4. The Laboratory Report

While the laboratory notebook is the primary record of a scientist’s work, it is not the way that the scientist conveys the results of that work to the world at large. Any report on your work stating and explaining results will be separate from the notebook.

In 2230L, the students complete datasheets not lab reports. Many of the questions on the 2230L datasheets were written to encourage students to begin to write like scientists. In 2240L, some of the experiments utilize datasheets but other experiments require a full lab report to be written.

The biggest difference between the notebook and the report is the intended audience. The notebook is written primarily for your own use, but the report is addressed to others. It might take the form of an article to be published in a scientific journal intended for the scientific community at large, a research update for one’s supervisor, or a project update submitted to a grant funding agency.

The report is more selective than the notebook. All data and observations are recorded in the notebook. In the report, you should be more selective. Choose the data and observations from the notebook that accurately convey the results of the experiment to the readers, and include these in the report. Do not include irrelevant data in the report. Use the data from your notebook as the basis for the report, but add explanations and discussion of the work to support your conclusions. These should be at an appropriate level for the intended readers, who are competent chemists who are not familiar with the specific experiment you have performed.

Selectivity and accuracy are both important in report writing. No one has the time or the inclination to sift through many lines of numbers to search for the few important ones. The same principle applies to the non-data sections. Don’t use three sentences to say what could be said in one. Be selective about what you include, but avoid the tendency to include only favorable data and results. Don’t omit data that do not fit your conclusions or preconceived ideas about what the results should be. That type of “selectivity” is unethical. Also, do not change or modify any data recorded in the notebook. This includes adding or dropping digits, even zeros. To do so is to falsify data. This is unethical. This behavior has resulted in scientists losing jobs\textsuperscript{1}, having patents invalidated, convictions thrown out\textsuperscript{2} and in extreme cases prison terms.

Format

There are a number of formats that are acceptable for lab reports in general. Usually, a particular journal publisher will define the format to be followed in that journal. \textit{In this class we require you to follow a particular format, which is described below.} Your instructor may be grading a hundred or
more reports per week. He or she will expect to find them in the following
format and may deduct points from or refuse to grade reports that are not in
this format.

Here are some comments on the 9 sections you will be required to
include in your lab report. Additional instructions on writing lab reports follow
this section.

1. **Title of Experiment**

   The title can come straight from this manual, the on-line manual, or the
course syllabus.

2. **Your Name**

3. **Date**

   This is the date on which you write the report.

4. **Introduction**

   This section serves as an introduction to the report by explaining why
the experiment was done and discussing some of the theoretical background of
the experiment. It should be no longer than one or two paragraphs and must
not be copied from any other source. It is not the same as the purpose
statement in the lab notebook. In the introduction be sure to state the exact
experiment that will be done including all relevant chemical names. State how
the success of the experiment will be assessed or measured. Be sure to include
citations to sources of material (such as the lab manual, on-line notes, or web
articles) that you used to write this section. Citations are typically superscripts
of numbers that correspond to the number of the reference from which the
material was taken.

5. **Equations and Structures**

   If you identify an unknown as part of your experiment, give the structure
of the compound here.

   If you run a chemical reaction, give the equation or equations for the
reaction or reactions. Equations should be balanced and include structural
formulas for the organic compounds involved. Do not simply list the individual
structures if a reaction has been carried out. Instead draw the starting
reagents separated by a “+”, have an arrow then draw all products (aA +bB
→cC + dD). It is appropriate to list the name of each material under each
structure.

   Your reaction may be hand drawn or made with ChemDraw only. Do not
“cut and paste” the reaction from another source. Instructions for downloading
ChemDraw, a chemical structure drawing program, may be found on the course web site.

If you purify a compound but do not synthesize it, do not include an equation (because there is none). Do not include structures of any compounds that are neither unknowns nor part of the equations.

Reaction conditions and catalyst typically are placed above the arrow. Solvent is typically placed below the arrow.

