**Title of Experiment**

Author’s name (that’s you!), Lab partners 1-X follow in alphabetical order by last name

Physical Chemistry Lab - Spring 2012

Date of experiment: MM/DD/2012

Date submitted: MM/DD/2012

**Abstract**

The abstract summarizes the goals of the experiment, the methods used to obtain those goals, and any numerical results which can be presented without further explanation. Numerical results should be presented with units and uncertainties. Do not use “new” abbreviations in the abstract – do NOT assume the reader has done this experiment. If the results suggest some flaw in our fundamental understanding of the science, OR if they suggest some flaw in the experiment itself, this should be mentioned here. The abstract should be no longer than 4 or 5 sentences, unless you really do have a shocking amount of results to present.

**1. Introduction**

The introduction describes the theory behind the experiment, and explains the goals laid out in the abstract. The introduction should include *information which was known before the experiment itself was conducted*. No new results should appear in the introduction. **Do not** simply reproduce the information provided in the handouts or the text: your introduction does not need to go into that level of detail. State the problem *in your own words*, and the means by which the problem will be solved. Be careful with your verb tenses. What you or others **did** should be presented in past tense, preferably in the passive voice. What the underlying theory **is** should be written in the present tense.

Because the class is quite large, I have to limit how long you can go on in this section. The introduction almost certainly has to be longer than one full page, but it should be no longer than three pages except in extraordinary circumstances (e.g., the “double-point” Kinetics experiment). To assist in keeping it brief, please don’t *derive* equations that are presented in the lab handouts. You can state where equations started:

 ∆H = mCP∆T (1)

and then proceed to talking briefly and generally about how you get from eq 1 to eq 2:

 ∆Hcal + ∆HCW + ∆HHW = 0 (2)

Note that Word allows for the use of subscripts and superscripts, and these have meaning in Chemistry. Do not ignore them. Failure to use proper scripting would completely destroy eq 3:

K∆TCW + mCWCPW∆TCW + mHMCPM∆THM = 0 (3)

**2. Experimental Section**

This is intended to be a very brief section. Do not repeat the instructions from the handouts; instead use *references* to recommend detailed sources of information if such is necessary. Note that this section is NOT written as an instruction manual to some third party. Do not provide a bulleted list of steps that someone should perform. Instead, describe what apparatus you used and what steps you followed *in paragraph form*. Use passive voice as much as possible, unless doing so would make your sentence tortured. Use past tense where appropriate. Indicate how many measurements were performed, the measurement conditions (if not specified in the instructions), any unusual events that occurred during the measurements that might have affected the results. Include any deviations from the procedure described in the handout.

This is also a likely place to include Figure 1, if you didn’t already in your introduction. Place Figure 1 in your report as close as possible to the sentence where you describe it. Do not fail to include a sentence *in the body of the report* where you “call” Figure 1, and proceed to describe it and its meaning. Several of our experiments are divided neatly into two or more parts. If this is true for any given experiment, feel free to create sections 2.1 and 2.2 with appropriate titles. This is especially useful if the two components use different apparatus.



**Figure 1**. A familiar figure from the sample JPC paper of the experimental apparatus. Note that the caption appears below the actual figure, and is not simply a title, but also a description. Don’t make the figure any bigger than it needs to be, nor so small that the fonts are unreadable.

**3. Results and Discussion**

The results section starts with the presentation of the *raw* data obtained. **Always** include your raw data, before you’ve done any calculations or manipulations. Tabulate the raw data. Show the results of calculations including error analysis. Present the final result with its error (i.e. T = 275±10ºC).Use tables and graphs as appropriate. Present the results of your data analysis **after** you have presented the relevant data! This is probably the first section where you’re likely to include Table 1. Just like Figure 1, Table 1 needs to be “called” in the body of your text, and the table needs to appear as close to that point as possible. The data in Table 1 is reproduced from the sample JPC paper. Note some important differences between Tables and Figures. Table captions appear **above** the table, and usually consist of a title only, not an explanation. Footnotes are often used to describe how these values are calculated, but may not be necessary if the text description is robust enough. Under no circumstances let Word split your table over two pages! This is pretty much the only valid reason to have a table appear somewhere other than right next to the paragraph in which it is described.

