

Guide for writing the strain energy report Experimental Chemistry I, CH 362 & 362H Winter term, 2009

Reports covering the second half of Experiment 1 would be appreciated by Feb 28 (R) or Feb 29 (F). The report should include the results of your bomb calorimetry work done by you and your partner(s) as well as your HyperChem calculations and error analysis. We are also asking that you report and discuss the significance of the average class values including the standard deviations for ΔH^0_c for each ester and the resultant S. Discuss how your values fit or don't fit with the class data.

For completeness, you will probably want to mention the source of your esters, but you can do that simply by referencing the forthcoming publications¹ of your and your partner's (or partners') syntheses in the *Journal of Experimental Chemistry I*. Similarly, you can reference the Chem 362 manual for the procedure, and not spend time writing this up for the report. Of course any significant departures from the referenced procedure (whether deliberate or accidental) should be noted.

As you know, an important component of this experiment is the error analysis. Error analyses are challenging to perform, and can be even more challenging to write up. Everyone should report estimated uncertainties for all key numerical results, together with something that would enable a patient reader to see how those uncertainties were arrived at. No fixed format of presentation is called for. You might consider summarizing all input to the uncertainty calculations in a table, and then give a brief description of the analysis. However, if you have worked hard to organize and annotate a spreadsheet, and think that a patient reader could follow your calculations, it would suffice to include a copy of the annotated spreadsheet as an appendix. (Some components of your spreadsheets might also appear as tables or figures in the body of the report.) We certainly don't expect anyone to word process a complicated error analysis for this report!

Please remember that the results of computer experiments are also associated with uncertainties. In the case of computer modeling with programs like HyperChem, the errors are typically more in the "systematic" category and less in the "random" category. That is, the problem with computer experiments is typically more a matter of accuracy than precision. However, since you spent much less time with HyperChem than with calorimeters, and it is challenging to make unbiased estimates for the uncertainties associated with the computed values, you don't have to attempt any error analysis on HyperChem results.

So far you know some things you *don't* need to spend a lot of time on as you write your report. But please do spend time thinking about your results, their significance, and their presentation. If you can provide some motivation and context for the work being reported, this is definitely appropriate. If you recognize limitations in the experiments as performed (and possibly avenues for addressing those limitations), please share this in your discussion. It also makes sense to pay special attention to the first things that a reader is likely to look at: the title, the abstract, and non-text elements like figures and schemes.² Finally, please try to interpret results (especially unanticipated or problematic ones), and not just report them. (If something seems to call for an explanation, but you can't provide one, it's often appropriate to point this out.) Discuss how your values fit or don't fit with the class data. If your results and data suggest a systematic error, try to identify it and discuss how your reported value for S is overestimated or underestimated as a result of the proposed error. Compare S +/- ΔS from calorimetry with the HyperChem values and with reference values for the strain in the isolated cyclopropane ring.

There is no length restriction or recommendation for this report, but a few standard journal pages would probably be adequate to report and discuss the significance of the second half of Experiment I. The report format described near the beginning of the Chem 362 lab manual is appropriate, though not required. If followed, the "experimental" section would probably be very short (assuming no special circumstances), the "results" section could be broken into two parts (experimental results and computer simulation results), and we hope that you will devote special attention to the discussion section.

Finally, we remind you that it is a good idea to proofread!

¹ You can ignore any problems with reviewers' comments, concerns about the *Journal of Experimental Chemistry I*, and so forth. The usual way to reference something not yet in print is to write "submitted" or "accepted" where you would normally find the journal's volume number, page number, and year.

² As for other write-ups, you should think of your potential reader as someone who has a degree in chemistry and has access to anything that you cite, but who knows nothing of Experimental Chemistry I at OSU. This individual is flipping through the new issue of the *Journal of Experimental Chemistry I*, and your goal is to capture and hold his or her attention, even though there are many other tempting articles in the new issue!