6. Data

The data in this section should be selected from the data recorded in your notebook. For many of the experiments the notebook data and the final report data will be exactly the same. Sometimes some of the data and observations recorded in the notebook will prove to be irrelevant to the final result of the experiment, and should be omitted from the report. This is especially true if you perform an experiment more than once to get it right. Be sure to include units and identifiers.

Do not eliminate data merely because it does not fit in with your conclusions. Your instructor may give you further guidance on how to select which data should be included and which should be omitted.

The data included in the lab report, must be exactly the same as it was recorded in the notebook. Do not change numbers. Do not add or drop digits, including zeros. To add a zero is to imply that a more precise measurement was taken than actually carried out. This is scientifically unethical. The data recorded in a scientific notebook is defined as permanent and unalterable.

When constructing this section, think about what would be the best way to present the data. Usually, numerical data are most easily understood if they are presented in a clearly labeled table arranged in some logical order. Do not forget to include units. Observations may also be placed in tables, but often they can be presented in narrative form instead.

7. Calculations

Most scientific reports do not have a calculations section. Such things as percent recoveries and percent yields are normally included as part of the data. However, your instructors need to be sure you know how to perform these calculations. Each synthesis you perform needs to have a calculation showing the determination of the limiting reagent, the maximum theoretical yield, and the percent yield. All calculations you perform should be shown in this section. Be sure to include all units and identifiers. Remember your significant figure rules.

In your final report, keep the calculations section separate from the data section. In experiments that do not involve any calculations, you should still include a heading for this section with the statement that there were no calculations in the experiment.
8. Conclusions

In this section, it is always reasonable to include a short summary of what was done and what was observed. Do not include a step by step reiteration of the procedure. The results of each analysis need to be clearly stated and explained. Be sure to come to some conclusions about the results of the experiment. These conclusions should be related to the purpose that you wrote in your lab notebook.

If the purpose of the experiment was to synthesize cyclohexanone oxime, then state if this material was successfully synthesized or not.

If the purpose included identifying an unknown, then the conclusions must include the identity of the unknown. Give your evidence, and explain how and why it is consistent with your proposed identity and not others.

If the purpose was to purify a compound, the conclusion should state the obtained purity of the material and whether the experiment was successful or not.

State all obtained analysis. Then explain what this information means in terms of purity and or identity of product.

You must have experimental evidence to support your conclusions, but your conclusions must go beyond merely restating the data. This is also the appropriate place to compare your data to literature data.

For example, melting point range is one measure of the purity of a product. If a product was synthesized and a melting point was taken, the melting point of the product would be listed. In the conclusions section you might have a statement such as the following. “The literature melting point value of resorcinol (1,2-dihydroxybenzene) is 111°C\(^2\). The melting point of the product was found to be 93-108°C. This low and wide melting point indicates that the obtained product is not very pure. The reason for this high degree of impurity may be the difficulty in removing all of the ethanol solvent.” Notice that this statement stated a conclusion (the product was impure), gave a reason for that conclusion (wide and low melting point range), and cited the particular experimental data that supported the statement (the melting point range of 93-108°C) as well as the literature melting point with a citation from which this information was taken.

In each experiment state the obtained percent recovery or percent yield. Explain reasons where material have gone missing if the percent is lower than 100 %, and explain where extra material might have come from if the percent is over 100%.

Some instructors provide a list of the topics you should be sure to cover in the first few reports. Check Blackboard for your class to see if such a list has been provided. This list is normally not provided for the last lab report since one of the objectives of this class is to teach you what to include and leave out when writing a good lab report.
9. References

This is a formal list of all the materials you utilized to conduct, understand or analyze your experiment. Do not include references of articles or books that you yourself have not read. Do not include all the references listed in an article you read, only include the reference to the article itself.

Normally the references used in CHEM 2240L will include the lab manual (either on-line or hard copy) and the on-line notes. Some reports may also contain other materials that were consulted. If literature data (melting points, densities, etcetera) was taken from another source, be sure to reference that source.

