Experiment Write-Up Expectations in Organic Chemistry 2 Lab (CHML 2211)

Please note the following descriptions constitute the complete list of expectations for each part of the experimental write-up. Also, listed directly below is a grading scheme for each category.

Excellent: ***if you meet or exceed the expectations for any given category you will obtain 100 % of the available points for that category.***
Good: ***if you meet an overwhelming majority but not all of the expectations (~75-99 % of the expectations) you will receive ~75-99 % of the points available for that category.***
Fair: ***if you meet a majority of expectations (~51-74 % of the expectations) you will receive ~51-74 % of the points available for that category.***
Poor: if you meet less then a majority of expectations (~25-50 % of the expectations) you will receive ~25-50 % of the points available for that category.
Very Poor: ***if you meet none or much less then even half of the expectations in the category (~0-24% of the expectations) you will receive ~0-24 % of the points for that category.***

Experimental write-up categories

Title of Experiment: Hand written complete title of experiment appears on the top of every page in the lab book that pertains to that experiment.

Signature and Date: Hand written signature including the full last name of the student and correct date, at the bottom of every page in the lab book that pertains to that experiment.

Purpose: A hand written brief description (2-3 sentences) of the experimental objectives, in the student's own words, which clearly identifies and states the chemistry and methods of characterization involved in the experiment.

Table of Chemicals: A table of the reactants, solvents, drying agents and products in the experiment must be included and each of these must be listed in its own row. There are 11 column headings: IUPAC name and common name, formula, structure, molecular mass, melting point, boiling point, solubility (in water), density, amounts to be used in the experiment, and the role. All chemicals used in the experiment must be listed and include correct units, spelling, amounts and roles (reagent/solvent/drying agent/product). An example of the format for a table of chemicals is shown below:

IUPAC name	Common name	Formula	Structure	Molecular Mass (units)	Melting point (units)	Boiling point (units)	Solubility (in water)	Density (units)	Amounts to be used (units)	Role of reagent

Sketches of Apparatus & Materials Used: All apparatus and materials used in the experiment hand drawn in PEN, not pencil.

Theoretical Yield Calculation: If applicable the following must be included and hand written: (1) a correctly balanced reaction equation, (2) a correct reaction mechanism, (3) a detailed

correct calculation of the number of moles of the reactants, (4) correct identification of the limiting reagent and (5) correct theoretical yield of product(s). All calculations, units and unit conversions must be clearly shown to gain full credit. The reaction mechanism(s) must include: curved arrow notation to account for electron flow, lone pairs of electrons, charges and correct molecular/ion structures. Reaction equations must be correctly balanced and show correct chemical formulae and reaction arrows. Solvents should not be included in the reaction equation, mechanism or any calculations.

Flow Chart: A brief outline for carrying out each experimental step in the students own words, and which can be hand written or typed. A standard diagram flow chart format to map out the procedural steps should be utilized with rectangles encompassing each action or instruction point. The action/instruction points should be correctly spelled and include correct chemical formulae, quantities and units.

Answers to PRE-LAB Questions: At least one written response will be required and must be answered such that all parts of every question are addressed in complete sentences. These must be spelled correctly and incorporate correct chemical formulae. Also, reaction mechanisms or equations will be required and must be fully shown/complete. The reaction mechanism(s) must include: curved arrow notation to account for electron flow, lone pairs of electrons, charges and correct molecular/ion structures. Reaction equations must be correctly balanced and show correct chemical formulae and reaction arrows.

Procedures and Observations: Procedures and Observations must be hand written directly into lab notebook, in third person, and as the student performs the experiment. The procedures and observations cannot be pre-written or pasted-in.

Correct formatting for this section: divide the page into two columns, with the left hand column labeled as “Procedures” and right column labeled as “Observations”.
For the *Procedures Column*: there must be an all inclusive step by step write up of the experimental procedure as was carried out by the student. This can be in point form or sentence format, but must include detailed instructions that could be easily duplicated by a third party to carry out this procedure/experiment. All procedural step descriptions should be spelled correctly.

For the *Observations Column*: each observation noted should correlate to the correct procedural step listed in the left hand column. An observation describes either what the student saw (e.g. color change, phase change, temperature change, relative distance traveled of compounds *versus* solvent from TLC separations etc.) or how much of a chemical the student measured/weighed out to use in any given step of the procedure or how much of the product was obtained as well as the product melting point (if applicable). Any chemical test(s) carried out must be included in this section with descriptive observations. The correct units must be recorded in this column.

Results & Calculations:
Results: If applicable should include the following:
1. Actual yield(s) (re-recorded from the observations section).
2. Melting point range(s) (re-recorded from the observations section).
3. Copies of IR and NMR spectra affixed (such that all four corners of the spectrum are taped down/glued into the lab notebook) and key vibrations labeled (for IR) and peak resonances

labeled (for NMR). Each spectrum must also have the molecular name and structure hand drawn on the spectrum.
4. Table(s) identifying functional groups by their vibrations and the corresponding group frequencies from any collected IR spectra and tables with NMR signal assignments which include signal splitting/multiplicity information as well integration for ^{1}H NMR.
5. Any TLC plate(s) must be taped in and labeled for the solvent front, elution spots and elution start line.
6. The results of the chemical test(s) should be briefly re-summarized from the observations section and any applicable chemical equation included.
7. TA signature(s) for product inspection will also appear here if required.

