umn.edu/8021/C4H6N2O2-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).

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.

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? Are there clear errors in the data? 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 find 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?). You can look at trends in bond lengths for different molecules, trends in energies—you can do *whatever you want*. To help you with planning, I am providing everyone with a *J. Chem. Ed.* article that describes some of the ideas that members of a past class had.

References, where provided, should be in *JACS* format. Note that if you find obvious errors in the data, these should be reported to Casey or 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).

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