Each reference should be cited (with a superscript) somewhere within the lab report.

Chemistry uses ACS style. Details of how to properly use ACS style can be found in *The ACS Style Guide A manual for Authors and Editors, 2nd Ed*, Ed J. S. Dodd, American Chemical Society: Washington D.C. 1997, pp173-229. This is available in the library. A summary of pertinent features of this book may be found at http://www.libraries.psu.edu/content/dam/psul/up/pams/documents/QuickGuideACS.pdf. This is a useful guide put together by Pennsylvania State University.


Materials gathered from the web also need to be referenced. A proper method of referencing web material is Author (if available), title of document, sponsoring institution, the full electronic address or URL, followed by date of access set within parenthesis. (An example; Thin Layaer Chromatography and Column Notes, Xavier University, http://www.xula.edu/chemistry/crs- orgleclab/Organic_Lab_1_2230L_Web_Files/10_TLC_&_%20Column_notes.pdf (accessed May 1, 2013).

If you get any part of the procedure from another published source, include that reference. If you perform an experiment using a procedure given in a handout or verbally by your instructor, give the procedure reference this way: "(Name of handout author or your instructor), personal communication."

Each reference should start with a number. If a particular fact or sentence was taken from a reference, then a small superscript of that reference number should be included after that bit of information. If a string of words was taken from a reference, those words needs to be set aside in quotes “…” and followed directly by a superscript denoting the reference from which they were taken. More information on proper referencing and an in-depth example may be found at the end of this chapter.
Other Lab Report Requirements

The laboratory report should be done on a computer using a word processing program. The document that you turn in must be a good quality printout. The font size for the text in the main body of the report should be 10 or 12. You can make the title larger if you so desire. Under no conditions will a handwritten or hand-printed report be accepted.

Some sections of the lab report are routinely added by hand. These include the reaction section and the calculations section.

A hard copy of the report is due at the beginning, not in the middle or end of the next class period. Points will be deducted for each 24 hours the report is late. An electronic copy of the lab report must be submitted to Turnitin in order to receive a grade for the work. The report may be submitted multiple times to Turnitin. Be sure to review the originality report of any submission and correct any inadvertent plagiarism.

The report must be entirely your own work and an honest report of that work. In some cases, the data in the report will have been obtained with a lab partner. In that case, you and your partner will necessarily have the same data. However, your partnership must not extend to the writing of the report. If material from another source is legitimately included, it must be properly attributed and the source cited in a footnote.

Presenting another person’s work as your own by copying it and not properly giving credit is plagiarism. It is a serious offense in any scholarly and scientific community. Depending upon the severity of the offence a few points may be removed from the report or a zero for the entire report may result. If a zero is given, an academic misconduct report will be filed with the Dean’s Office. A major infraction may result in you receiving an F in this course. In the same vein, all data must be your own and reported just as obtained in the laboratory. Any copying, altering, inventing, or fudging of data is also unethical and will be treated as cheating.

When writing the report, imagine that the reader will be a competent chemist, but unfamiliar with the experiment that you are describing. Don’t explain general things that a chemist would know, but do explain the particular experiment.

Don’t leave necessary things out, but try to be brief and to the point. Your instructor will not be impressed with flowery language and is an expert at recognizing padding. The lab report is not the place for poetry or creative prose. Complete and concise writing will lead to the highest grades.

You must follow the rules of grammar and good writing. Use complete sentences and correct punctuation. Your instructor will deduct points for poorly written lab reports. If you discover that you need help with the writing aspects of the notebook, your instructor can give you a referral to the Writing Center, or you can take the initiative and go yourself. The writing center is a great resource. It is located in room 105 of the St. Joseph’s Academic and Health Resource Center.
**Additional Information Regarding Proper Referencing and Avoidance of Inadvertent Plagiarism.**

Within every first year English course at XULA, plagiarism has been discussed. It is the student’s responsibility to ensure they do not plagiarize. The Plagiarism Statement put out by the English Department is helpful to recognize what is plagiarism and how to avoid it. [http://www.xula.edu/english/documents/plag.pdf](http://www.xula.edu/english/documents/plag.pdf) The Writing Resource Center (St. Joseph 106) can assist students with their writing assignments.