Calculations: If applicable include the following:
1. Re-evaluation of theoretical yield.
2. Calculation of percentage (%) yield.
3. Density calculations.
4. R_f value calculations based on the distances recorded in the observations section.

The correct units must be used throughout this section and all unit conversions and calculations must be shown clearly and in detail to gain full credit.
Key vibrations in the diagnostic region of IR spectra (above 1500 cm^{-1}) and which correspond to major functional groups present in a given molecule must be identified on each spectrum. In addition, key secondary IR vibrations of the unique functional groups, usually already assigned from the diagnostic region, must also be assigned in the fingerprint region (1500-500 cm^{-1}). All IR vibration labels on the spectra must clearly show the functional group and the nature of the vibration (e.g. stretch or bend).
All resonance signals should be assigned on the NMR spectra. These labels must correlate to either the correct proton or carbon-13 atoms (for ^{1}H or ^{13}C NMR respectively) in the hand-drawn labeled molecular structure on each spectrum. For ^{1}H NMR spectra the integral ratios must be shown on the spectrum. The table(s) summarizing ^{1}H NMR spectra must clearly identify how many protons are represented by each resonance signal as well as the multiplicity of each signal.

Discussion & Conclusion: Discussion and Conclusion section must be hand written directly into the lab notebook, in third person, using complete sentences, with correct spelling and units and in paragraph format. No point form allowed and NO SUBHEADINGS! If required complete equations should be included using correct chemical formulae formatting (e.g. water must written as H_2O not H2O!)

Summary: The first part of the Discussion and Conclusion section should consist of a summary of the experiment in 2-3 sentences (do not include procedural descriptions). Specifically, go over the main points of the science/chemistry in the experiment.

Characterization of Product and General Discussion: In this part of the Discussion and Conclusion section pertinent experimental results obtained by the student must be re-quoted, such as: melting point, density, TLC/column chromatography and chemical test results and IR and NMR data. Each quoted experimental result in turn should be compared with known literature values and a conclusion must be drawn regarding the purity of the product obtained by the student. If the product is determined to be impure the specific source of the impurity must be

identified and correctly named (e.g. if there is any starting material still present, or a reaction intermediate or if there is a potential solvent contamination due to lack of drying time).

A further requirement for IR and NMR data analysis is a thorough interpretation of the obtained spectra. For the IR data discussion, the significant bands which are characteristic of the expected functional groups must be identified in the experimental data and then compared to the literature values. If there are two IR spectra obtained in the experiment (e.g. for the starting material and product or for two different products or for an intermediate and the product) these must also be compared to one another. For the NMR data discussion, the significance of where the signals are observed in the spectrum as these relate to the electronic environment of the nuclei under observation should be explained and their multiplicity as well as molecular symmetry (in relation to the NMR spectra of the molecule) should be addressed.

A further requirement for TLC data analysis is a thorough discussion of the polarity of the compounds under analysis with respect to how far they eluted on the TLC plate or down a chromatographic column and as compared to one another (e.g. a comparison of the starting material polarity compared to intermediate and/or product polarity may be required).
Relevant questions will be posted on blackboard that must be answered in this part of the Discussion and Conclusion section to further help explain the chemistry in the experiment. The inclusion of chemical equations may be required.

Error Analysis: In this section of Discussion and Conclusion, if it was previously shown that the product contained impurities (such as starting material etc.), then specific suggestions must be made as to what changes in the procedure would allow for a purer product or a better yield if there were no impurities in the product. If any other errors that lead to diminished product purity or yield can be identified these should be discussed in detail in this section. Suggestions that more lab time be allocated for purification purposes will not be accepted as valid procedural changes. For identification of errors in the experiment procedures general statements of "human error" or "faulty equipment" are insufficient in detail and cannot be used to account for impurities or low yields of product. You must be specific in all cases as to the sources of the error and for any proposed procedural changes.

Wrap-Up: The Discussion and Conclusion section should be concluded with a brief re-summarization in 2-3 sentences of the outcome from the experiment, including a comment on its applicability for the chemistry principles being examined in the experiment.

Citations: At the end of the Discussion and Conclusion section a full citation list for any referenced data obtained from the literature that was used in any part of the experimental write-up (specifically: Table of Chemicals, Answers to Assigned PRE-LAB Questions, and Results and Calculation, and Discussion and Conclusions sections) must be included. A minimum of two citations are required, however all references used must be included in the list of citations to gain full credit. Citations must be hand-written (not pasted-in).

Certification: The following certification must appear handwritten (not pasted-in) and exactly as shown below at the end of the experimental write-up:
"I certify that this is my own work, and I understand that if I am found to be in violation of the honor code, I will be subject to the highest penalty."