# Guide for writing the strain energy report
# Experimental Chemistry I, CH 362 & 362H
# Winter term, 2021

The report should include the results of your bomb calorimetry work done by you and your partner(s) and error analysis, as well as your Gaussian calculations. We look forward to reading what you have to say about the significance of your results in terms of the ideas presented on strain energy and bonding in the cyclopropane ester.

For completeness, you will probably want to mention the source of your esters, but you can do that simply by referencing the forthcoming publications[1] of your and your partner's (or partners') syntheses in the *Journal of Experimental Chemistry I*. Give a succinct overview of one experimental run. This can be the calibration or a run for either ester. Of course any significant departures from the referenced procedure (whether deliberate or accidental) should also 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 (e.g., $\Delta H^{o}_{c}$, S and C) 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 using PM6 semi-empirical methods in Gaussian, 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 Gaussian 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 Gaussian 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 $S \pm \Delta S$ from calorimetry with the Gaussian values and with reference values for the strain in the isolated cyclopropane ring.

There is no length restriction or recommendation for this report, but four or five pages of text (12 pt font, double spaced) not including figures and tables would probably be adequate to report and discuss the significance of the second half of Experiment I. There is no page limit on appendices or supplemental materials section. 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 calorimetry results and computational chemistry results), and we hope that you will devote special attention to the discussion section. Some ideas for this are presented below:

Suggestions for Discussion Section:

1. Please include some discussion on bonding in the two ring systems due to the bond angles, etc. For example, bent

bonds might be suspected in the cyclopropyl ring compared with the cyclohexyl ring which has the tetrahedral geometry. You might want to refer to your organic chemistry text on bonding in cycloalkanes. If you do, this text should be in your reference section for your paper.
2. Please include some discussion on the Gaussian experiment in which you also calculated strain energy and compare this strain energy with the literature value for strain energy for both the isolated cyclopropane and cyclohexane. For example, you might consider the effect of hyper-conjugation in the orbital calculation showing the LUMO for the cyclopropane ring and it's carbonyl group but not in the LUMO for the cyclohexane ring and it's carbonyl group. Note: you might also recall the lecture on rotation about the carbonyl group on cyclopropane carboxylic acid and the energy barrier that is evident from this higher order calculation as evidence for this interaction between the ring and the carbonyl group. Also, consider whether the bonding effects you see based on MO calculations are supported by what you see in the IR spectrum.
3. The data for Calorimetry can have some experimental bias possible in data collection and handling. Here are a few things that you might want to consider:

a) Reading the thermometer - parallax viewing - recording data points and times
b) Bias in the plateau region for both the upper and lower slope calculations which will effect $\Delta T$
c) Were runs reproducible to within 1% ? This includes two H-ester and two P-ester runs and the calorimeter constant determination was also within 1% of the acceptable value for your calorimeter system
d) You might also suggest some reasons why methyl salicylate was a good standard based on structure and thermodynamic constants

4. We are looking for a discussion of the significant results of these experiments. This can be fairly long, at least a page, and should refer the reader to any previous figures in the body of your paper to clarify your discussion. Remember that the calorimetry experimental results are usually considered the correct results for the strain energy for these isomeric esters.

Lastly:
5. Please do not forget to provide annotated spreadsheets - like the one shown in the lab manual - and the plots including the trendlines with slopes and intercepts for each run - two H-ester, two P-ester, and C the calorimeter constant. Please put the spreadsheets, plots, and compiled results from Gaussian into an appendix section or a supplemental materials section.
6. This is a significant paper since you have worked on Project 1for six weeks so we expect an exceptional effort on your part and this paper is worth 200 pts.
7. You are welcome to submit your own paper instead of a group paper if you prefer.

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

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[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!