Many students have difficulty reading about an experiment then writing about that experiment without inadvertently plagiarizing. The key is to first read, process and understand what is written. Then explain what is going on in your own words. It should sound like you wrote it, not like the manual or a textbook.

If you read a passage in an on-line article that gave you some ideas about things you could include in your introduction but you do not copy them word for word, make sure you cite the reference with a number in a superscript or within parentheses, and list that article after the number used in your list of references.

For example: Diels-Alder reactions are efficient methods to make six
membered rings in a single synthetic step\(^3\).

If you take a string of words (4 or more) directly from another source and place it within your document, these need to be set aside in quotes and a superscript number added to the end which corresponds to the entry in the references from which it was taken. For example: “The Diels-Alder reaction is an important synthetic tool because it produces new six-membered rings with a high degree of stereoselectivity.”\(^4\)

If a value such as a volume or density or amount of time was taken from a document, then a superscript number needs to be added directly after the value which corresponds to the entry in the references from which it was taken. Density of acetic anhydride = 1.081 g/mL\(^5\)

Let us look at one particular case in more depth for added clarification. An introduction into an experiment in a textbook begins with the following paragraph:\(^6\)

An important property of diastereotopic ligands is that they are chemically nonequivalent toward achiral as well as chiral reagents, and that they can be distinguished by physical probes, most particularly by NMR spectroscopy. The environments of diastereotopic groups are topologically nonequivalent. A consequence of this nonequivalence is that they experience different shielding effects and have different chemical shifts in the NMR. (Enantirotopic groups have the same chemical shift).
One student is totally confused and in a bit of panic. For the introduction of their lab report they copy this entire description because they decide that if it is very confusing it must be very important. This student does not bracket the passage in quotes and does not list the source of this passage in their reference list. This student receives a zero on their entire report and an academic misconduct form documenting this plagiarism is filed at the Dean’s Office. Don’t do this!

A second student is also confused. This student does not surround the passage in quotes but does place a “6” at the end of the passage. This 6 corresponds to the entry in the reference list from which this passage was taken. This student gets 5 points (10%) taken off of their lab report and receives additional instruction as to how to properly reference sources.

A third student includes the entire passage in their introduction. They set the passage aside in quotes and places a superscript 6 at the end of the passage. This 6 corresponds to the entry in the reference list from which this passage was taken. This student gets no points taken off for this manner of referencing. Overall their introduction is not very clearly composed and awkward to read so they get a 1 point deduction.

A forth student rereads the passage twice more, reads the passage preceding this paragraph and thinks a bit. This student adds the following sentence to their report introduction;

Diastereomeric ligands including protons react differently toward chiral and achiral reagents. Diasteromeric ligands including protons have different shifts in the NMR. Diasterotopic protons will be found at slightly different locations along the 1H NMR x-axis (ppm), while enatiomeric protons have the exact same chemical shift.6

This student understood what was meant and integrated it into a well composed complete introduction. This student received a perfect score on this section.

Being able to read a scientific passage, distill out the important bits of information and restate this in your own words is a valuable skill to possess. Knowing how to properly site and reference sources is a required ability in any well respected and knowledgeable scientist.

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EXAMPLE OF ORGANIC LABORATORY REPORT  [ Each segment starts with an explanation of what is expected in brackets]

1. Title [List the title of the experiment] Diels-Alder reaction of Cyclohexadiene and Maleic Anhydride

2, 3. Name, Lab Time, and Date [Self explanatory] A.M. Brilliant, Monday 11:00, January 25, 2012

4. Introduction [Explain the brief theoretical background and benefit or value of the experimental procedure. State the exact reaction that will be carried out and state how the product will be analyzed. ] Diels-Alder reactions are an important method of forming 6 member rings in a single step. Diels-Alder reactions are one of the most unique and useful synthetic transformations available. In this experiment maleic anhydride was reacted with 1,3-cyclohexadiene to form Bicyclo[2.2.2]octa-5-ene 2,3-dicarboxylic acid anhydride (hereafter referred to as ‘product’). The product purity was determined by melting point. The percent yield was calculated. This section is normally ~10% of grade.