**Table 1: Parameters Used for the Calculation of *γ*w**

|  |  |
| --- | --- |
| parameter | value |
| average gas flow velocity, *u*j  | 21.4 cm s-1 |
| liquid flow velocity at the interface, V  | 6.8 cm s-1 |
| temperature, *T*  | 294 K |
| average thermal speed of HONO, *ω*  | 3.6 × 104 cm s-1 |
| Henry’s law coefficient, *H*  | 61 M atm-1 |
| acid dissociation constant, *K*a  | 4.9 × 10-4 M |
| aqueous phase diffusion coefficient, *D*aq  | * 1. × 10-5 cm2 s-1
 |

Somewhere here is probably where you’ll get to your first graph of your data. All graphs should be prepared using a suitable graphing program. Data points should be evident and the best line or curve drawn through the points should be given. You should have error bars. If the error bars are too small to be seen, the figure caption should say so. In cases of data that should describe a straight line, apply a linear least-squares regression routine and quote the values of the slope, intercept, and correlation coefficient (or residuals). If the data are fit to a nonlinear curve, the nature of the curve (exponential, polynomial, etc.) should be stated and the best-fit equation given. Graphs are simply a special case of figures, and should be treated the same. Figure 2 is sure to follow after I name it here, and remind you that you’ve seen it before in the JPC sample paper. Note the caption! It’s telling you a *lot* of important stuff here. First and foremost it’s pointing out what you should *see* when you look at the graph.



**Figure 2**. [HONO]/[HONO]0 as a function of the contact time for the gas, *t*. The pH of the aqueous solution was prepared at 11.0 (solid circles) and 7.0 (open circles). Inset shows the semilogarithmic plot of the relative concentration of HONO, indicating that the [HONO]/[HONO]0 decreases exponentially with the contact time.

This section is also where you’ll get to *describing* the calculations you’re doing. You will be emailing me a copy of your Excel spreadsheet showing the data analysis, so I don’t want to you show me all of your calculations. A sample calculation is useful if the process is hard to explain. If you repeat the same calculation multiple times, only one explanation/sample is required. Any further results should simply be presented, perhaps in a handy table?

Once you have arrived at all of your numerical results and their associated errors, it is time to move on to discussing them. Included here are a restatement of the values calculated from the data, interpretation of the results, assessment of error, limitations of the method, and suggestions for improvement. Are the results expected? Why or why not? How do your results compare with known or literature values? In addition, include in the discussion answers to any questions which were presented in the lab procedure itself. **Do not** separate the questions from the rest of the text with numbers or bullet points; these answers should flow naturally from the thought processes used to describe how your results fit in to the physical models used in the course.

This discussion part is **hard**. Expect to struggle with this section. Expect to not know the “right” answer to the question of why things went wrong. If you posit a theory about how something went numerically wrong, follow that thought to its conclusion – if your initial value of some experimental measurement X was probably too high, how high was it likely to be? If it were that high, what would your final answer for some solved parameter Y be? Is that different enough to explain the discrepancy?

You will also discuss precision and accuracy here. Which of these values most affects your results? What measurements and terms in the calculations are primarily responsible for those errors? Also consider - what assumptions/approximations were you forced to make in doing this experiment? How good are those assumptions, and how do they affect your final answer? What could you do differently in the lab or in your calculations to minimize these uncertainties?

This section is likely to be long. If it’s less than a page, that probably means that you haven’t thought very hard about your results, and you probably won’t get many points for this section. But if it’s longer than 3 pages of text (i.e., not counting figures and tables), then you need to be more concise. As with the Experimental Section, if the experiment is naturally subdivided into discrete components, feel free to split up section 3 into 3.1, 3.2, etc.

**4. Conclusions**

 This is a restatement of the most important findings of the paper. Like the abstract, this contains relevant facts about the experimental methods, but it is not as limited in its length. It does still have to be only one paragraph, no matter how earth-shattering your results may be. Expand on the key findings, and on the key failings of the experiment. Postulate on what could be done differently. Declare whether the experiment was a success or a failure. Importantly, *no new material appears in the conclusion* – everything here has already been stated in the discussion, but now you’re pulling all those crucial facts together in to one place. The only exception is that you might include a projection into the future about what to do next or how to do things differently… but it certainly wouldn’t hurt if that material was also in the Discussion.

**5. References (optional)**

References should be indicated throughout the paper using superscripted numerals which then appear with the corresponding references at the end of the paper, like so.

1. University of Massachusetts at Boston, Chemistry 314. http://alpha.chem.umb.edu/chemistry/ch314/documents/exp2HeatCapacity09.pdf (2-24-09)
2. J. Doe, J. Müller, *Journal*, **Year**, *Issue*, Page 1.
3. J. Müller, *Title of book*; Wiley: Chichester, 1990; p. 51-60.

**6. Appendix (optional)**

Remember that this report is designed to be *read*. Any long detailed calculations that might break the continuity of the results and discussion section should be moved here. If you choose to do this, you must say so at the point in the results section where it *would* have been included. Sample calculations longer than a page go here.