5. Chemical Reactions- [Write a balanced chemical equation representing the reactions which occur during the lab. Don’t simply list the reagents used. This can be neatly hand drawn or computer drawn using ChemDraw. Don’t simply plunk in some image from the internet.] This section is normally ~15% of grade.

\[
\text{1,3-cyclohexadiene} + \text{maleic anhydride} \xrightarrow{\Delta} \text{Product}
\]

6. Data and Observations [This portion is selected from the data you recorded in your notebook while carrying out the experiment. Every experiment should have observations. Take

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5 CRC Handbook of Chemistry and Physics, 65th Edition, CRC Press, 1984, C-70
some time to organize this data into a visually and intellectually reasonable manner. Be sure to include units and the appropriate number of decimal places. The hard data must be EXACTLY the same as what was recorded in the notebook. Changing numbers in any way will get points deducted.] This section is normally 10-20% of grade- but you can't do the rest of report without it.

Volume of 1,3-cyclohexadiene = 1.76 mL
Density of cyclohexadiene = 0.8471 g/mL
Mol. Wt. cyclohexadiene = 80.14 g/mol
Starting mass of Maleic Anhydride = 2.574 g
Mol. Wt. Maleic Anhydride = 98.06 g/mol
Mass of collected product = 1.903 g
Mol. Wt. Product = 178.18 g/mol

The 1,3-cyclohexadiene was a clear colorless liquid.
The maleic anhydride was a white grainy solid.
The product ‘fell’ out of solution as a white snow-like solid.
White crystalline product collected via vacuum filtration.
Product was rinsed with about 1 mL of cold methanol.
Some product stuck on filter paper.

Melting point of product = 142.3-145.5°C
Literature melting point of product = 147°C

7. Calculations. [Include a clear list of all calculations performed including appropriate units. Must determine the limiting reagent based on maximum amount of product (not starting material) that will form. Points will be deducted for erroneous use of significant figures. This is often better done by hand as it is difficult to type clear equations without a special add-on equation editor program.] This section is normally 20-25% of grade.

Grams of product from 1,3-cyclohexadiene (“CHD” used for abbreviation of Cyclohexadiene) =
\[
\frac{1.76 \, \text{ml} \_ \text{CHD}}{1 \, \text{ml} \_ \text{CHD}} \times \frac{0.8405 \, \text{g} \_ \text{CHD}}{1 \, \text{mol} \_ \text{CHD}} \times \frac{1 \, \text{mol} \_ \text{Prod}}{1 \, \text{mol} \_ \text{CHD}} \times \frac{178.18 \, \text{g} \_ \text{Prod}}{1 \, \text{mol} \_ \text{Prod}} = 3.29 \, \text{g} \_ \text{prod}
\]

(note: The vol. of CHD has 3 s.f., the mol wt of CHD has 4 s.f., the mol wt of Prod has 5 s.f. The “1”s are exact numbers so they have an infinite number of s.f. The number with the smallest number of sig figs is the vol of CHD with 3. Therefore the answer will have 3 s.f.)

Grams of product from Maleic Anhydride (“MA” used for abbreviation) =
\[
\frac{2.574 \, \text{g} \_ \text{MA}}{98.06 \, \text{g} \_ \text{MA}} \times \frac{1 \, \text{mol} \_ \text{MA}}{1 \, \text{mol} \_ \text{MA}} \times \frac{1 \, \text{mol} \_ \text{Prod}}{1 \, \text{mol} \_ \text{MA}} \times \frac{178.18 \, \text{g} \_ \text{Prod}}{1 \, \text{mol} \_ \text{Prod}} = 4.672 \, \text{mass} \_ \text{Prod(g)}
\]

(note: Both the mass of MA and mol.wt of MA have 4 s.f. The mol wt of Prod has 5. The “1”s are exact numbers so they have an infinite number of s.f. Therefore the answer has 4 s.f.)
Determine L.R. Since 3.29 g is less than 4.672 grams, the limiting reagent is 1,3-cyclohexadiene. The theoretical maximum amount of product which can form is 3.29 g.

\[
\text{% Yield Product} = \frac{1.903\text{ g}_\text{Product}}{3.29\text{ g}_\text{product}} \times 100\% = 57.7\% \text{ yield}_\text{Product}
\]

(note: The actual mass has 4 s.f. The theo. Max. amount of product has 3 s.f. Therefore the answer has 3 s.f.)

8. Discussion and Conclusions. (This should explain what you did, what you observed (your results), what this indicates, and what this indicates. Discuss the results you obtained; not simply restating what was done. Comment on ALL yields and purities. Explain where sources of error could have originated. Be sure to state if the objectives of the experiment were successfully met or not. It is good to start out discussing the overall reaction. Give a brief reintroduction into the experiment, then explain what was done and chemically explain all key steps involved. Do not use “I”, “we”, “our” or other pronouns. Write in the passive voice. Instead of “I heated 40 ml of water”, write “Forty ml of water was heated.”). This section is normally ~25-33% of grade. A list of topics you need to be sure are covered in this section are often listed on blackboard. Consult with your instructor on this.

Diels-Alder reactions are a highly efficient way to synthesize cyclohexene rings\(^7\). In this experiment a Diels-Alder reaction was carried out between 1,3-cyclohexadiene and maleic anhydride to form a new bicyclic ring adduct, Bicyclo[2.2.2]octa-5-ene 2,3-dicarboxylic acid anhydride\(^8\). The reaction was carried out by combining cyclohexadiene and maleic anhydride in a small round bottom flask fitted with a condenser. The reaction was allowed to heat for approximately 30 minutes in a gently boiling water bath. During the course of the reaction the formation of a white precipitate was observed. The formation of a new solid from a previously clear solution indicated a reaction was taking place and a new material was being formed. The solution was removed from the water bath and allowed to cool to room temperature, then placed in an ice/water slurry to reduce the temperature further and decrease the solubility of product. More white crystals formed.

The material was removed from the round bottom flask and the crystals were collected via suction filtration. The solid was weighed and the percent yield calculated. A 57.7% yield resulted. This is not awful but is also not particularly good either. One reason this yield may be low is that it was quite difficult to remove all of the solid from the round bottom flask. Hence material was lost.

The sparkly white appearance of the product indicates a reasonably high purity product. The observed melting point of 142-145°C is close to, but a bit lower than the literature melting point of 147°C. The closeness of the obtained melting point to the literature value supports the identity of the product to be the desired cycloadduct. This slight deviation and breadth of melting points indicate a reasonably high purity, but also indicates that a small amount of
impurities are present. One possible origin of these impurities is that the sample was not allowed to fully dry before the melting point was taken.

Overall the synthesis of relatively high purity and moderate yield of Bicyclo[2.2.2]octa-5-ene 2,3-dicarboxylic acid anhydride was a success.

9. References (This section can go directly after reaction, or at end of report as is typical) (List, in ACS format all references which were used to carry out the reaction, write the introduction, conclusion or to obtain literature values of chemical properties. Do not include any references that you did not actually read. Do not list the references that another book has listed, unless you yourself have also read them.) This section is normally ~5% of grade.

9. ACS style guide can be found in the library or a quick reference sheet can be found on the course web-site.

Revised June 7, 2017 S. L. Weaver

11 ACS style guide can be found in the library or a quick reference sheet can be found on the course web-site.